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MONTE CARLO DIRECT SIMULATION TECHNIQUE

USER'S MANUAL

Prepared Under Contract NAS 9-11207
"Space Shuttle Vehicle Reentry Flow-Field Analysis"
for NASA Manned Spacecraft Center
Houston, Texas

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"Space Shuttle Vehicle Reentry Flow-Field Analysis"
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SUMMARY

This document represents the User's Manual for the Monte Carlo Direct Simulation Technique, a set of 1108 computer programs which describe the rarefied flow field around various bodies reentering the earths atmosphere at high angle of attack. The programs were developed under NASA/MSC Contract NAS 9-11207 involving a study of reentry flow fields around various surfaces representative of the MSC Space Shuttle Orbiter Vehicle. Seven Monte Carlo flow field programs are described: SLAB, DRUM SLAB I and DRUM SLAB II (for flat plates), ORBITER, DRUM ORBITER I and DRUM ORBITER II (for Orbiter fuselage cross sections), and 3-D (for a 3-D representation of the Orbiter). A general description of the Monte Carlo technique is given in the User's Manual together with a relationship of the technique to the Boltzmann Equation. A description of parameters are given together with input descriptions, input forms, dimension statements, flow charts, and output descriptions for each of the programs.

1. INTRODUCTION

Computer programs to describe the flow field about the space shuttle orbiter vehicle at high altitudes have been developed. These programs employ a new numerical kinetic theory method called the Monte Carlo Direct Simulation Technique.

A two-dimensional program to compute rarefied flow about a flat plate of finite thickness at angle of attack, intended to investigate rarefaction effects on the flow about orbiter lifting surfaces, has been completed. A number of production runs have been executed with this program.

Another two-dimensional program describes flow about an infinite cylinder at angle of attack. The cylinder cross section is a box section on the bottom and a cylinder section on the top, intended to simulate those portions of the orbiter fuselage which are free of end effects, at the lower altitudes where complete orbiter vehicle calculations would be difficult. A number of production cases have been executed with this program.

A general, flexible three-dimensional program which can describe any body shape (defined by input data) has been developed. A simple test case for flow past two plates joined together at right angles has been executed. A test case has also been run for a body representing a portion of the orbiter vehicle fuselage and wing at angle of attack.

This report describes the simulation technique and provides user instructions for the above computer programs. Results of the production calculations are described in a companion document.

2. GENERAL DESCRIPTION OF THE MONTE CARLO SIMULATION TECHNIQUE

The method has been briefly described in the published literature and References 1 through 15 contain results obtained with it. Reference 10, 12 and 14 in particular contain discussions of the basic reasoning underlying the methods and outline its theoretical justifications.

The approach is to conduct numerical experiments with a model gas on a digital computer. The real gas is simulated by a collection of molecules which may be thought of as a representative sample of the many billions of molecules in the corresponding real gas.

To begin the calculation, a small number of molecules (on the order of several thousand) is set in uniform motion in a field of size sufficient to contain the disturbance caused by the body. The molecules are distributed uniformly in space, and their velocity components are assigned by sampling randomly from a distribution which is Maxwellian about the freestream velocity. Two position and three velocity coordinates for each molecule are stored in the computer. The body is instantaneously inserted in the stream, and the motion of the molecules is computed in a region surrounding the body. The molecular paths between collisions are computed exactly, but collisions are treated statistically. The calculation procedure consists of holding all molecules motionless for a time interval, ΔT_M, while collisions are computed everywhere in the field. ΔT_M is made small compared to the mean free time per molecule, $\overline{T}$, so as to produce a small distortion for most molecular paths. Molecules are then allowed to move with their new velocities for the time interval ΔT_M and are then once again held motionless in their new positions while another collision cycle takes place.

Molecules which strike the body during this time interval are immediately re-emitted with a new velocity chosen according to the assumed reflection law.

Collisions should be said to be prescribed rather than to occur since the detailed checking of paths to find intersections is not done. The prescription must be such that the collision frequency for molecules in each region of velocity space is appropriate to the local distribution of molecular velocities and further, no assumptions as to the shape of that distribution should be made. The distribution of free paths is then

correct. A sampling scheme which implicitly produces this by assigning a time interval to each collision can be described as follows:

1) The flow field is divided into a network of cells of varying size selected such that the changes in flow properties across a cell are small. The molecules in the cell can then be taken to represent the distribution at a point. Pairs of molecules are selected at random from a particular cell without regard to their location in the cell and are retained for collision with probability proportional to their relative velocity raised to an exponent m whose value depends upon the molecular model. For hard spheres, $m = 1$. For molecules repelling with the force law, $F = kr^{-\nu}$, $m = \nu - 5/\nu - 1$.

2) For pairs of molecules which have been accepted for collision a line of impact and azimuth angle in the center of mass reference frame are selected and the conservation laws are applied. For hard spheres these are selected at random. For power law molecules the dimensionless impact parameter $W = b(K/m^* v_r^2) - 1/\nu - 1$ is selected with probability proportional to W and the azimuth angle is selected at random. The new direction of the relative velocity is found from the deflection integral. (22)
The range of possible impact parameters is truncated at a maximum value which corresponds to a deflection angle of approximately 10°. Collisions producing deflections smaller than this are neglected as contributing negligibly to transport.

3) At each collision, a time counter for the cell in which it occurs is advanced by an appropriate amount. For hard spheres

$$\Delta T_N = \frac{2}{N_c} (A\ n\ V_r)^{-1}$$

For power law molecules

$$\Delta T_N = \frac{2}{N_c} \left\{ \pi\ W_m^2 \left(\frac{K}{m^*}\right)^{\frac{2}{\nu-1}} n\ V_r^{\frac{\nu-5}{\nu-1}} \right\}^{-1}$$

where ΔT_N = time increment for the collision

A = hard sphere collision cross section

b = impact parameter

n = molecule number density

N_c = number of molecules in the cell

V_r = relative velocity

W_m = dimensionless impact parameter cutoff

K = constant in force law

m^* = reduced mass

ν = exponent in force law

This sampling scheme produces a collision frequency for pairs of molecules proportional to the product of the local number density and the relative velocity of the pair, raised to the appropriate exponent. Molecules move, therefore, an average distance between collisions equal to the local mean free path. The collision frequency and mean free path produced by this collision process have been studied previously.[23]

As the calculation progresses, the flow field evolves toward the steady state. After a time interval has passed sufficient for the mean flow to traverse a distance of a few body lengths (on the order of 6), the flow is considered to be sufficiently close to the steady state. Recording is then begun, at an interval set large enough to prevent correlation, of flow field properties and the number of molecules involved in computing them. Steady state values of these properties are determined accurately by computing a cumulative average of these instantaneous samples. Similarly, a cumulative average of body surface properties is computed as molecules strike the body. In this way a collection of simulated molecules numbering many orders of magnitude less than the collection of molecules in the corresponding real gas flow is constrained to behave in the mean as does the collection of real molecules, and by continuing the calculation for a long enough time an accurate description of the flow can be built up.

As the movement interval and cell size are made to approach zero and the number of molecules approaches the actual number in a gas, we believe the Monte Carlo solution will approach an exact solution of the equations of motion of the collection of molecules. Our consideration is, of course, always restricted to gases of moderate and low densities.

The computer storage requirements to straightforwardly simulate flows with large density variations are large since the number of molecules to be followed would vary directly as the density. To achieve an adequate sample size in the region with lowest density, most of the computational labor would be needlessly spent in producing a far larger than required sample size in the regions of high density. To circumvent this a system of weighting is used in which molecules are assigned different statistical weights in different regions of the flow. When a molecule crosses to a region with a higher statistical weight, it stands a certain probability of being removed from the calculation. Conversely, if the molecule crosses to a region with a lower factor, it is duplicated the appropriate number of times. In a certain sense the molecules are only carriers of information, and it is most efficient to have more carriers, i.e., more points to represent velocity space, where the gradients are large and fewer where they are small. The appropriate weighting factors must be applied when number density is computed, since a molecule in a region for which the factor is k represents k times as many actual molecules as a molecule in a region where $k = 1$.

In addition to the net force and heat transfer to the body, this method provides a detailed description of the flow; viz,

1) flow field properties: density, temperature, velocity, etc., everywhere in the region surrounding the body.

2) local values on the body surface of pressure, skin friction, number flux, heat transfer, etc.

3) the distribution function everywhere in the gas.

The method does not require an initial estimate of the solution; instead the steady state solution is found as the large time limit of the unsteady solution. It should be recalled that the motions of the molecules are

followed exactly, and the flow field is divided into cells solely for the purpose of computing collisions. The key feature of the technique is that the collisional statistics and corresponding mean properties in the gas are determined by sampling with the correct probability for individual events from the collection of molecules representing the gas. Quantities such as the local mean free path and local collision frequency are not prescribed but are derived from the sampling procedure.

2.1 BOUNDARY CONDITIONS

The set of molecules in each cell will change as the molecules are moved and appropriate conditions must be applied at the boundaries of the region being simulated. The upstream boundary normal to the freestream direction is treated as a source of molecules with velocity components representative of the downstream moving molecules in the equilibrium freestream. Any molecule which moves back upstream across this boundary is regarded as being "lost" and is removed from the store. The plane of symmetry along the x-axis is regarded as a specularly reflecting surface in two-dimensional flows. The outer and rear surfaces present greater difficulties. A procedure has been developed which usually introduces only a small reflected disturbance and which becomes exact in free molecule flow. This is to regard a molecule as "lost" if it moves outward across the boundary but, if it moves inward from the boundary during the time interval Δt_m through a distance greater than its original distance from the boundary, it moves to the new position and a similar molecule is added in the original position. The latter part of this procedure should only be applied to those molecules with properties similar to the freestream molecules.

In practice it has been found adequate for hypersonic flows to simply remove from the calculation all molecules which move outward across a downstream boundary, and neglect the few inward traveling molecules. The downstream boundaries must be placed sufficiently far from the body for the flow to accelerate to supersonic velocity.

2.2 TYPE OPTION

The molecules are divided into three distinct classes at any point in the flow by reference to their past histories; viz,

Class I - freestream molecules which have not been affected by the body

II - molecules which at some time in their past history have struck and been reflected from the body

III - molecules which have been indirectly affected by the body by collisions in the gas.

Class I molecules transfer to Class II when they strike the body and transfer to Class III when they collide with a member of either II or III. Class III molecules transfer to Class II when they strike the body. Molecules once in Class II remain there. G. A. Bird originated this classification scheme and has used it to display the simulated molecule motion on a cathode ray tube which is then photographed in triple exposure with the molecules of each class taking on a different color.[7]

This option can be utilized by the use of the LS1 and LS2 flags in the input data. The required storage is increased and the array dimensioning in the program must be set accordingly.

2.3 STATISTICAL FLUCTUATIONS

This method is a probabilistic numerical experiment. Accordingly, the value of any quantity computed is a statistical estimate which has a sample size (the number of molecules involved) and standard deviation associated with it. The standard deviation σ should decrease roughly inversely as the square root of sample size, but it is impossible to make accurate a priori estimates of expected scatter. Calculations have been made to identify the approximate relationship between sample size and magnitude of scatter. The scatter was found to be close to Gaussian with standard deviation as shown in the following table.

Property	Sample Size	Standard Deviation
Surface Pressure, etc.	350	$\sigma_x = 7\%\ x$
	1000	3%
Flow Field Density, temperature, etc.	1300	4%
	4500	3%

Table I. Standard Deviation

The body surface is divided into segments and a cumulative average of the flux of energy and momentum to each segment is recorded. What results then for a quantity such as surface pressure is a sequence of points each of which represents the average pressure on a segment. Representative results for flow over a flat plate are shown in Reference 11.

2.4 MOLECULAR MODEL OPTION

Four monatomic molecular models are available: rigid elastic spheres, and power law models with exponents 12, 9 and 5. Their effects in continuum flows are illustrated by the way in which transport properties vary with temperature. This is shown by the Chapman-Enskog expressions shown in the table below for three of these.

Model	Viscosity	Mean Free Path	Mean Free Time
Hard spheres	$\mu \sim T^{1/2}$	$\lambda \sim \frac{1}{n}$	$\bar{t} \sim \frac{1}{n\,T^{1/2}}$
12th power molecules, $F = K\,r^{-12}$	$\mu \sim T^{15/22} \sim T^{0.68}$	$\lambda \sim \frac{T^{2/11}}{n}$	$\bar{t} \sim \frac{1}{n\,T^{7/22}}$
Maxwell molecules, $F = K\,r^{-5}$	$\mu \sim T$	$\lambda \sim \frac{T^{1/2}}{n}$	$\bar{t} \sim \frac{1}{n}$

Table II Molecular Models

Recent experiments in argon suggest a value for the viscosity-temperature exponent of 0.68. Moreover, a plane shock wave density profile computed with this Monte Carlo technique for 12th power molecules is in excellent agreement with an experimental profile for a Mach 8 shock in argon,[24] hence there is some reason to believe the 12th power molecules adequately represent the properties of argon. Hard spheres are seen to have a mean free path independent of temperature and are the "hardest" molecules of the three. The transport properties of air, such as viscosity, are believed to be approximated at temperatures of 300°K and above by hard spheres and by 9th power molecules at lower temperatures.

Maxwell molecules have a mean free time independent of temperature and are the "softest," i.e., encounters with very small impact parameter can result in negligible deflection if the relative velocity is high enough. Thus, the faster molecules in the distribution can have quite long free paths.

The constant K in the force law is determined for the power law models in terms of the hard sphere collision cross section by matching the freestream viscosity of the hard sphere gas. This also fixes the magnitude of an effective mean free path for these models.

An energy sink model is available to approximately represent molecules with either two or three internal degrees of freedom.

3. RELATIONSHIP OF BIRD DIRECT SIMULATION TECHNIQUE TO THE BOLTZMANN EQUATION

3.1 THE BOLTZMANN EQUATION

The Boltzmann equation for a monatomic gas can be written

$$\frac{\partial(nf)}{\partial t} + \vec{u}\,\frac{\partial(nf)}{\partial \vec{x}} = \iiint_{-\infty}^{\infty} n^2\,(f'f_1' - ff_1)\,A(v_r)\,v_\gamma\,d\vec{u}_1$$

where $f(\vec{u}, \vec{x}, t)$ is the normalized distribution function, $\vec{u}$ is the molecular velocity, A is the collision cross section, $d\vec{u}$ is an element of velocity space, n is number density, and a prime denotes post collision quantities.

The righthand side of this equation is the collision term, and the lefthand states that, in the absence of collision, nf remains constant if one moves along with the molecules in phase space. In the Monte Carlo method, the distribution function is replaced by a finite number of simulated molecules located, at any instant, at particular points in phase space. The paths of these molecules are followed exactly in phase space and the lefthand side of the Boltzmann equation is obviously satisfied.

The collision term can be subdivided into the gain and loss terms, the latter representing the rate of scattering by collisions out of the phase space element du dx per unit volume of the element. This rate may be derived from the Monte Carlo procedure by the following argument.

3.2 REQUIRED COLLISION RATE

We first make the approximation of uncoupling molecular movement and the determining of collisions over a short time interval. What remains is the problem of statistical sampling for the appropriate collisions; i.e., given the time interval T, prescribe an appropriate number and kind of collisions for that interval.

From the righthand side of the Boltzmann equation, the collision rate in the region of phase space du dx is

$$d\dot{N} = du\,dx \iiint_{-\infty}^{\infty} n^2\,ff_1\,A\,v_r\,du_1$$

where A is the total collision cross section for encounters with relative velocity v_r, a function of v_r in general.

The total collision rate for the volume of physical space dx is obtained by integrating again over velocity space (we now count each encounter of a pair of molecules as two collisions)

$$\dot{N} = n^2 \, dx \iiint_{-\infty}^{\infty} du \iiint_{-\infty}^{\infty} du_1 \; ff_1 \; A \cdot v_r$$

$$= N \, n \, \overline{Av_r}.$$

where $N = n \cdot dx$ is total number of molecules in dx.

To prove that the Monte Carlo sampling scheme is consistent with the Boltzmann righthand side we must show that over a given time interval T:

1. The number of collisions in each small region of velocity space relative to the number in other regions is correct; i.e., has Boltzmann form.
2. The total number of collisions in interval T is correct.

We first divide velocity space into R regions, each of volume du.

We then can write the discrete analogue of $d\dot{N}$ as:

$$d\dot{N} = \sum_{j=1}^{R} N_i \frac{N_j}{dx} A \cdot v_{ri-j} = N_i \frac{N}{dx} (\overline{Av_r})_i$$

where

$(\overline{Av_r})_i$ = average value for the product (Av_r) for a molecule in region du_i in collisions with molecules in all other regions

N_i = number of molecules in region $du_i = n \, f_i \, du_i \, dx$

N_u = number in region $du_j = n \, f_j \, du_j \, dx$

3.3 MONTE CARLO SAMPLING PROCEDURE

We now discuss the Monte Carlo sampling procedure. We select pairs of molecules at random in velocity space, which means that the <u>expected number</u> of pairs from regions i and j in S pair selections is:

$$\frac{N_i}{N} \cdot \frac{N_j}{N} \cdot S$$

where N is total number of molecules. (S is left arbitrary for the moment--in fact it will be determined indirectly by assigning a time interval to each collision and stopping the selection when the intervals add up to equal T.)

Prescribing collisions to occur with probability Av_r, the <u>expected number</u> of pairs to collide (number which would occur in a large sample) from regions i and j is:

$$\frac{S}{N^2} \cdot N_i \cdot N_j \cdot \frac{(Av_{ri-j})}{(Av_r)_{max}}$$

where $(Av_r)_{max}$ is the maximum value of the product (Av_r) for any two regions.

Summing up over all regions, i.e., overall j, <u>the expected total number</u> of collisions in region i in S pair selections is:

$$\frac{S}{N^2(Av_r)_{max}} \sum_{j=1}^{R} N_i \cdot N_j \cdot Av_{ri-j}$$

$$= \frac{S}{N^2(Av_r)_{max}} N_i \sum_{j=1}^{R} N_j \, Av_{ri-j}$$

$$= K \, N_i \cdot N \cdot (\overline{Av_r})_i$$

where

$$K \equiv \frac{S}{N^2 (Av_r)_{max}}$$

Hence total scattering rate out of region i is proportional to $N_i \cdot N(\overline{Av_r})_i$ which, according to the Boltzmann equation, is correct relative to other regions.

We now sum over velocity space once more, overall i, to get total collision rate.

First define:

N_{coll} = number of collisions in S pair selections

= 2 x total number of pairs accepted for collision

Therefore

$$N_{coll} = 2 \times \frac{1}{2} K \sum_{i=1}^{R} N_i \, N(\overline{A \cdot v_r})_i = K \, N^2 \cdot \overline{Av_r}$$

where

$$\overline{Av_r} \equiv \frac{1}{2} \cdot \frac{1}{(N^2/2)} \sum_i^R \sum_j^R N_i \, N_j \, Av_{ri-j} = \frac{1}{N^2} \sum_i^R \sum_j^R N_i \, N_j \, Av_{ri-j}$$

Now

$$\dot{N} \equiv \frac{N_{coll}}{T} = \frac{K \, N^2 \, \overline{Av_r}}{T}$$

where T is the sum of all the time intervals assigned to the collisions. Further, we showed earlier that the mean or expected value of total collision rate obtained by integrating the Boltzmann righthand side over velocity space is $N \, n \, \overline{Av_r}$.

$$\frac{N_{coll}}{T} \text{ and } N \, n \, \overline{Av_r}$$

If we left the interval to be assigned to each collision as undetermined and ask what ΔT would produce identity for the two expressions:

$$\frac{N_{coll}}{T} \text{ and } N\ n\ \overline{Av_r}$$

since

$$\frac{N_{coll}}{T} = \frac{K\ N^2\ \overline{Av_r}}{\frac{1}{2} \times K \sum_i \sum_j (N_i\ N_j\ Av_{ri-j} \cdot \Delta T)}$$

we would find that one possibility is:

$$\Delta T = \frac{2}{N} \frac{1}{n\ \overline{Av_r}}$$

For then

$$\frac{N_{coll}}{T} = \frac{N^2\ \overline{Av_r}}{\frac{1}{n\ N\ \overline{Av_r}} \cdot \sum_i \sum_j N_i\ N_j\ Av_{ri-j}}$$

$$= N\ n\ \overline{Av_r}$$

However, another possibility is:

$$\Delta T = \frac{2}{N} \frac{1}{n\ Av_{ri-j}}$$

for which we find

$$\frac{N_{coll}}{T} = \frac{N^2\ \overline{Av_r}}{\frac{1}{Nn} \sum_i \sum_j N_i\ N_j}$$

$$= N\ n\ \overline{Av_r}$$

The second way is more efficient since the quantity $\overline{Av_r}$ need never be computed, but they both produce the Boltzmann collision rate. Hence as the uncoupling interval and the cell size are made small, and the number of simulated molecules is made large, the Monte Carlo solution tends to a solution of the Boltzmann equation, differing only by random statistical error.

4. DESCRIPTION OF PARAMETERS

4.1 PRINCIPAL APPROXIMATIONS

4.1.1 Molecular Motion and Collisions

The molecular motion and molecular collisions are uncoupled over an interval Δt_m; that is, the molecules move for Δt_m without collision and then are held fixed in position while the appropriate collisions for the interval are prescribed. Δt_m must be made sufficiently small compared to the local mean free time so that distortions in the particle paths are small. In practice there clearly will be some distortion - the free time for a very fast molecule can be quite small and it would be prohibitive to set Δt_m to cope with the smallest free time.

4.1.2 Division Into Cells

Physical space is divided into cells. The molecules in each cell are taken to represent the distribution function at a point while collisions are prescribed; that is, their actual positions are temporarily ignored. A molecule which undergoes a collision would then move during the next cycle from its actual position (unchanged during the collision process) with its new velocity. Molecules which did not have a collision would, of course, also move from their actual (unchanged) positions with unchanged velocity. The size of each cell is selected to be sufficiently small compared to distances in which there are significant changes in the distribution function. Again, in practice there unquestionably will be distortion in some parts of the distribution function - the cell size is set so as to keep this small. It has been found that the cells can be set surprisingly large without introducing errors easily detectable in the moments of the distribution function. This is due to the fact that the actual position of each molecule in the cell is not changed during the collision process. Even though molecules at opposite ends of a large cell are prescribed to collide, the only error incurred is that due to using all the molecules in the cell to estimate the local velocity distribution and density surrounding each molecule. The magnitude of the error would then depend upon how the local velocity distribution and density differ from the average for the cell.

4.2 SAMPLING CELL ARRANGEMENT

The general rule for selecting the cell sizes is that the change in flow properties across each cell should be small. It is difficult to give specific rules which are flexible enough to cover all situations. The only reliable way is to first visualize what the average free paths are for various classes of molecules in all regions of the flow.

4.2.1 Discussion of Mean Free Paths

The Chapman-Enskog first approximation to the viscosity coefficient μ, contains a length; viz,

$$\lambda_\infty \equiv \frac{32}{5\pi} \frac{\mu}{m\, n\, \overline{C}}$$

where $\overline{C}$ is mean thermal speed

n = number density

m = molecular mass

If we wish to visualize the gas as composed of rigid elastic spheres of diameter $\sigma = (\sqrt{2}\pi\, \lambda_\infty\, n)^{-1/2}$, λ_∞ is the mean free path in a frame of reference moving at the fluid mechanical velocity (for a gas nearly in equilibrium). If we choose instead to visualize point centers of inverse power repulsion, $F = Kr^{-\nu}$, λ_∞ is just a reference length which is related to the transport cross section for viscosity θ_V[25] by

$$\theta_V = \frac{1}{\sqrt{2}\, \lambda_\infty\, n}$$

θ_V may be thought of as that part of the total scattering cross section which contributes non-negligibly to viscosity. The Chapman-Enskog second approximation to μ introduces only a very weak dependence on ν into the

proportionality constant which becomes

$$\frac{32}{5\pi\ (1 + \varepsilon)}$$

where

$\varepsilon = 0 \qquad \nu = 5$

$\varepsilon = .016 \qquad \nu =$ (hard spheres)

Thus whether we visualize the gas molecules as billiard balls or as point masses surrounded by force fields, we influence only very slightly the magnitude of the reference length and an "effective size" for the molecule deduced from viscosity in this way. Most experimentalists take the viscosity of their test gas at the freestream temperature and compute this length and call it the mean free path.

In general λ_∞ is not a length of great usefulness as far as deducing how many collisions have occurred; however, since we wish to make direct comparisons with experiment, we adopt it as our length scale. This should not cause any difficulty as long as one takes care in inferring what the collision process looks like.

In calculations for point centers of inverse power repulsion the force fields do not extend to infinity but are cut off. The range of the dimensionless impact parameter

$$b \left(\frac{m^* V_r^2}{k}\right)^{\frac{1}{\nu-1}}$$

is truncated and hence molecular encounters which result in a deflection less than a prescribed minimum (approximately 10°) are ignored. The viscosity of the power law gas is affected negligibly by this approximation, and it is

then appropriate to consider λ_∞ an "effective mean free path" for these models also, with the same limitations as to physical significance as for hard spheres. The constant k in the force law is found by matching the viscosity of a hard sphere gas at the freestream temperature. For the power law models the transport cross section for viscosity varies with the relative velocity of encounter V_r; viz,

$$\theta_v \sim \left(\frac{k}{V_r^2}\right)^{\frac{2}{\nu-1}}; \quad \lambda \sim \left(\frac{k}{V_r^2}\right)^{-\frac{2}{\nu-1}} \cdot \frac{1}{n}$$

and for a gas nearly in equilibrium:

$$\theta_v \sim \left(\frac{k}{T}\right)^{\frac{2}{\nu-1}}; \quad \lambda \sim \left(\frac{k}{T}\right)^{-\frac{2}{\nu-1}} \cdot \frac{1}{n}$$

Now the mean free path in a flowing gas is a function of the frame of reference of the coordinate system. For a coordinate system fixed in the body, the general rule to compute the mean free path for molecules of a given class (i) (whose velocity is V) in collisions with another class (e) is:

$$\lambda_{i-e} = \frac{V_i}{f_{i-e}} = \frac{V_i}{A\, n_e\, \overline{V}_{r_{i-e}}}$$

where

f_{i-e} = collision frequency

A = collision cross section

n_e = number density of molecules of class (e)

$\overline{V}_{r_{i-e}}$ = mean relative velocity for collisions between the two classes

It has long been recognized that a number of important such mean free paths can be defined (1, 31, 32, 33, 26, 19, 20, 21). The hierarchy of mean free paths, all computed in a frame of reference fixed in the body, which are relevant in the zone near the body leading edge where freestream and emitted molecules collide is shown for hard spheres and Maxwell molecules, $\nu = 5$, in Table 3 where:

λ_{e-i} = mean free path of molecule emitted from body with respect to incident freestream molecules

λ_{i-e} = mean free path of incident freestream molecule with respect to emitted molecules from body

Table III. Mean Free Paths Near Leading Edge for Representative Body Shapes

	Cone		Flat Plate	
	Cold Wall $T_w \approx T_\infty$	Hot Wall $T_w \approx T_0$	Cold Wall $T_w \approx T_\infty$	Hot Wall $T_w \approx T_0$
	Hard Sphere Molecules			
$\lambda_{e-i} \sim$	$\frac{\lambda_\infty}{M_\infty}$	λ_∞	$\frac{\lambda_\infty}{M_\infty}$	λ_∞
$\lambda_{i-e} \sim$	$\lambda_\infty \frac{(r/r_b)}{\chi}$	$M_\infty \lambda_\infty \frac{(r/r_b)}{\chi}$	λ_∞	$M_\infty \lambda_\infty$
	Maxwell Molecules			
$\lambda_{e-i} \sim$	λ_∞	$M_\infty \lambda_\infty$	λ_∞	$M_\infty \lambda_\infty$
$\lambda_{i-e} \sim$	$M_\infty \lambda_\infty \frac{(r/r_b)}{\chi}$	$M_\infty^2 \lambda_\infty \frac{(r/r_b)}{\chi}$	$M_\infty \lambda_\infty$	$M_\infty^2 \lambda_\infty$

The mean free path for collisions among freestream molecules, λ_{i-i}, is $\approx M_\infty \lambda_\infty$ for all situations tabulated above and we ignore λ_{e-e}. The quantity in the table is the ratio of free molecule flux to the surface for a cone to that for a flat plate. For slender cones at hypersonic cold wall conditions, χ is also approximately the ratio of free molecule pressure, heat transfer and shear stress for these two geometries.

For a slender cone the density in the emitted stream near the body drops off approximately as r_b/r where r_b is the body radius, and this factor is included to account for this.

In attempting to understand leading edge flow it is important then to realize that:

1. at hypersonic speeds the mean free paths for different classes of encounter can differ considerably, e. g., $\lambda_{i-i}/\lambda_{e-i} \sim M_\infty^2$

2. body geometry has an important influence on the free paths of incident molecules, λ_{i-e}

3. mean free paths for the extremes of collision cross section variation, hard spheres and Maxwell molecules, differ by the factor M_∞

4.2.2 Values of Mean Free Path for Various Flow Geometries

We shall compute some typical values of the important mean free paths for a few typical flow geometries.

1. Near the leading edge of a flat plate with cold walls at zero angle of attack in a hypersonic hard sphere gas:

$$\overrightarrow{M = 25} \quad \overrightarrow{\lambda_{i-e}} \quad \frac{\nwarrow \lambda_{e-i}}{\text{Wall temperature } T_W = T_\infty}$$

a) The mean free path for self-collisions among the free stream molecules is:

1) in a coordinate system moving at the freestream velocity:

$$\lambda_{i-i} = \frac{\overline{C}_\infty}{A\, n_\infty\, \overline{v}_{r_\infty}}$$

where

$\overline{C}_\infty$ = freestream molecular thermal speed

now,

A = constant (because of hard sphere gas assumption)

$\overline{v}_{r_\infty} = \sqrt{2}\ \overline{C}_\infty$ since the free stream gas is in equilibrium

$$\lambda_{i-i} = \frac{1}{\sqrt{2}\ A\ n_\infty} = \lambda_\infty$$

2) in a coordinate system fixed in the body:

$$\lambda_{i-i} = \frac{V}{A\ n_\infty\ \overline{v}_{r_\infty}} \approx M_\infty\ \lambda_\infty$$

since $\overline{v}_r$ is independent of the coordinate system and is still $= \sqrt{2}\ \overline{C}_\infty$.

b) The mean free path (near the leading edge) for the molecules emitted from the plate colliding with free-stream molecules is: (henceforth we only consider a coordinate system fixed in the body):

$$\lambda_{e-i} = \frac{\overline{C}_W}{A\ n_\infty\ \overline{v}_{r_{e-i}}}$$

where $\overline{C}_W$ = mean thermal speed at wall temperature =

$$\sqrt{T_W/T_\infty}\ \cdot\ \overline{C}_\infty$$

$$\overline{v}_{r_{e-i}} = (U_\infty + \overline{C}_W) \approx U_\infty \approx M_\infty \cdot \overline{C}_\infty$$

$$\therefore\ \lambda_{e-i} = \frac{\sqrt{T_W/T_\infty}}{A\ n_\infty\ M_\infty} \approx \lambda_\infty/M_\infty = \lambda_\infty/25$$

hence the cold wall and hypersonic speed has created a free path near the wall which is extremely small compared to λ_∞.

c) The mean free path (near the leading edge) for freestream molecules colliding with emitted molecules is:

$$\lambda_{i-e} = \frac{U_\infty}{A\ n_i\ \overline{v}_{r_{i-e}}}\ U_\infty$$

where n_i = number density of emitted molecules, whose approximate magnitude near the leading edge will lie between n_∞ and $10\,n_\infty$.

$$\overline{v}_{r_{i-e}} = (U_\infty + \overline{C}_W) \approx U_\infty$$

$$\therefore \quad \lambda_{i-e} \approx \lambda_\infty \text{ to } \lambda_\infty/10$$

Referring to Table III we can see that if instead of hard spheres we consider Maxwell molecules, whose cross section $\sim K/v_r$, then λ_{i-e} and λ_{e-i} increase by the factor M_∞ (K is the force constant, whose magnitude has been adjusted so that $A(v_r = \overline{C}_\infty)$ is equal to the hard sphere value).

Similarly, if we consider hard sphere molecules but an adiabatic wall (for which $\overline{C}_W \approx U_\infty$) then λ_{i-e} and λ_{e-i} also increase by the factor M_∞.

Note that we have considered only the region very near the leading edge where n_i, n_e and $\overline{v}_{r_{i-e}}$ can be readily estimated. As we go further back along the plate the relative velocity becomes closer to the local mean thermal speed and the densities can vary widely, hence it becomes more difficult to make estimates. However, in practice it is found that the most demanding region is near the leading edge, where the cell height normal to the plane should be $\approx \lambda_\infty/M_\infty$. In the regions beyond the leading edge this requirement can be relaxed, and the required cell height can approach λ_∞.

2. A flat plate set normal to the flow - The preceeding flow situation contained the feature that, no matter how long the plate, the very rarefied region near the leading edge is still present, a typical slender body feature. For the plate normal to the flow we have a blunt body situation. If the plate height is of the order of λ_∞, then the entire flow is rarefied and molecules emitted from the wall will collide with free-stream molecules to a significant extent. Applying the previous reasoning we would find that

$$\lambda_{e-i} \approx \frac{\sqrt{T_W/T_\infty}\,\overline{C}_\infty}{A\,n_\infty\,(U_\infty + \overline{C}_W)}$$

and for a cold wall and hard sphere molecules λ_{e-i} is again $\approx \lambda_\infty/M_\infty$.

The flux of incoming molecules is now $\approx n_\infty U_\infty$ and n_e is $\approx n_\infty (U_\infty/\overline{C}_W)$, hence for a cold wall, $n_e \approx n_\infty M_\infty$ and λ_{i-e} is also close to λ_∞/M_∞. Hence the required cell size normal to the plate is also $\approx \lambda_\infty/M_\infty$ for the rarefied blunt body.

If the body size exceeds λ_∞ by an order of magnitude or more then a sizeable disturbance is built up and the mean free paths in the disturbance become closer to λ_∞. Near the plate the cold wall will create a very dense layer in which the mean free path will be determined by the density. However, it has been found that making the cell height of the order of λ_∞ in this region does not introduce significant error.

Angles of attack between 0 and 90° produce a mixture of the slender body and blunt body flow situations and will have to be considered individually.

4.3 REQUIRED NUMBER OF SIMULATED MOLECULES

The required number of molecules to be used in the simulation calculation is determined principally by requirements of the statistical sampling procedure and is independent of the actual number of molecules in a gas. Calculations have been made with the number density of simulated molecules differing by an order of magnitude, with results at a given sample size completely consistent between the two calculations. This point is discussed at length in Reference 12. In general it is found that during the calculation the minimum average number of molecules in any cell should be 4 for near-continuum flows and 20 for near-free-molecule flows.

The number of actual molecules in a real gas at the conditions being represented can be found in the following way:

Specify body size D and Knudsen number Kn. These determine the freestream mean free path $\lambda = Kn \cdot D$. Given λ, the altitude represented can be found by consulting altitude tables for the particular model atmosphere chosen. In addition, viscosity measurements for the particular gas of interest specify the molecule collision cross section A as a function of temperature. The actual number density in the freestream which is being simulated, n, can then be computed:

$$n = \frac{1}{\sqrt{2}\, A\, \lambda}$$

If in the simulation, INM molecules populate a field of total volume V, then each simulated particle of statistical weight 1 represents a number of actual molecules equal to:

$$n/(INM/v)$$

The magnitude of this number has some bearing on how "real" the statistical fluctuations in the simulation are, as discussed in Reference 12. However it is completely irrelevant for all other aspects of the simulation.

4.4 IMPORTANT TIME INTERVALS

4.4.1 Movement Interval, DTM = $\Delta T_M/\bar{t}_\infty$

For computational purposes the Monte Carlo direct simulation technique uncouples the movement of the molecules and the collisional process. Molecular trajectories are followed exactly while the collisions are computed statistically. An important parameter in this calculation is the movement time interval DTM (measured in terms of the freestream mean time between collisions). During this time molecules are moved using the molecular coordinates and velocities of the previous time. The molecules are then held at a constant position while the appropriate number of collisions are computed in each cell, modifying the molecular velocities. The value for DTM should theoretically be chosen so that the movement time interval is small compared to the smallest time between collisions; i. e., the smallest mean free time.

The mean free time is defined by:

$$\bar{t} = \frac{1}{\text{collision frequency}} = \frac{1}{A\, n\, \bar{V}_r}$$

In the freestream:

$$\bar{t}_\infty = \frac{1}{\sqrt{2}\, A\, n_\infty\, \bar{c}_\infty} = \frac{\lambda_\infty}{\bar{c}_\infty}$$

Locally in the gas:

$$\bar{t} = \frac{1}{(n/n_\infty) \cdot (\bar{V}_r/\bar{c}_\infty)} \cdot \bar{t}_\infty$$

Thus for molecules emitted from a cold body with $\bar{c}_w \approx \bar{c}$, the mean free time for collisions with freestream molecules would be: $\bar{t}/\bar{t}_\infty = 1/(V_\infty/\bar{c}_\infty) \approx 1/M_\infty$ and this would dictate the approximate size of ΔT_M to be $\bar{t}_\infty/M_\infty$.

In the programs the quantity ΔT_M is normalized by a reference time $t_r = \lambda_\infty/V_m$ where V_{m_∞} is the freestream most probable thermal speed (which is close to $\bar{c}_\infty$). Thus for all practical purposes the input variable DTM can be assumed to be $\Delta T_M/\bar{c}_\infty$.

In practice it is found the ΔT_M can be varied within fairly wide limits without incurring serious error. To understand this we take a look at the mean free times for molecules of various speeds.

Consider a region of physical space of width dx containing molecules of differing velocities, as shown in the sketch below. Let $\bar{t}$, $\bar{c}$ and λ be the mean free time, mean thermal speed and mean free path for all the molecules in region dx. We consider three small classes of molecules according as their velocity

$v \ll \bar{c}$

$v \approx \bar{c}$

$v \gg \bar{c}$

Restricting this discussion to molecules with constant cross section A, the mean free time and mean free path for each class are as follows:

In general

$$\frac{\lambda_v}{\lambda} \approx \frac{v}{A\ n\ \overline{v}_r} \cdot A\ n = \frac{v}{\overline{v}_r}$$

$$\frac{\overline{t}_v}{\overline{t}} \approx \frac{A\ n\ \overline{c}}{A\ n\ \overline{v}_r} = \frac{\overline{c}}{\overline{v}_r}$$

Then for

$$v << \overline{c};\quad \frac{\lambda_v}{\lambda} \approx \frac{v}{\overline{c}} << 1$$

$$\frac{\overline{t}_v}{\overline{t}} \approx \frac{\overline{c}}{\overline{c}} = 1$$

for

$$v \approx \overline{c};\ \frac{\lambda_v}{\lambda} \approx \frac{v}{\overline{c}} \approx 1$$

$$\frac{\overline{t}_v}{\overline{t}} \approx \frac{\overline{c}}{\overline{c}} \approx 1$$

for

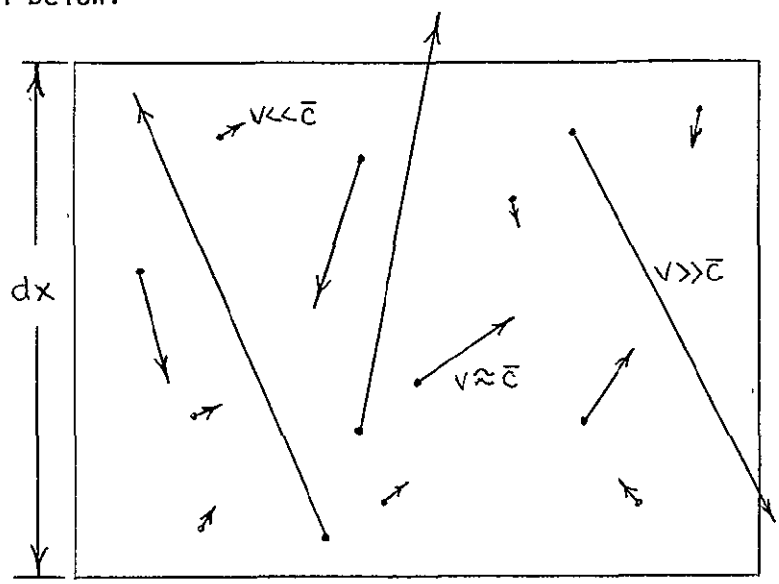
$$v >> \overline{c};\ \frac{\lambda_v}{\lambda} \approx \frac{v}{v} = 1$$

$$\frac{\overline{t}_v}{\overline{t}} \approx \frac{\overline{c}}{v} << 1$$

consider a small interval of time:

$$\Delta t = \varepsilon \cdot \bar{t} \quad \text{where } \varepsilon \text{ is } < 1.$$

The movements of the three classes of molecules during this interval are as shown below.



In general, for any v, the distance traveled during Δt is:

$$v \cdot \Delta t = \varepsilon \cdot \frac{v}{\bar{c}} \cdot \lambda$$

The magnitude of dx during the simulation will typically be $\approx \lambda$.

Therefore, for $v \ll \bar{c}$

$$\frac{v \cdot \Delta t}{dx} = \frac{v \cdot \Delta t}{\lambda} \ll \varepsilon$$

$$\frac{v \cdot \Delta t}{\lambda_v} = \varepsilon$$

for $v \approx \bar{c}$

$$\frac{v \cdot \Delta t}{dx} = \frac{v \cdot \Delta t}{\lambda} = \frac{v \cdot \Delta t}{\lambda_v} \approx \varepsilon$$

for $v >> \bar{c}$

$$\frac{v \cdot \Delta t}{dx} = \frac{v \cdot \Delta t}{\lambda} = \frac{v \cdot \Delta t}{\lambda_v} >> \varepsilon$$

Thus we see that both for slow moving molecules, $v << \bar{c}$, and for molecules moving with the average speed for the gas, $v \approx \bar{c}$, the requirements on ε are not very severe. By definition the change in flow properties in the distance λ cannot be large, and it is found that even for values of $\varepsilon \approx 1$ the distortion in molecular paths does not have significant effect on macroscopic gas properties. The very fast molecules ($v >> \bar{c}$) for which $v \cdot \Delta t/\lambda_v >> \varepsilon$, pose the most severe problem. Values of $\varepsilon \approx 1$ do cause distortion of their paths since they would move in one collision cycle a distance large compared to their mean free path. However, there are relatively very few fast moving molecules and this distortion is not a serious error. In practice ΔT_M can be set approximately equal to the minimum value of $\bar{t}$ in the flow field.

At low Knudsen numbers where the distribution function is nearly Maxwellian the mean relative velocity can be related to the local temperature and the time between collisions is

$$\frac{\bar{t}}{t_\infty} \sim \frac{1}{\frac{n}{n_\infty}\sqrt{\frac{T}{T_\infty}}}$$

In any case DTM should not exceed 0.2. At moderate Knudsen numbers the smallest time between collisions occurs near the walls and the relative velocity is $\bar{v}_r \approx u_\infty + \bar{c}_w \approx u_\infty$ and the local time between collisions is

$$\frac{\bar{t}}{t_\infty} \sim \frac{1}{\frac{n_2}{n_\infty} M_\infty}$$

where n_2 is the number density near the wall and M_∞ is the freestream Mach number.

At very high Knudsen numbers the limiting factor for determining DTM is the size of the flow field since the complete disturbance is not always contained within the flow field. The movement time interval, DTM, in this case is chosen to be smaller than the time to traverse the flow field.

4.4.2 Sampling Time Interval, ΔT_S

This is the interval at which the molecular information is sampled during the steady state period. Ideally it should be set equal to the smallest of the following times:

a) Time to change cell population by convection (where B_W is cell width)

$$\Delta T_S = \frac{B_W}{U}$$

Normalizing by reference quantities

$$\frac{\Delta T_S}{\bar{t}_\infty} = \frac{B_W/\lambda_\infty}{U/\bar{c}_\infty}$$

b) Time to change the velocity distribution in the cell due to collisions (where $\bar{t}$ is mean free time)

$$T_S = \bar{t}$$

Normalizing

$$\frac{\Delta T_S}{\bar{t}_\infty} = \frac{\bar{t}}{\bar{t}_\infty} = \frac{1}{(n/n_\infty)\ (\bar{v}_r/\bar{c}_\infty)}$$

Now since B_W, U, and $\overline{t}$ vary throughout the flow, it is even more difficult than for ΔT_M to define rules for selecting ΔT_S. However, there is no way in which a bad guess for ΔT_S can affect the operation of the simulation. The only effect would be in efficiency. If too small a value is selected, the samples will not be independent and the true sample size is less than the computed sample size. If too large a value is selected, some useful information is not being recorded and the length of the calculation is less than it need be. A useful rule of thumb which has worked well in practice is to set $\Delta T_S = 2 \times \Delta T_M$.

5. PROGRAM SLAB

5.1 DESCRIPTION

Program SLAB computes the flow about a slab of arbitrary thickness at arbitrary angle of attack. The flow field extends both above and below the slab centerline. There are allowed six weighting factor zones (or layers) in the upper field; two are allowed in the lower field. The entire flow field is divided into "A" level cells with an integral number in front of, along, and behind the body; and an integral number above and below the centerline. Any one rectangular region of "A" cells may be broken up into "B" cells. Similarly any one rectangular portion of "B" cells may be broken up into "C" cells.

Cell number one is the "A" cell located at the left boundary just above the centerline. Numbering increases along rows moving up the flow field until the upper field is filled. The next sequentially numbered cell is the "A" cell at the left boundary just below the centerline. Numbering then increases along rows and down the flow field until the entire field is populated with "A" cells. The next number is the lower left "B" cell above the centerline. Similarly, "B" cell numbering increases to the right and up the field, then to the right and down the field. "C" cells are numbered similarly.

The characteristic dimension is the body length. The Knudsen number and physical quantities are referenced to it. The flux of molecular number, momentum, and energy to an arbitrary number of segments on the body are recorded. Wetted length is referenced to the zero angle of attack stagnation point and increases around the body clockwise. The origin of the cell coordinates is on the body centerline at the leading edge. At positive angle of attack the upper field is to windward. In order to set up the input data for a particular calculation some engineering calculations must be made along with some estimates of the expected flow field.

All physical quantities are non-dimensionalized with respect to characteristic physical quantities. The reference length is the free stream mean free path (λ_∞). The reference velocity is the most probable molecular speed ($v_{m_\infty} = \sqrt{2RT_\infty} = \sqrt{2/\gamma}\, a_\infty$ where a_∞ is the freestream sound speed), while the

reference density and temperature are those in the freestream (ρ_∞, T_∞). Surface quantities are output in coefficient form as described in the SLAB program output description.

The important parameters that must be considered in setting up the input data are the freestream speed ratio ($S = u_\infty / v_{m\infty} = \sqrt{\gamma/2}\, M_\infty$, where M_∞ is the freestream Mach number), the Knudsen number referenced to the length of the plate ($AKN = \lambda_\infty / L$), the wall temperature ratio ($TR = T_W / T_\infty$), the angle of attack (ALP in degrees), the ratio of the plate length to the plate half-thickness (ALENR), the fraction of molecules striking the walls which will be specularly reflected (PSPR), (the remaining fraction is diffusely reflected from the surface), and the molecular model.

The molecular model is specified by the parameters IØPT, KCØL, WAM, NI and TFF. For monatomic gases IØPT = 0 and NI = 0 (number of internal degrees of freedom). Four different types of monatomic gases can be considered: hard sphere molecules (KCØL = 0) and power-law molecules where the inter-molecular repulsive force is inversely proportional to the fifth, (Maxwell molecules) ninth or twelfth power of the separation distance (KCØL = 5, 9, 12). When power-law molecules are considered a cutoff parameter (WAM) must be input. The cutoff parameter corresponds to molecular deflection angles being used to specify whether or not a collision has occurred. For example, for 5th-power molecules a value of 1.45 for the cutoff parameter means that collisions in which the deflection angle is less than 10° are not considered. Similarly, for 9th and 12th power molecules the corresponding values for the cutoff parameter are about 1.3 and 1.2. Some caution should be exercised here since a small increase in WAM can cause the computation time to increase dramatically without a corresponding increase in the accuracy of the results. That is, time will be spent calculating weak collisions which do not affect the flow field. Another molecular model which is considered is that for rough hard spheres (IØPT = 1). This is an exact dynamical model that has three internal degrees of freedom (NI = 3). The remaining molecular model is the energy-sink molecular model (IØPT = 2). This is an approximate model in which a fraction (proportional to TFF) of the translational energy is transferred into the internal degrees of freedom (NI). For a gas representing nitrogen the transfer factor (TFF) is 0.1. This value was obtained by comparing

calculations of the transport in strong shock waves to a corresponding experiment in nitrogen.

The specification of the above input data is all that is physically needed to determine the flow field. The problem is now to set up the cell arrangement and the movement time interval to calculate the flow field using the Monte Carlo program. The basic philosophy is to place the smallest cells where the largest gradients in flow properties are located. For cold wall temperatures there is usually a large density gradient close to the plate and at angle of attack there is a shock wave located within the flow field.

The first step is to estimate the total extent of the disturbance that is expected. This will provide the location of the outer boundaries. There is some guesswork involved here and sometimes it is necessary to make several runs in order to refine the cell structure. There are three levels of cells that are available: A level or primary cells, B level cells and C level cells. NL is the number of cell levels used in the calculation. The number of primary cells from the leading to the trailing edge of the plate (NC) is always an integer. Other than this the cell arrangement is independent of the body geometry. The flow field boundaries are located by specifying the number of primary cells in front of, behind, above and below the plate (NF, NR, NHU and NHL) and by setting the ratio (CR) of the height to width of A level cells. When the gradients normal to the plate are much larger than the gradients along the plate (for long plates at high angle of attack), the value of CR may be chosen less than 1, say 0.2.

The B (or second) level cells can be placed in the flow field where gradients exist in the flow field. Typically, they are placed near the body or, for blunt bodies, along the stagnation line. A given rectangular block of A level cells NCA by NHUA (or NHLA) in the x and y directions (along and normal to the plate) is divided into a block of B level cells MW by MHU (or MHL) in extent. The left hand boundary of the region where B cells are located is determined by specifying NFA - the number of A level cells in front of (to the left of) the B level region. The lower (upper) boundary of the B cells in the upper (lower) field is always along the axis of the slab. Similarly, a rectangular block of B level cells NCB x NHUB (or NHLB) is divided into a block of C level cells LW x LHU (or LHL). NFB

determines the left hand boundary of the block of C level cells. The surface of the plate is divided into segments in order to compute the distribution of the pressure, skin friction, heat transfer, etc. on the body. It is usually convenient to make the size of surface divisions equal to the local cell width. NDUL, NDUS, NDUT, NDLT, NDLS, NDLL are the number of divisions on the upper leading face, upper side, upper trailing face, lower trailing face, lower side and lower leading face.

Weighting factors can be set at horizontal boundaries (which must lie along a primary cell boundary) across which simulated molecules are duplicated or removed from the calculation. The weighting factors are set by specifying LD(i) and LF(i) i = 1,5 in the upper field and LDL and LFL in the lower field. LD (i) represents the number of primary cells from the centerline to the weighting factor boundary and LF is the weighting factor which is applied across this boundary. The cumulative weighting factor for each weighting factor zone (LWF) is calculated within the program and represents the number of particles which move about as a cluster. Near the centerline in both the upper and lower regions the weighting factor is always one (LWF = 1). When a simulated molecule crosses a weighting factor boundary from a region of lower weighting factor to a region of higher weighting factor, the particle remains in the calculation with a probability proportional to the ratio of the two weighting factors. When crossing the weighting factor boundary from a region of higher weighting factor to a region of lower weighting factor, a simulated molecule is duplicated proportional to the ratio of the two weighting factors. If the simulated molecules can be thought of as clusters of particles, then crossing from a higher to a lower weighting factor zone causes the cluster to break up into the component particles.

The weighting factor zones serve additional functions in the drum versions of the SLAB program. There the molecular quantities are broken up into blocks for storage on the 1108 drum system. For the "hopped-up" drum version the cell information is also broken up into blocks for storage on the drums.

The flow field is initially populated with simulated molecules by specifying the initial number of molecules, INM. During the course of the computation the number of molecules will build up with time until a steady

state is reached. The maximum number of molecules that are allowed in the calculation is MNM. If the actual number of molecules builds up beyond this number the calculation will stop and a diagnostic will be written out. INM should be chosen so that there are an adequate number of molecules in the various cells. Typically, there should be at least four molecules in a freestream cell in order for the collisions to be computed properly. The number MNM is also used to dimension the BN1 array which contains the properties of each simulated molecule.

If desired, each molecule can be labelled as to its molecular "type". Type 0 molecules are freestream molecules; type 2 molecules are those which have struck the body at some time; and type 1 molecules have had a collision at some time with either a type 2 or another type 1 molecule. Type 1 molecules are therefore indirectly aware of the presence of the body.

When it is desired to keep track of the molecular "type" several things must be done. First, LS1 must be set equal to MNM; otherwise, LS1 is unity. The dimension of ITP is the maximum number of molecules MNM, one dimension of NTSC is the total number of divisions on the plate LS2 = NDUL + NDUS + NDUT + NDLT + NDLS + NDLL and one dimension of NBC and NBCT is the total number of cells, NBX.

The total number of cells, NBX, is used in dimensioning the qualities associated with the properties of the cells. The number of primary cells is (NHU + NHL)* (NF + NC + NR); the number of second level or B cells, if any, is MW* (MHU + MHL); and the number of C cells is LW* (LHU + LHL).

If the rough sphere molecular model is chosen for the computation then the rotational velocities WX, WY, WZ must be dimensioned by the maximum number of molecules MNM. Similarly, if the energy sink molecular model is used the rotational energy ER must be dimensioned by MNM. In either case the cell quantities used to compute the rotational temperature, TER and TRA, must be dimensioned by the total number of cells NBX.

In the Monte Carlo method, the flow field is divided into cells for the purpose of calculating collisions. One way that oversized cells can be used without hurting the accuracy of the calculation too much is through the use of an option where the second molecule of the molecular pair is selected so that the separation distance is not too large. This is done

by specifying AMDX and AMDY the maximum allowable X and Y separation distance (in mean free paths). When AMDX is zero this option is not used and molecular pairs are selected at random from the molecules within a cell.

The Monte Carlo calculation is a time dependent calculation and there exists an unsteady flow time at the beginning of each calculation during which time the flow field evolves. The flow field then reaches a steady state, TST, and then the cells are sampled at time intervals, DTS, long enough to prevent correlations between succeeding samples. Typically, TST is chosen to be roughly the order of the time for a freestream molecule to traverse the flow field. DTS is usually chosen to be two or three times DTM. The flow field information is printed at time intervals DTP. This is usually set at some multiple of DTS and is typically chosen to be smaller than TST so that some unsteady flow field information is obtained. The Monte Carlo calculation can be terminated by setting the parameter TLIM. This is measured in terms of the mean collision time. Alternatively this parameter can be set to a large value and the job can be terminated by specifying the maximum run time on the job card.

There are several features or options which are not checked out for the program at this time. Therefore, set the following values: NSA = 0, L1= 1, L2 = 1, IPLØT = 0, INBX = 0, NPR = 0, and TMAX = 0. The final input parameter for the unpacked SLAB program is NSR which is chosen to be an arbitrary odd integer. NSR gives the initialization for the random number generator. Although the program is computed using random numbers, these numbers come in a definite sequence so that a run can be duplicated exactly if all the input including NSR, is the same.

If NSR is different, a different sequence of random numbers is used in the calculation and the results will be different. The averaged quantities for two similar runs, except for NSR, can be compared to give an idea of the statistical scatter inherent in this type of calculation. Typically, the statistical scatter is inversely proportional to the square root of the sample size.

Before the Monte Carlo calculation can be performed the dimensioning of the various arrays within the program must be checked. The "BN" arrays must be dimensioned to be consistent with the input variables on the input cards. The "CØMMØN/S ARRAY/" statement in SLAB (main program), MSLAB and RSTART must be modified. If "type" molecules are being used the following variables must also be dimensioned in SLAB (main program): ITP, NTSC, NBC and NBCT. These dimensions should be consistent with the data that is input. If IØPT is different from zero the variables for calculation of rotational temperature (TER and TRA) must be dimensioned in SLAB. For the rough sphere molecular model WX, WY and WZ must be dimensioned MNM. For the energy sink molecular model ER must be dimensioned MNM. There are three 1108 versions of the SLAB program: the "unpacked" SLAB version which is the basic program, the drum SLAB version in which the "432" high-speed drums are used for the storage of the molecular quantities, called DRUM DRUM SLAB I, and the "hopped-up" drum SLAB version in which the "432" drum system is also used for the storage of the cell quantities, called DRUM SLAB II.

The following description for the cell arrangement is applicable to the "unpacked" SLAB version and the DRUM SLAB I version. The cell arrangement for the "hopped-up" DRUM SLAB II version will be described later.

In both of the drum versions of the SLAB program the flow field is divided into blocks (NBLK = number of blocks). In the drum SLAB I version the molecular quantities x, y, u, v, w are broken up along horizontal boundaries which correspond to the weighting factor zones and are stored on the "432" hi-speed drum unit. The appropriate molecular quantities are read into core when calculations are to be performed on a given block. When the molecules move from one block to another, they are stored in temporary "Q-arrays". The dimension of the Q-arrays is (NBLK, MNQ) where NBLK and MNQ are input quantities. The upper and lower boundaries of the flow field are input as YM and YL and must be input to be consistent with CR and the total number of cells in the vertical direction. In the drum versions the quantity MNM Is the maximum number of molecules within a block. If the number of molecules builds up beyond MNM within a block, a molecule is removed at random and the weighting factor of that block is modified.

Some general considerations that have to be taken into account are that the MSC 1108 has a core size of 53,000 decimal words and the program itself requires about 17,000 decimal words for the instructions (with all the variable dimensions set equal to one).

<u>1108 Core Size = 53,000 words</u>

Drum version of SLAB for 1108

Instructions - 17,347 words

i.e., The core required to load a run with:

1. IØPT = 0
2. ITP option turned off
3. MNM = 1
4. NBX = 1

5. ND = 1

6. NBLK = 1 (# of Blocks)

7. MNQ = 1 (length of the Q-arrays)

For a given run with IØPT = 0 and ITP turned off:

Core = 17,347 + 7(MNM-1) + 26(NBX-1) + 9(ND-1) + 7(NBLK·MNQ-1)

I. If ITP is turned on, add:

4(NBX-1) + (MNM) + (NBLK·MNQ-1)

II. If IØPT = 1 add

3(MNM-1) + 2(NBX-1) + ND + 3(NBLK·MNQ-1)

III. If IOPT = 2 add

(MNM-1) + 2(NBX-1) + ND + (NBLK·MNQ-1)

5.2 CONSTRUCTION OF CELL PICTURES

The cell arrangement and body geometry are independent, with the sole exception that the total length of the body always spans an integer number of primary cells, NC. All lengths are scaled by λ_∞; however, to facilitate construction of the cell picture, it is helpful to select a scale on which it is also convenient to represent the primary cell width, b_W. In the following discussion, all variable names in lower case letters represent dimensional quantities, all variable names in upper case letters are dimensionless Fortran variables. The few exceptions for this are specifically noted.

Brief Definitions:

$$\ell_t/\lambda_\infty = 1/AKN$$

$$b_W/\lambda_\infty = 1/(NC \cdot AKN)$$

$$b_h/\lambda_\infty = CR/(NC \cdot AKN) \quad ; \quad (b_h/b_W \equiv CR)$$

$$2 \cdot \ell_t/h = ALENR$$

$$h/\lambda_\infty = 2/(AKN \cdot ALENR)$$

Complete definitions for the following cell geometry variables can be found in the input description: CR, NC, NF, NR, NHU, NHL, NL, NFA, NCA, NHUA, NHLA, MW, MHU, MHL, NFB, NCB, NHUB, NHLB, LW, LHU, LHL. The construction of the second and third level cell arrangement is obvious from the definitions in the input description.

Restrictions on the cell geometry are:

1) The body centerline must be contained within the second and third levels or form a boundary for those levels.

2) The third level must be nested within the second level.

3) The second and third level cells must not straddle primary cell boundaries at which weighting is done, i.e., the weighting boundaries must lie along cell boundaries for any level.

The body and primary cell structure for Program SLAB Sample Case are shown in Figure 1. The complete cell picture is shown in Figure 2 with a blown-up view of the third level cells shown in Figure 3.

PROGRAM SLAB SAMPLE CASE

CONSTRUCTION OF BODY AND CELL GEOMETRY

(ONLY PRIMARY CELLS SHOWN)

AKN = .0556

ALENR = 26 = $\frac{l_t}{h/2}$

NC = 9

$b_w/\lambda_\infty = 1/(9 \cdot .0556) = 2.0$

$h/2\ \lambda_\infty = .69$

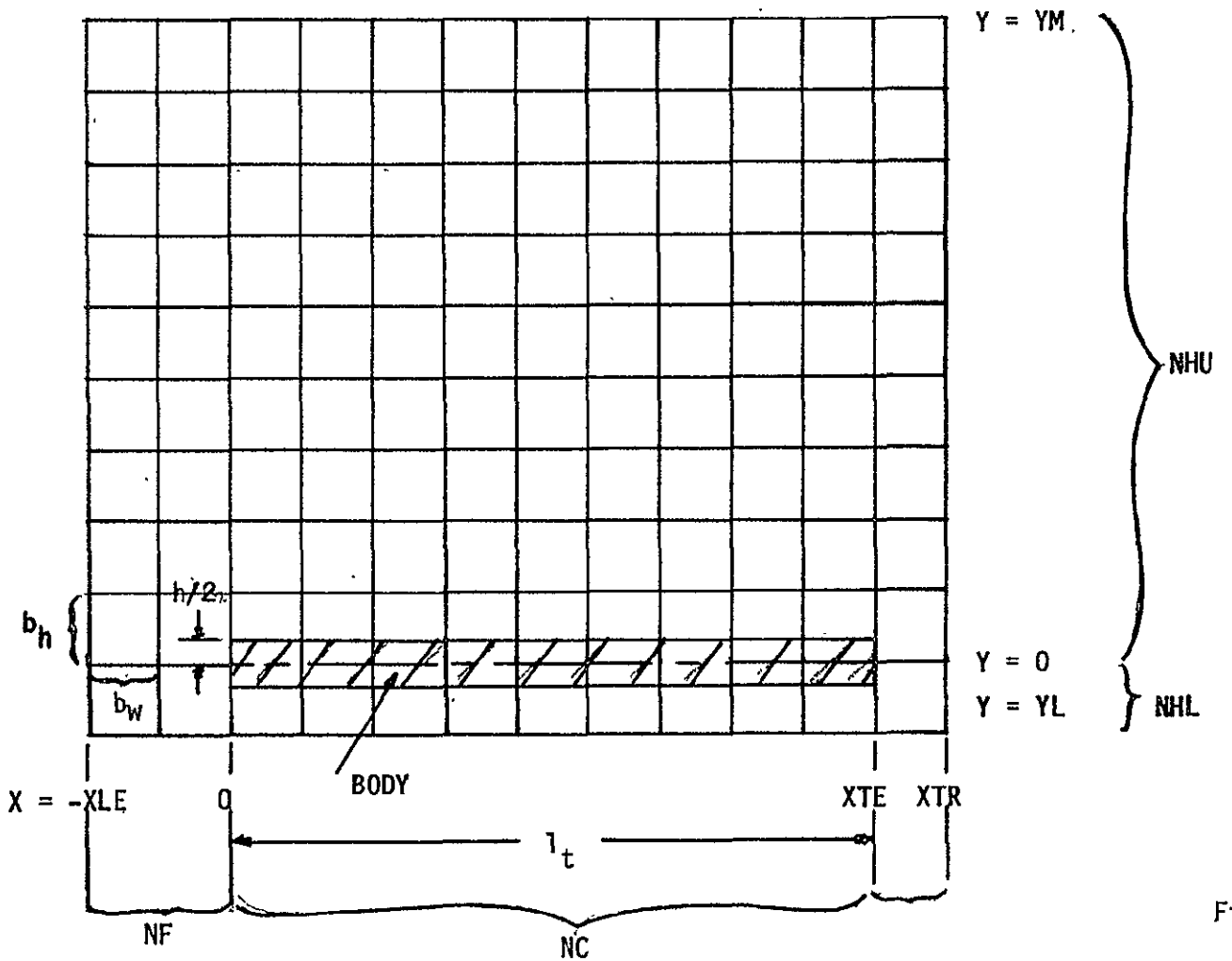


Figure 1.

PROGRAM SLAB SAMPLE CASE

COMPLETE CELL PICTURE

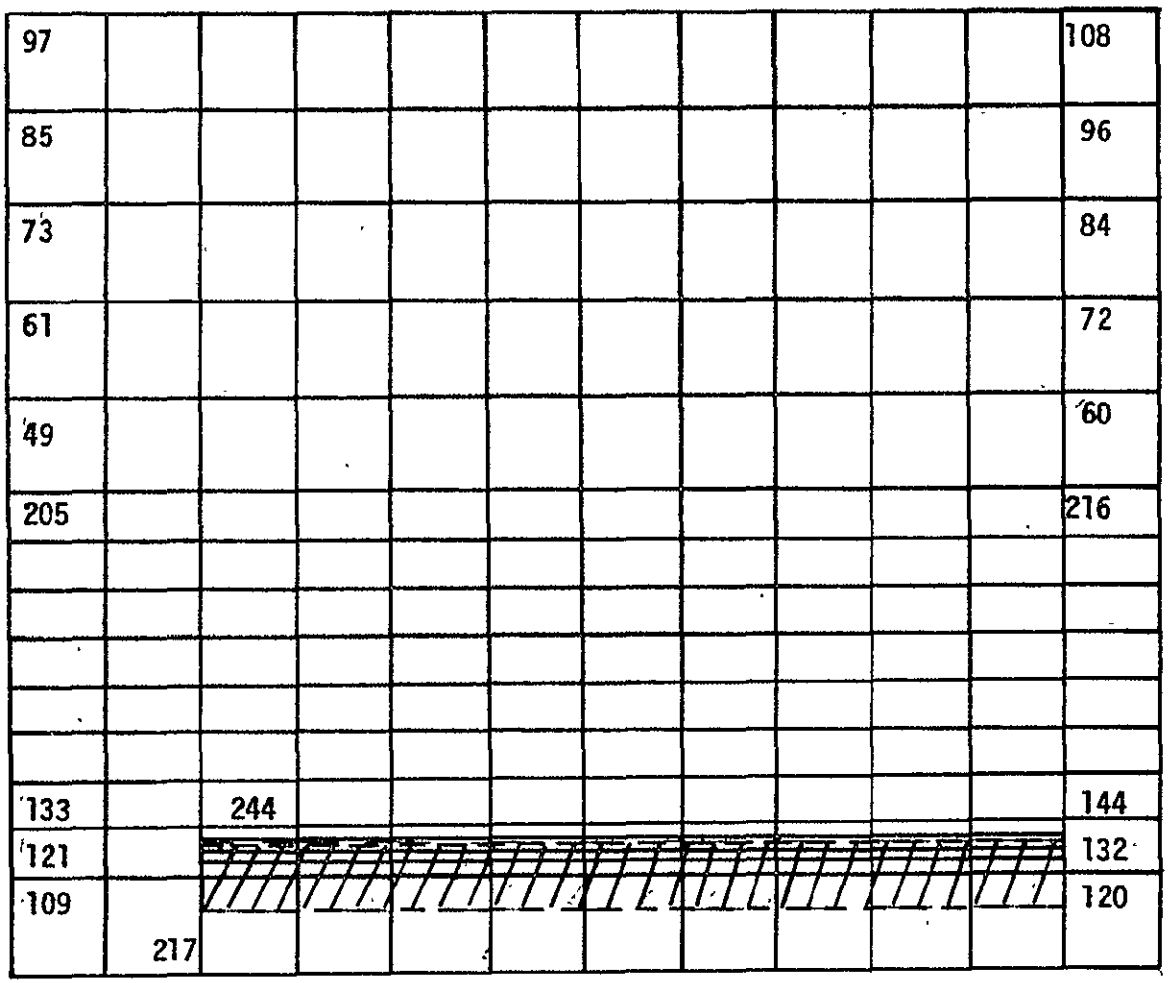


Figure 2

PROGRAM SLAB SAMPLE CASE

BLOWN-UP VIEW OF 3rd LEVEL CELLS

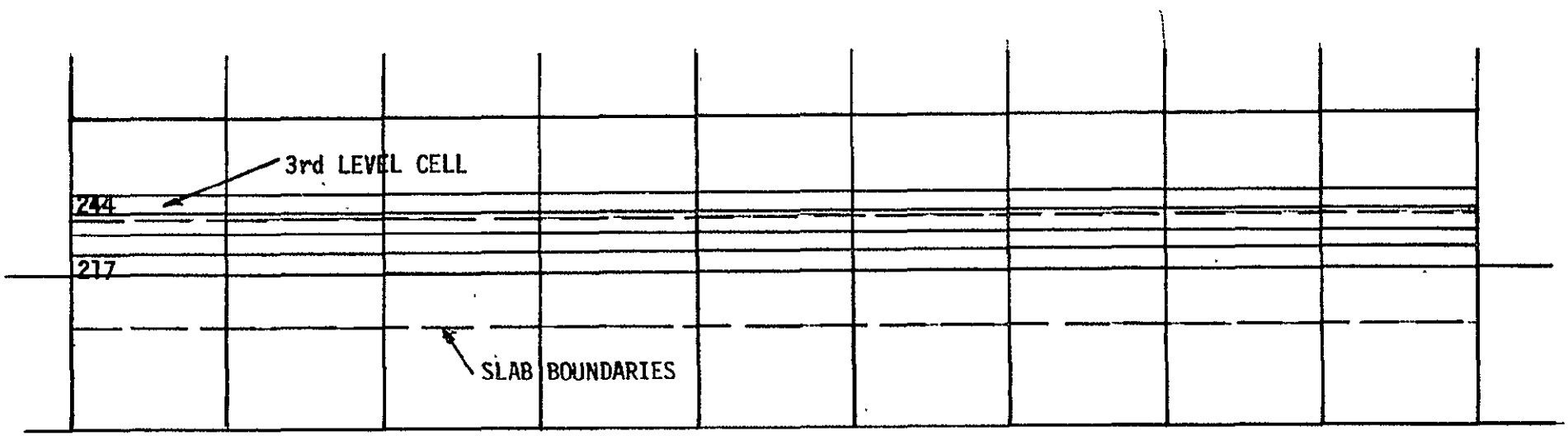


Figure 3

5.3 EXPLANATION OF WEIGHTING FACTORS IN PROGRAM SLAB

The statistical weight of particles varies among a number of horizontal zones in the flow field. The input data array LD(i), LF(i) specifies horizontal boundaries in the flow field (which must lie along a primary cell boundary) across which changes occur in the number of simulated particles which a particle in the molecular table represents. One can think of the particles which have statistical weight greater than one as representing a cluster of an integer number of particles which move about together.

Define: LD = Primary cell boundary at which weighting is done
LF = Weighting factor applied

The values used for Program SLAB Sample Case are shown below:

Weighting Input Data for Program Slab Sample Case

i	LD(i)	LF(i)
1	4	2
2	9	1
3	9	1
4	9	1
5	9	1
	LDL = 1	LFL = 1

LWF = Weighting factor for the zone or layer, i.e., the number of particles which move about as a cluster. The zone arrangement for this sample case is shown in Figure 4 with a schematic of how particles crossing zone boundaries are handled.

PROGRAM SLAB SAMPLE CASE

EXPLANATION OF WEIGHTING FACTORS

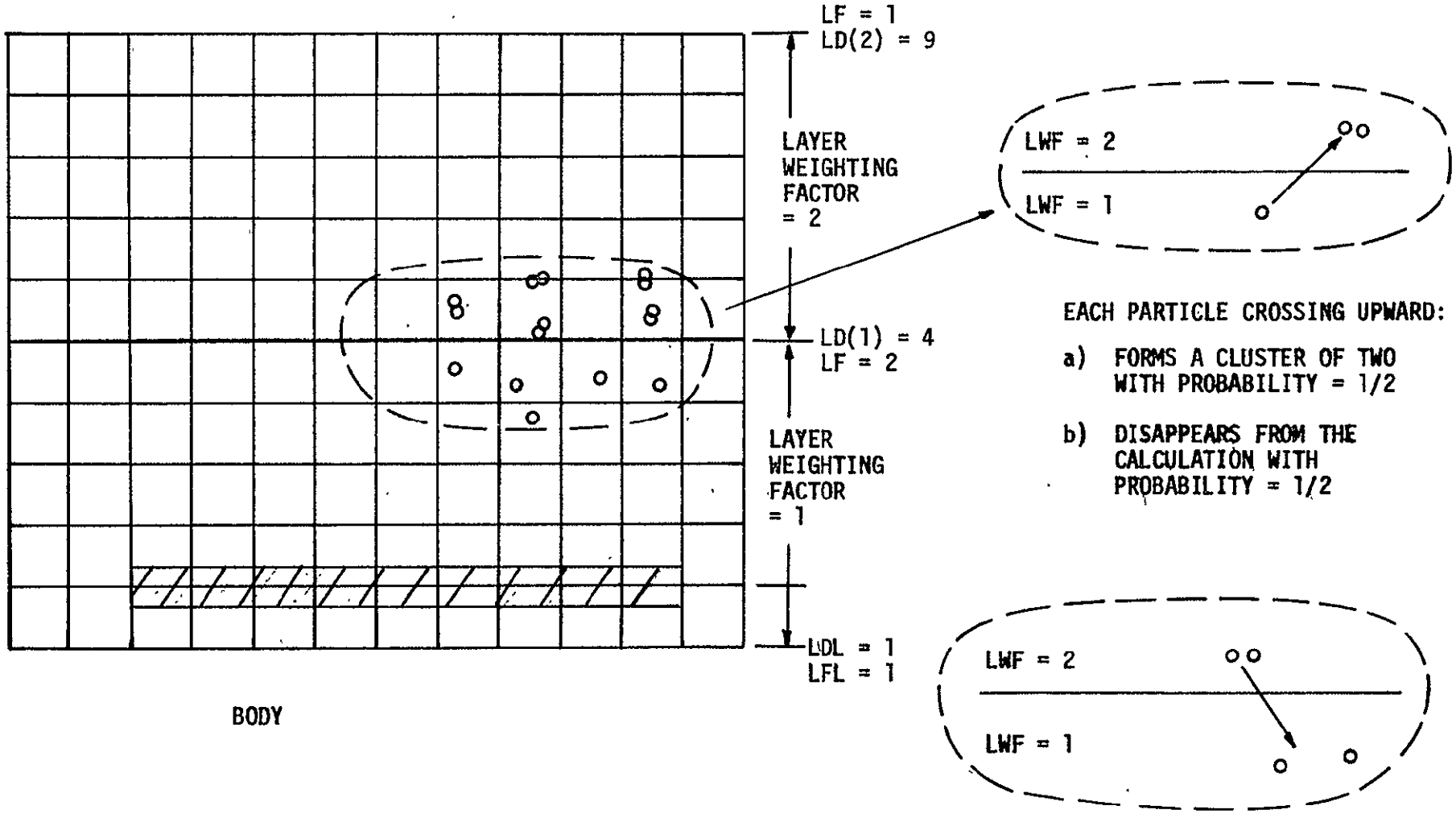


Figure 4

5.4 SLAB PROGRAM SUBROUTINES

Main Program	Function
MAIN	Computes molecular movement and collisions with the body

Subroutines	
MSLAB	Initialization routine, computes initial field coordinates and velocities
VELOC	Computes rough sphere velocities
ENTER	Enters molecules at boundaries of the field
SAMPLE	Takes sample of fluid velocity and temperature
NUMB	Re-stores molecules in cells after movement cycle
ERF	Computes error function
CORENT	Computes values for number of molecules to be entered on boundaries
TDWT	Computes weighting factors for each layer in the field
RSTART	Restarts the calculation at end of previous run
GETV	Computes inter-molecular collisions
SETTD	Computes initial velocities and locations of molecules at beginning of calculation
RANF	Computes pseudo random numbers

5.5 SLAB PROGRAM INPUT DESCRIPTION

Card 1 - (9I6 format)

ISTART	- Restart option flag (= 1 normal start, = 0 restart)
NSA	- No longer used, set = 0
L1	- No longer used, set = 1
L2	- No longer used, set = 1
LS1	- Number of cells for molecule type output (LS1 = 1 if output is not requested)
LS2	- Maximum number of body divisions for molecule type output (LS2 = 1 if output is not requested)
IPLØT	- No longer used, set = 0
NSR	- Initial random number
IØPT	- Molecule designation flag -- 0 - Monatomic 1 - Rough spheres 2 - Energy sink

Card 2 - (6F10.4 format)

AKN	- Knudsen number based on body length
S	- Speed ratio
TR	- Ratio of surface temperature to freestream temperature
CR	- Ratio of height to width of first level cells
YAW	- No longer used, set = 0.0
ALP	- Pitch angle of attack in degrees

Card 3 - (10I6 format)

NC	- The number of first level cells along the body
NF	- The number of first level cells in front of the body
NR	- The number of first level cells behind the body
NHU	- The vertical number of first level cells in the upper field
NHL	- The vertical number of first level cells in the lower field
INM	- Initial number of molecules
MNM	- Maximum number of molecules
KCØL	- Power law repulsion model exponent
INBX	- No longer used by the program, set = 0
NPR	- No longer used by the program, set = 0

Card 4 - (8I6 format)

NL	- Number of cell levels
NFA	- Number of first level cells in front of the second level region
NCA	- Horizontal number of first level cells to be divided into second level cells
NHUA	- Vertical number of first level cells to be divided into second level cells in the upper field
NHLA	- Vertical number of first level cells to be divided into second level cells in the lower field
MW	- Horizontal number of second level cells in the upper field (same number in lower field)
MHU	- Vertical number of second level cells in the upper field
MHL	- Vertical number of second level cells in the lower field

Card 5 - (7I6 format)

NFB	- Number of second level cells in front of the third level region
NCB	- Horizontal number of second level cells to be divided into third level cells
NHUB	- Vertical number of second level cells to be divided into third level cells in the upper field
NHLB	- Vertical number of second level cells to be divided into third level cells in the lower field
LW	- Horizontal number of third level cells
LHU	- Vertical number of third level cells in the upper field
LHL	- Vertical number of third level cells in the lower field

Card 6 - (12I6 format)

LD(1)	- Number of primary cells from the centerline to the first weighting factor boundary in the upper field
LF(1)	- Weighting factor applied across the first weighting factor boundary in the upper field
LD(2)	- Number of primary cells from the centerline to the second weighting factor boundary in the upper field
LF(2)	- Weighting factor applied across the second weighting factor boundary in the upper field

. .
. .
. .
. .

LF(5) - Weighting factor applied across the fifth weighting factor boundary in the upper field

LDL - Number of primary cells from the centerline to the lower field internal weighting factor boundary

LFL - Weighting factor applied across the lower field internal weighting factor boundary

Card 7 - (5F10.4 format)

DTM - Movement time interval

DTS - Sampling time interval

DTP - Print time interval

TST - Steady flow time

TLIM - Time limit for problem

TMAX - No longer used, set = 0

Card 8 - (5F10.4 format)

PSPR - Molecular reflection option flag

0 - Diffuse reflection from body
$0 < PSPR \leq 1$ - Specular reflection percentage

WAM - Impact parameter cut off for the power law collision routine

AMDX - Maximum separation X-distance for collisions option

AMDY - Maximum separation Y-distance for collisions option

ALENR - Ratio of body length to body half-height measured from the centerline

Card 9 - (6I6 format)

NDUL - Number of divisions on the upper leading face

NDUS - Number of divisions on the upper side

NDUT - Number of divisions on the upper trailing face

NDLT - Number of divisions on the lower trailing face

NDLS - Number of divisions on the lower side

NDLL - Number of divisions on the lower leading face

Card 10 - (2F10.4 format)

NI - Number of internal degrees of freedom

TFF - Transfer factor

5.5.1 SLAB Program Input Forms

CARD (11I6)

ISTART	6	
NSA	12	0
L1	18	1
L2	24	1
LS1	30	
LS2	36	
IPLØT	42	0
NSR	48	
IØPT	54	

CARD 2 (6F10.4)

AKN	10	
S	20	
TR	30	
CR	40	
YAW	50	0.0
ALP	60	

CARD 3 (12I6)

NC	6
NF	12
NR	18
NHU	24
NHL	30
INM	36
MNM	42

KCØL	48	
INBX	54	0
NPR	60	0

CARD 4 (12I6)

NL	6
NFA	12
NCA	18
NHUA	24
NHLA	30
MW	36
MHU	42
MHL	48

CARD 5 (12I6)

NFB	6
NCB	12
NHUB	18
NHLB	24
LW	30
LHU	36
LHL	42

CARD 6 (12I6)

LD(1)	6
LF(1)	12
LD(2)	18
LF(2)	24
LD(3)	30

LF(3)	36	
LD(4)	42	
LF(4)	48	
LD(5)	54	
LF(5)	60	
LDL	66	
LFL	72	

CARD 7 (6F10.4)

DTM	10	
DTS	20	
DTP	30	
TST	40	
TLIM	50	
TMAX	60	0

CARD 8 (6F10.4)

PSPR	10
WAM	20
AMDX	30
AMDY	40
ALENR	50

CARD 9 (12I6)

NDUL	6
NDUS	12
NDUT	18
NDLT	24
NDLS	30

NDLL 36

CARD 10 (6F10.4)

NI 10

TFF 20

Dimension (must be < 35,000)

ITP(N)

NTSC(2,ND)

NBC(2,LS1)

NBCT(2,LS1)

BN1(MNM,7)

BN2(NBX, 25)

BN3(1,12)

BN4(ND,9)

BN5(1,5)

NBX = (NHU+NHL) (NC+NF+NR) + MW(MHU+MHL) + LW(LHU+LHL)

ND = NDUL + NDUS + NDUT + NDLT + NDLS + NDLL

LS1 = NBX; for type molecule option
1 ; otherwise

N = MNM; for type molecule option
1 ; otherwise

IOPT = 2 { ER(MNM), TRA(NDX), TER(NDX) }

IOPT ≠ 2 { ER(1), TRA(1), TER(1) }

5.5.2 SLAB Program Dimension Statements

Four FØRTRAN dimension statements must be changed with each run as follows:

BN ARRAYS - These must be consistent with the dimensions on the input variable load sheet. The "CØMMØN/SARRAY/" statement must be modified in the following three routines:

SLAB - (Main program)

MSLAB

RSTART

TYPE MOLECULES - The first dimension statement in SLAB (main program) must be consistent with the dimension on the load sheet regarding the following four arrayed variables:

ITP

NTSC

NBC

NBCT

5.6 SLAB PROGRAM OUTPUT DESCRIPTION

The following is a description of the SLAB program output after the establishment of steady flow. As the molecules move in the flow field, a record is kept of collisions with the body surface. With each collision, appropriate amounts are added to the counters for the total flux, drag, and heat transfer. The variables for the appropriate surface segment on the body are also modified. The rates of increase of these quantities with time after the establishment of steady flow give the required flux, drag, and heat transfer coefficients; and the distribution of flux pressure, skin friction, and heat transfer around the surface.

All physical quantities are non-dimensionalized. Distances are referenced to the free stream mean free path. Velocities are normalized to the most probable molecular peculiar velocity in the freestream (i.e., $\sqrt{2RT_\infty}$). Densities and temperatures are also referenced to the freestream values.

Flux, drag, and heat transfer are output in coefficient form according to the following conventions:

The total number flux coefficient is defined by,

$$\frac{\text{NUMBER/UNIT TIME}}{n_\infty U_\infty A}$$

where

n_∞ is the freestream number density

U_∞ is the freestream velocity

A is a reference area taken to be the length of the slab side times a unit length in the z direction (i.e., magnitude is that of the body length)

The total drag coefficient is defined by,

$$\frac{\text{DRAG}}{\frac{1}{2}\rho_\infty U_\infty^2 A}$$

where ρ_∞ is the freestream density. The total drag is broken up into a component due to the incident molecules and one due to the reflected molecules. Also the axial drag or drag in the z direction is calculated and normalized as above. It too is broken up into components due to the incident and the reflected molecules.

The total heat transfer coefficient is defined by,

$$\frac{\text{HEAT TRANSFER/UNIT TIME}}{\frac{1}{2}\rho_\infty U_\infty^3 A}$$

The heat transfer is broken up into components along the slab surfaces where the coefficient in these cases is redefined as,

$$\frac{\text{HEAT TRANSFER/UNIT TIME}}{\frac{1}{2}\rho_\infty U_\infty^3 A_{ref}}$$

where A_{ref} is the area of the segment being considered and has a magnitude equal to the length of that segment.

5.6.1 Distribution Around Surface

The next block of output is the distribution of physical quantities at each division around the surface of the body. The following quantities

are output for each division.

WETTED LENGTH -- (denoted "ANGLE" in some program versions) -- location of that division around the body perimeter in units of freestream mean free path. It is assumed zero at the zero angle of attack stagnation point and increases clockwise around the body. The value for any division is taken at the intersection of that division and the next clockwise division.

TOTAL NUMBER -- number of molecules to have hit body along the division since the beginning of steady state time.

NUMBER FLUX -- defined in coefficient form as:

$$\frac{\text{WEIGHTED NUMBER/UNIT TIME}}{n_\infty U_\infty A_{div}}$$

where A_{div} is the reference area of that division and has magnitude equal to the length of that division.

SHEAR STRESS -- (denoted "THETA STRESS" in some program versions) -- defined in coefficient form per unit area as:

$$\frac{\text{SHEAR STRESS/UNIT AREA}}{\frac{1}{2}\rho_\infty U_\infty^2 A_{div}}$$

Z STRESS -- component of shear stress in the z direction defined as:

$$\frac{\gamma_Z\text{/UNIT AREA}}{\frac{1}{2}\rho_\infty U_\infty^2 A_{div}}$$

where γ_Z is that component of the shear stress in the z direction.

PRESSURE -- defined as pressure in coefficient form as:

$$\frac{p}{\frac{1}{2}\rho_\infty U_\infty^2 A_{div}}$$

where p is the pressure on that division.

TRANSLATIONAL HEAT TRANSFER -- the heat transfer imparted to the body from the kinetic energy of impinging molecules along each division - defined as:

$$\frac{\text{TRANSLATIONAL H. T./UNIT TIME}}{\frac{1}{2}\rho_\infty U_\infty^3 A_{div}}$$

ROTATIONAL HEAT TRANSFER -- the heat transfer imparted to the body from the internal energy of impinging molecules along each division - defined as:

$$\frac{\text{ROTATIONAL H. T./UNIT TIME}}{\frac{1}{2}\rho_\infty U_\infty^3 A_{div}}$$

TYPE 1 -- (applicable only with "type molecule" option) -- this is the percentage of the actual number of molecules hitting that division subject to these restrictions:

1) molecules cannot have hit the body previously
2) molecules have had a molecular collision with either a molecule that has hit the body, or a collision with another type 1 molecule.

TYPE 2 -- (applicable only with "type molecule" option) -- this is the percentage of the actual number of molecules hitting that division which have hit the body previously.

5.6.2 Flow Field Information

NUMBER	- Cell number
X	- x coordinate of the cell center. The leading edge corresponds to x = 0.
Y	- y coordinate of the cell center. The body centerline corresponds to y = 0.
SAMPLE	- Actual number of molecules used to compute properties for the cell
NUMBER DENSITY	- Cell density normalized to the freestream density
X VEL	- Average x velocity of molecules in the cell normalized to the most probable molecular peculiar velocity in the freestream
Y VEL	- As above for y velocity
Z VEL	- As above for z velocity
TEMP	- Cell temperature normalized to the freestream value. It is the average of x, y, and z temperatures below.

X TEMP	- Cell temperature associated with the x component of the kinetic energy. It is normalized to 1 in freestream.
Y TEMP	- As above for y component
Z TEMP	- As above for z component
ROTATIONAL TEMP	- Cell temperature associated with the internal energy of molecules in the cell
TYPE 1	- Density of type 1 molecules normalized to cell density
TYPE 2	- Density of type 2 molecules normalized to cell density

6. DRUM SLAB I AND II PROGRAMS

6.1 DESCRIPTION OF MASS STORAGE BLOCKS

6.1.1 General

(i) The existing weighting factor regions; e.g., 1, 2, 3, are used as the separate storage blocks (even if all weighting factors are set = 1).

(ii) A non-integer weighting factor WF(n) is read in for each block (this replaces both LF(n) and LWF(n). LD(n) is now the number of primary cells (the total from the axis) to the outer radius of each region.

(iii) MNM is now the maximum number of molecules in each block. If the number exceeds this, one molecule is removed at random and an appropriate change is made to the weighting factor WF for the block. This means that there will never be an "excess molecule" stop; instead, the number in the affected block will level off with MNM as the maximum of the fluctuations.

(iv) LPF is now the cell number. This should save sufficient time in the indexing to more than balance the computational time increases elsewhere.

(v) Auxiliary storage is manipulated

- (i) to enter initial state of molecules
- (ii) to calculate collisions and move molecules
- (iia) if a buffer storage is filled during this process
- (iii) to enter buffer storages and set cross-reference arrays
- (iv) to sample molecules.

If (iia) does not occur, the auxiliary storage is scanned only twice each DTM.

(vi) Flow charts for the Drum Programs are shown in Figs. 5 and 6.

6.1.2 Changes to Data

(1) Read in integer NBLK

(2) Read in WF( ) and LD( ) for each block

WF(1) must = 1

LD(NBLK) must = NH

(3) INM remains the total number of molecules initially set up

FLOW CHART FOR DRUM PROGRAMS

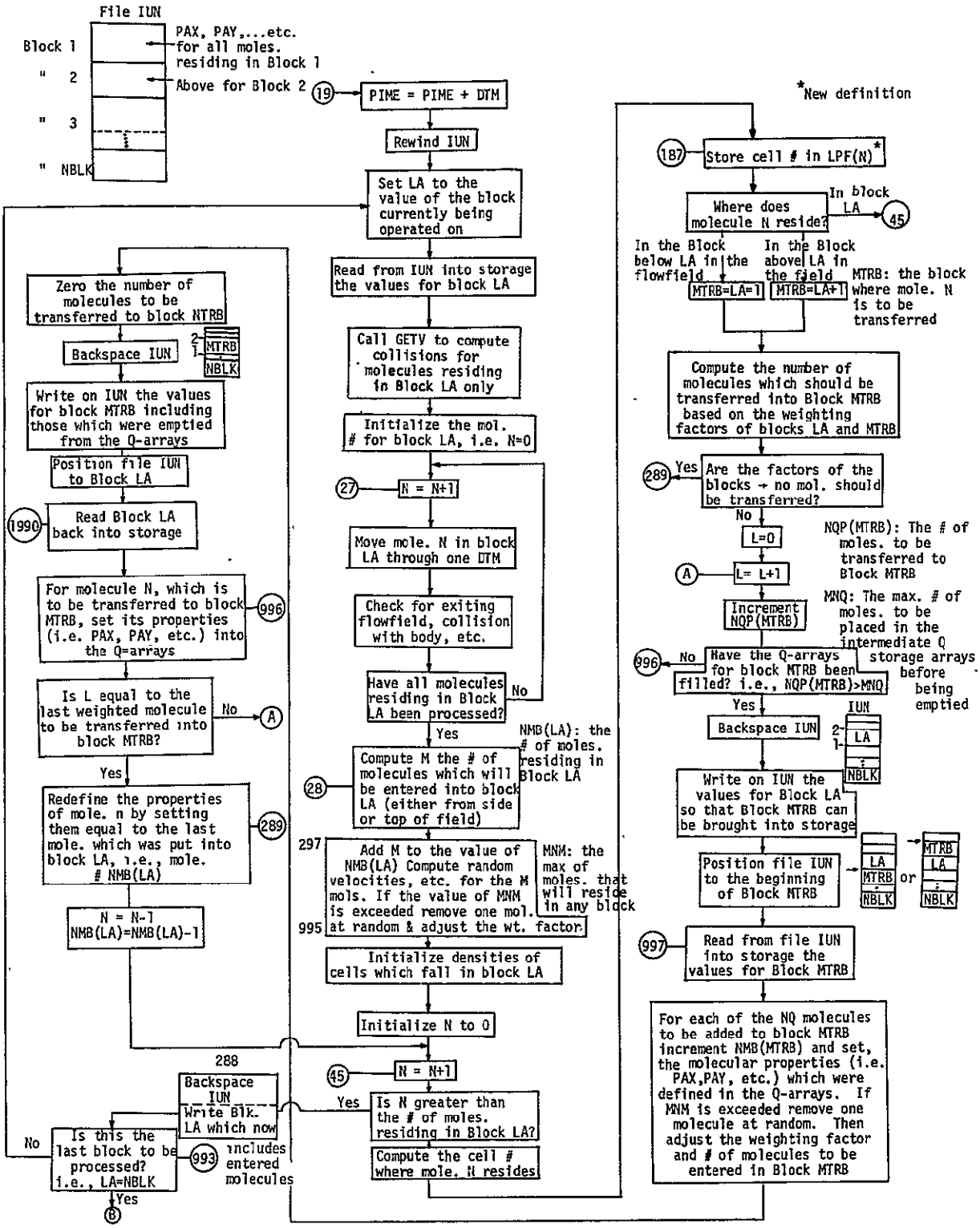
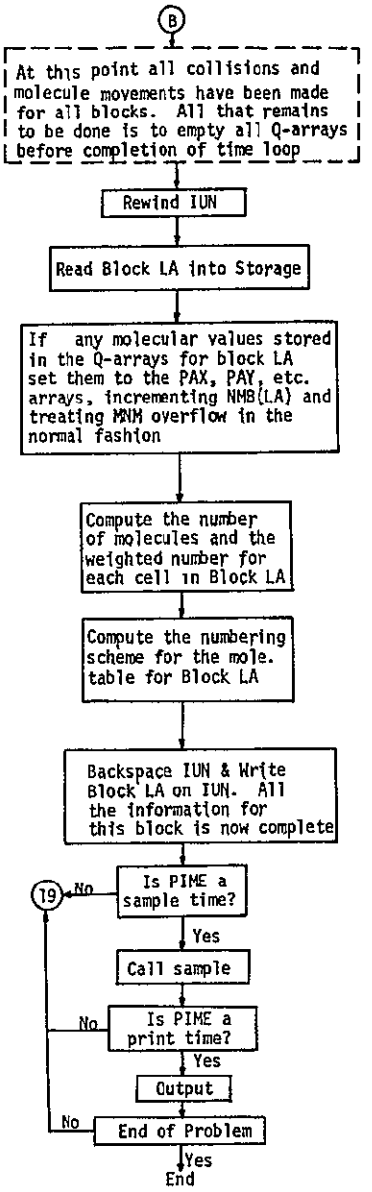
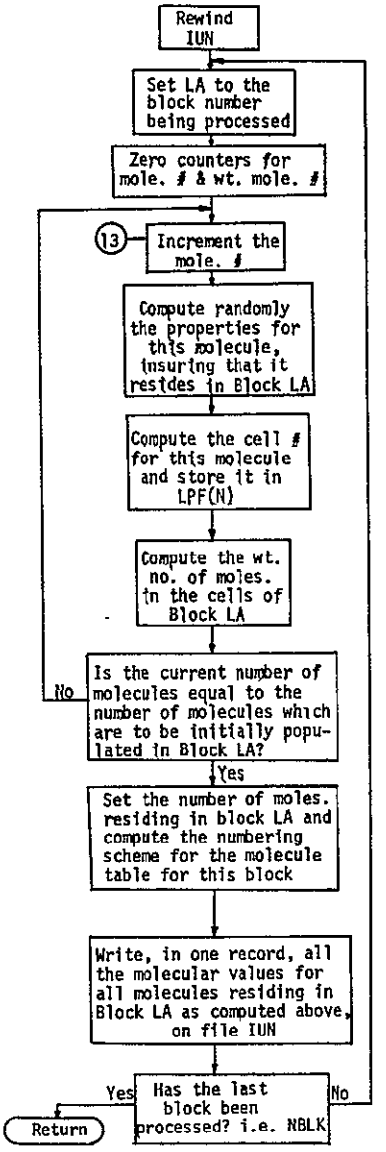


FIGURE 5

FLOW CHART FOR DRUM PROGS. (CONTD.)



SETTD



SAMPLE

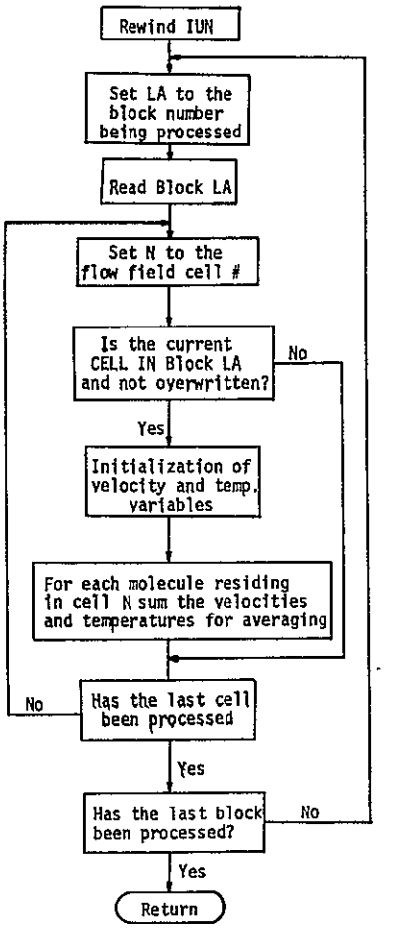


FIGURE 6

(4) Read MNQ the maximum number of molecules in buffer storage arrays QPAX, etc. -- equal to the second dimension of Q PAX, etc. (if the number in one buffer storage exceeds the limit, it is emptied immediately, so that MNQ need only be sufficiently large to prevent excessive record shuffling).

6.1.3 Modifications to Variables

Deleted variables and arrays

LF(5)

LWF(5)

New variables and arrays

NBLK the number of blocks

WF(1 to NBLK) weighting factor for block (NBLK is the number of blocks)

NMB(1 to NBLK) the number of molecules in the block

LL(1 to NBLK) the initial (factored) number in the block

NBF(cell) is now REAL (non-integer weighting factors equal real factored number)

NTSF(surface elements) is now REAL

NBFC(1 to NBX) the block in which cell falls

QPAX(1 to NBLK, MNQ)
QPAY(1 to NBK, MNQ)
etc. for all molecule storage
} Buffer storage for each region

NQP(NBLK) the number of molecules in each buffer storage

ENT & REM have dimensions NBLK +1

Changes

LPF(N) is now the cell in which the molecule numbered N lies

LD now has dimensions equal to number of blocks

6.2 DRUM SLAB I and II PROGRAM SUBROUTINES

Main Program — Function

MAIN

Sub-routines	
MSLAB	Initialization routine, computes initial field coordinates and velocities
VELOC	Computes rough sphere velocities
SAMPLE	Takes sample of fluid velocity and temperature
ERF	Computes error function
CORENT	Computes values for number of molecules to be entered on boundaries
TDWT	Computes weighting factors for each layer in the field
RSTART	Restarts the calculation at end of previous run
GETV	Computes inter-molecular collisions
SETTD	Computes initial velocities and locations of molecules at beginning of calculation
RANF	Computes pseudo random numbers
STORE	Transfers blocks of information from core to drum and vice-versa

NOTE: Subroutines ENTER and NUMB are no longer used.
The functions of ENTER are carried out in MAIN.
The functions of NUMB are carried out in MAIN also.

The cell arrangement for a sample case using the DRUM SLAB I and DRUM SLAB II Programs are shown in Figures 7 and 8, respectively.

DRUM SLAB I SAMPLE CASE

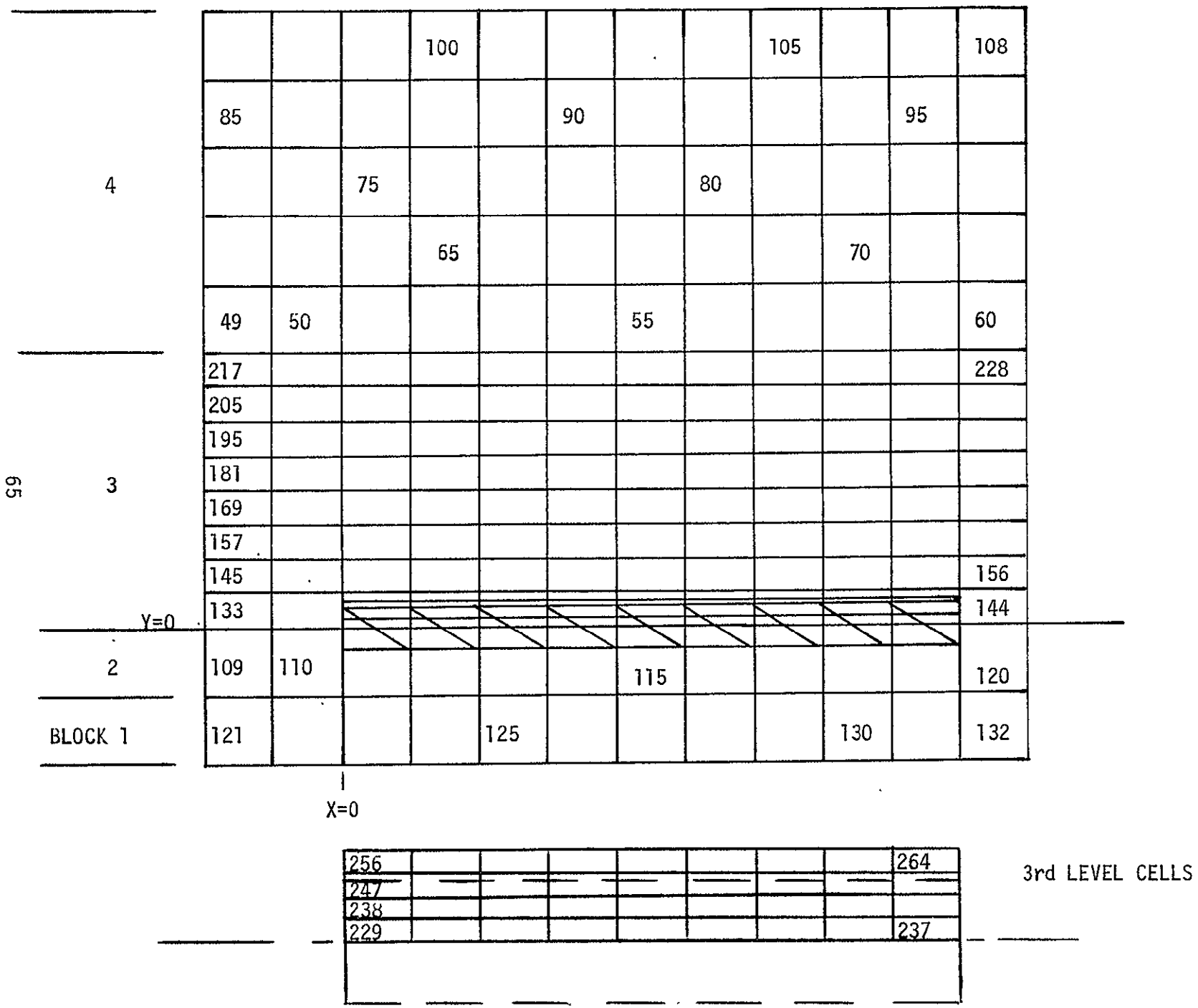


FIGURE 7

			50					55					60
	LD(3) = 9				40					45			
BLOCK 5	WF(3) = 2	25					30					35	
				15					20				
		1	2	3	4	5					10		
					100	101	102	103	104	105	106	107	108
		85					90					95	
	WF(2) = 1			75					80				
BLOCK 4	LD(2) = 4					65					70		
			50					55					60
		37	34	39	40	41	42	43	44	45	46	47	48
BLOCK 3	LD(1) = 1 WF(1) = 1	25	26	27	28	29	30	31	32	33	34	35	36
		13	14										
BLOCK 2	WF ≡ WF(1) = 1	1	2	3	4	5	6	7	8	9	10	11	12
BLOCK 1	LDL = 1 WFL = 1	1	2	3	4	5	6	7	8	9	10	11	12

DRUM SLAB II SAMPLE CASE

FIGURE 8

6.3 DRUM SLAB I PROGRAM INPUT FORM*

CARD 1 (11I6)

ISTART	6
NSA	12
L1	18
L2	24
LS1	30
LS2	36
IPLØT	42
NSR	48
IØPT	54

CARD 2 (6F10.4)

AKN	10
S	20
TR	30
CR	40
YAW	50
ALP	60

CARD 3 (12I6)

NC	6
NF	12
NR	18
NHU	24
NHL	30
INM	36
MNM	42
KCØL	48
INBX	54
NPR	60

*NOTE: Input description for this program is the same as that of the SLAB Program except: NBLK= total no. of blocks in the field and MNQ= maximum allowable no. of molecules in a Q array.

DRUM SLAB I PROGRAM INPUT FORM (contd.)

CARD 4 (12I6)

NL	6
NFA	12
NCA	18
NHUA	24
NHLA	30
MW	36
MHU	42
MHL	48

CARD 5 (12I6)

NFB	6
NCB	12
NHUB	18
NHLB	24
LW	30
LHU	36
LHL	42

CARD 6 (12I6)

NBLK	6
MNQ	12

CARD 7 (12I6)

LD(1)	6
LD(2)	12
LD(3)	18
LD(4)	24
LD(5)	30
LD(6)	36
LD(7)	42
LD(8)	48
LD(9)	54
LD(10)	60
LD(11)	66
LDL	72

DRUM SLAB I PROGRAM INPUT FORM (contd.)

CARD 8 (12F6.0)

WF(1)	6
WF(2)	12
WF(3)	18
WF(4)	24
WF(5)	30
WF(6)	36
WF(7)	42
WF(8)	48
WF(9)	54
WF(10)	60
WF(11)	66
WFL	72

CARD 9 (6F10.4)

DTM	10
DTS	20
DTP	30
TST	40
TLIM	50
TMAX	60

CARD 10 (6F10.4)

PSPR	10
WAM	20
AMDX	30
AMDY	40
ALENR	50

DRUM SLAB I PROGRAM INPUT FORM (contd.)

CARD 11 (12I6)

NDUL 6

NDUS 12

NDUT 18

NDLT 24

NDLS 30

NDLL 36

CARD 12 (6F10.4)

NI 10

TFF 20

Dimension

ITP(N)

NTSC(2,ND)

NBC(2,LS1)

NBCT(2,LS1)

BN1(MNM,7)

BN2(NBX,26)

BN3(1,12)

BN4(ND,9)

BN5(1,5)

$$NBX = (NHU+NHL)(NC+NF+NR) + MW(MHU+MHL) + LW(LHU+LHL)$$

$$ND = NDUL + NDUS + NDUT + NDLT + NDLS + NDLL$$

$$LS1 = \begin{cases} NBX; & \text{for type molecule option} \\ 1\ ; & \text{otherwise} \end{cases}$$

$$N = \begin{cases} MNM; & \text{for type molecule option} \\ 1\ ; & \text{otherwise} \end{cases}$$

$$IØPT = 2 \begin{cases} ER(MNM) \\ TRA(NBX) \\ TER(NBX) \end{cases}$$

$$IØPT \neq 2 \begin{cases} ER(1) \\ TRA(1) \\ TER(1) \end{cases}$$

DRUM SLAB I PROGRAM INPUT FORM (contd.)

Q Array Dimensioning

PERMANENT
- QPAX
- QPAY
- QPAU
- QPAV
- QPAW
- LAMQ
- LPRQ

OPTIONAL
- ITPQ
- QER
- QWX
- QWY
- QWZ

Permanent Q Arrays Must Be Dimensioned (NBLK,MNQ)

SET ITPQ(1,1) QER(1,1) QWX(1,1) QWY(1,1) QW2(1,1)
IF TYPE OPTION, ENERGY SINK, OR ROUGH SPHERES ARE NOT CALLED FOR

TOTAL
STORAGE

NBX*

MNM*

ND*

NBLK*MNQ*

INSTRUCTIONS

6.4 DRUM SLAB I PROGRAM DIMENSION STATEMENTS

Four FØRTRAN dimension statements must be changed with each run as follows:

BN ARRAYS - These must be consistent with the dimensions on the input variable load sheet. The "CØMMØN/SARRAY/" statement must be modified in the following three routines:

MAIN PROGRAM

Subroutine MSLAB

Subroutine RSTART

TYPE MOLECULES - The second dimension statement in MAIN PROGRAM must be consistent with the dimension on the load sheet regarding the following four arrayed variables:

ITP

NTSC

NBC

NBCT

Q ARRAYS - The third dimension statement in MAIN PROGRAM must be consistent with the dimension on the load sheet regarding the following arrayed variables:

QPAX

QPAY

QPAU

QPAV

QPAW

LAMQ

ITPQ

LPFQ

QER

QWX

QWY

QWZ

INTERNAL ENERGY - In the fifth dimension statement in MAIN PROGRAM, HTROT must be dimensioned ND if IOPT = 2.

In the sixth dimension statement in MAIN PROGRAM, ER must be dimensioned MNM if IOPT = 2.

In the seventh dimension statement in MAIN PROGRAM, TER and TRA must be dimensioned NBX if IOPT = 2.

If IOPT = 0, all these may be dimensioned (1).

6.5 DRUM SLAB II PROGRAM INPUT DESCRIPTION*

Card 1 - (9I6 format)

ISTART	- Restart option flag (= 1 normal start, = 0 restart)
NSA	- No longer used, set = 0
L1	- No longer used, set = 1
L2	- No longer used, set = 1
LS1	- Number of cells for molecule type output (LS1 = 1 if output is not requested)
LS2	- Maximum number of body divisions for molecule type output (LS2 = 1 if output is not requested)
NSR	- Initial random number (can be any non-zero odd integer)
IPLØT	- No longer used, set = 0

Card 2 - (6F10.4 format)

AKN	- Knudsen number based on body length
S	- Speed ratio
TR	- Ratio of surface temperature to freestream temperature
CR	- Ratio of height to width of first level cells
YAW	- No longer used, set = 0.0
ALP	- Pitch angle of attack in degrees

Card 3 - (10I6 format)

NC	- The number of first level cells along the body
NF	- The number of first level cells in front of the body
NR	- The number of first level cells behind the body
INM	- Initial number of molecules
MNM	- Maximum number of molecules
KCØL	- Power law repulsion model exponent
INBX	- No longer used by the program, set = 0
NPR	- No longer used by the program, set = 0

Card 4 - ( )

NBLK	- Total number of blocks in the field (2 in lower field, NBLK-2 in the upper field)
MNQ	- Maximum allowable number of molecules in a Q array

*NOTE: Program not yet operational

YM - Vertical coordinate to upper field boundary

YL - Vertical coordinate to lower field boundary

Cards (5) to (4 + NBLK) (12I6 format) (LA = block number)

NL(LA) - Number of cell levels in block (LA)

NH(LA) - Vertical number of first level cells

NFA(LA) - Number of first level cells in front of the second level region

NCA(LA) - Horizontal number of first level cells to be divided into second level cells

NHA(LA) - Vertical number of first level cells to be divided into second level cells

MW(LA) - Horizontal number of second level cells

MH(LA) - Vertical number of second level cells

NFB(LA) - Number of second level cells in front of the third level region

NCB(LA) - Horizontal number of second level cells to be divided into third level cells

NHB(LA) - Vertical number of second level cells to be divided into third level cells

LW(LA) - Horizontal number of third level cells

LH(LA) - Vertical number of third level cells

Card 5 + NBLK - (12I6 format)

LD(1) - Number of primary cells from centerline to upper boundary of the first block

LD(2) - Number of primary cells from the centerline to the upper boundary of the second block

⋮

LD(NBLK) - Number of first level cells from centerline to upper boundary of last block

LDL - Number of first level cells from centerline to lower boundary of block adjacent to the slab in the lower field

Card 6 + NBLK

WF(1) - Weighting factor for molecules in block 1

WF(2) - Weighting factor for molecules in block 2

⋮

WF(NBLK) - Weighting factor for molecules in block NBLK

WFL - Weighting factor for molecules in block adjacent to lower field boundary

Card 7 + NBLK (5F10.4 format)

DTM	- Movement time interval during unsteady portion of calculation
DTS	- Sampling time interval
DTP	- Print time interval
TST	- Steady flow time
TLIM	- Time limit for problem
TMAX	- No longer used, set = 0
DTM2	- Movement time interval during steady portion (after TST)

Card 8 + NBLK - (5F10.4 format)

PSPR	- Nolecular reflection option flag 0 - Diffuse reflection from body $0 < PSPR \leq 1$ - Specular reflection percentage
WAM	- Impact parameter cutoff for the power law collision routine
AMDX	- Maximum separation X-distance for collisions option
AMDY	- Maximum separation Y-distance for collisions option
ALENR	- Ratio of body length to body height measured from the centerline

Card 9 + NBLK

AMDXL	- Left hand boundary of rectangular region for collision partner restriction option
AMDXR	- Right hand boundary of rectangular region for collision partner restriction option
AMDYB	- Lower boundary of rectangular region for collision partner restriction option
AMDYT	- Upper boundary of rectangular region for collision partner restriction option

Card 10 + NBLK - (6I6 format)

NDUL	- Number of divisions on the upper leading face
NDUS	- Number of divisions on the upper side
NDUT	- Number of divisions on the upper trailing face
NDLT	- Number of divisions on the lower trailing face
NDLS	- Number of divisions on the lower side
NDLL	- Number of divisions on the lower leading face

Card 11 + NBLK - (2F10.4 format)

NI	- Number of internal degrees of freedom
TFF	- Transfer factor

6.6 DRUM SLAB II PROGRAM WITH NEW CELL SCHEME

Card 1

ISTART	6
NSA	12
L1	18
L2	24
LS1	30
LS2	36
IPLØT	42
NSR	48
IØPT	54

Card 2

AKN	10
S	20
TR	30
CR	40
YAW	50
ALP	60

Card 3

NC	6
NF	12
NR	18
INM	24
MNM	30
KCØL	36
INBX	42
NPR	48

Card 4

NBLK	6
MNQ	12
YM	22
YL	32

Card 5

NL(1)
NH(1)
NFA(1)
NCA(1)
NHA(1)
MW(1)
MH(1)
NFB(1)
NCB(1)
NHB(1)
LW(1)
LH(1)

Card 6

NL(2)
NH(2)
.
.
.
.
LH(2)
.
.

Card (NBLK + 4)

NL(NBLK)
.
.
.
LH(NBLK)

Card (NBLK + 5)

LD(1)
LD(2)
.
.
.
LD(NBLK - 2)
LDL

Card (NBLK + 6)

WF(1)
WF(2)
.
.
.
WF(NBLK - 2)
WFL

Card NBLK + 7

DTM
DTS
.
.
.
TMAX
DTM2

Card (NBLK + 8)

PSPR
WAM
AMDX
AMDY
ALENR

Card (NBLK + 9)

AMDXL

AMDXR

AMDYB

AMDYT

Card (NBLK + 10)

NDUL

NDUS

NDUT

NDLT

NDLS

NDLL

Card (NBLK + 11)

NI

TFF

6.7 DRUM SLAB II PROGRAM INPUT FORM

CARD 1 (11I6)

ISTART	6
NSA	12
L1	18
L2	24
LS1	30
LS2	36
IPLØT	42
NSR	48
IØPT	54

CARD 2 (6F10.4)

AKN	10
S	20
TR	30
CR	40
YAW	50
ALP	60

CARD 3 (12I6)

NC	6
NF	12
NR	18
INM	24
MNM	30
KCØL	36
INBX	42
NPR	48

CARD 4 (12I6)

NBLK	6
MNQ	12
YM	22
YL	32

DRUM SLAB II INPUT FORM (contd.)

CARD 4+NBLK (12I6)

NL(i) 6
NH(i) 12
NFA(i) 18
NCA(i) 24
NHA(i) 30
MW(i) 36
MH(i) 42
NFB(i) 48
NCB(i) 54
NHB(i) 60
LW(i) 66
LH(i) 72
NL(i) 6
NH(i) 12
NFA(i) 18
NCA(i) 24
NHA(i) 30
MW(i) 36
MH(i) 42
NFB(i) 48
NCB(i) 54
NHB(i) 60
LW(i) 66
LH(i) 72
NL(i) 6
NH(i) 12
NFA(i) 18
NCA(i) 24
NHA(i) 30
MW(i) 36
MH(i) 42
NFB(i) 48
NCB(i) 54

DRUM SLAB II INPUT FORM (contd.)

CARD 4+NBLK (12I6) (contd.)

NHB(i) 60

LW(i) 66

LH(i) 72

CARD 5+NBLK (12I6)

LD(1)

LD(2)

LD(3)

LD(4)

LD(5)

LD(6)

⋮

LD(NUBLK)

LDL

CARD 6+NBLK (12I6)

WF(1)

WF(2)

WF(3)

WF(4)

WF(5)

WF(6)

⋮

WF(NUBLK)

WFL

CARD 7+NBLK (7F10.4)

DTM 10

DTS 20

DTP 30

TST 40

TLIM 50

TMAX 60

DTM2 70

DRUM SLAB II INPUT FORM (contd.)

CARD 8+NBLK (6F10.4)

PSPR 10

WAM 20

AMDX 30

AMDY 40

ALENR 50

CARD 9+NBLK (6F10.4)

AMDXL 10

AMDXR 20

AMDYB 30

AMDYT 40

CARD 10+NBLK (12I6)

NDUL 6

NDUS 12

NDUT 18

NDLT 24

NDLS 30

NDLL 36

CARD 11+NBLK (6F10.4)

NI 10

TFF 20

CØMMØN
/CELL/

NBC(2,NBX)

NBCT(2,NBX)

NTSC(2,ND)

ITP(MNM)

TER(NBX)

TRA(NBX)

DRUM SLAB II INPUT FORM (contd.)

CØMMØN
/MARRAY/

BN1(MNM,7)

BN3(1,12)

BN4(ND,9)

BN5(1,5)

CØMMØN
/CARRAY/

BN2(NBX,25)

DIMENSION

ER(MNM)

WX(MNM)

WY(MNM)

WZ(MNM)

Q Array Dimensioning

PERMANENT
- QPAX
- QPAY
- QPAU
- QPAV
- QPAW
- LAMQ
- LPRQ

OPTIONAL
- ITPQ
- QER
- QWX
- QWY
- QWZ

DRUM SLAB II INPUT FORM (contd.)

Permanent Q Arrays Must Be Dimensioned (NBLK,MNQ)

SET ITPQ(1,1) QER(1,1) QWX(1,1) QWY(1,1) QWX(1,1)
IF TYPE OPTION, ENERGY SINK, OR ROUGH SPHERES ARE NOT CALLED FOR

TOTAL
STORAGE

NBX*

MNM*

ND*

NBLK*MNQ*

INSTRUCTIONS

7. ØRBITER PROGRAM

7.1 ORBITER PROGRAM INPUT DESCRIPTION

Card 1 - (9I6 format)

ISTART	- Restart option flag (operational for ISTART = 1 only)
NSA	- Number of cells for velocity distribution sampling, set = 0
L1	- Flag for velocity distribution sampling, set = 1
L2	- Number of divisions for distribution function, set = 1
LS1	- Number of cells for molecule type output LS1 = 1 if output is not requested
LS2	- Maximum number of body divisions for molecule type output. LS2 = 1 if output is not requested
IPLØT	- Plotting option flag (use IPLØT = 0 only)
NSR	- Initial random number
IØPT	- Molecule designation flag -- 0 - Monatomic 1 - Rough spheres 2 - Energy sink

Card 2 - (5F10.4 format)

AKN	- Knudsen number based on diameter
S	- Speed ratio
TR	- Ratio of surface temperature to freestream temperature
CR	- Ratio of height to width of first level cells
YAW	- Yaw angle in degrees

Card 3 - (10I6 format)

NC	- The number of first level cells along the body
NF	- The number of first level cells in front of the body
NR	- The number of first level cells behind the body
NH	- The vertical number of first level cells
ND	- The number of divisions along the body
INM	- Initial number of molecules
MNM	- Maximum number of molecules
KCØL	- Power law repulsion model exponent
INBX	- No longer used by the program
NPR	- Number of probes

Card 4 - (11I6 format)

NL	- Number of cell levels
NFA	- Number of first level cells in front of the second level region
NCA	- Horizontal number of first level cells in the second level region
NHA	- Vertical number of first level cells in the second level region
MW	- Horizontal number of second level cells
MH	- Vertical number of second level cells
NFB	- Number of second level cells in front of the third level region
NCB	- Horizontal number of second level cells in the third level region
NHB	- Vertical number of second level cells in the third level region
LW	- Horizontal number of third level cells
LH	- Vertical number of third level cells

Card 5 - (10I6 format)

LD(1)	- Number of primary cells from the centerline to the first weighting factor boundary
LF(1)	- Weighting factor applied across the first weighting factor boundary
LD(2)	- Number of primary cells from the centerline to the second weighting factor boundary
LF(2)	- Weighting factor applied across the second weighting factor boundary
LF(5)	- Weighting factor applied across the fifth weighting factor boundary

Card 6 - (5F10.4 format)

DTM	- Movement time interval
DTS	- Sampling time interval
DTP	- Print time interval
TST	- Steady flow time
TLIM	- Time limit for problem
TMAX	- No longer used

Card 7 - (5F10.4 format)

PSPR	- Molecular reflection option flag 0 - Diffuse reflection from body $0<PSPR\leq 1$ - Specular reflection percentage
WAM	- Collision cut-off parameter
AMDX	- Maximum separation X-distance for collisions option
AMDY	- Maximum separation Y-distance for collisions option
ALENR	- Ratio of flat side body length to radius

Card 8 - (3I6 format)

NDF	- Number of divisions on the leading face
NDS	- Number of divisions on the side
NDC	- Number of divisions on the cylinder

Card 9 - (2F10.4 format)

NI	- Number of internal degrees of freedom
TFF	- Transfer factor

7.2 ORBITER PROGRAM INPUT FORM

CARD 1 (11I6)

ISTART	6
NSA	12
L1	18
L2	24
LS1	30
LS2	36
IPLØT	42
NSR	48
IØPT	54

CARD 2 (6F10.4)

AKN	10
S	20
TR	30
CR	40
YAW	50

CARD 3 (12I6)

NC	6
NF	12
NR	18
NH	24
ND	30
INM	36
MNM	42
KCØL	48
INBX	54
NPR	60

CARD 4 (12I6)

NL	6
NFA	12
NCA	18
NHA	24
MW	30
MH	36
NFB	42
NCB	48
NHB	54
LW	60
LH	66

CARD 5 (12I6)

LD(1)	6
LF(1)	12
LD(2)	18
LF(2)	24
LD(3)	30
LF(3)	36
LD(4)	42
LF(4)	48
LD(5)	54
LF(5)	60

CARD 6 (6F10.4)

DTM	10
DTS	20
DTP	30
TST	40
TLIM	50
TMAX	60

CARD 7 (6F10.4)

PSPR 10

WAM 20

AMDX 30

AMDY 40

ALENR 50

CARD 8 (12I6)

NDF 6

NDS 12

NDC 18

CARD 9 (6F10.4)

NI 10

TFF 20

Dimension

ITP(N)

NTSC(2,ND)

NBC(2,LS1)

NBCT(2,LS1)

BN1(MNM,7)

BN2(NBX,25)

BN3(1,12)

BN4(ND,9)

BN5(1,5)

$$NBX = NH(NC+NF+NR) + MH \cdot MW + LH \cdot LW$$

$$ND = NDF + NDS + NDC$$

$$LS1 = \begin{cases} NBX; & \text{for type molecule option} \\ 1\ ; & \text{otherwise} \end{cases}$$

$$N = \begin{cases} MNM; & \text{for type molecule option} \\ 1\ ; & \text{otherwise} \end{cases}$$

The BN arrays appear in "ØRBIT," "MØRBIT," and "RSTART." The remaining arrays are in "ØRBIT."

7.3 ORBITER PROGRAM DIMENSION STATEMENTS

Four FØRTRAN dimension statements must be changed with each run as follows:

BN ARRAYS - These must be consistent with the dimensions on the input variable load sheet. The "CØMMØN/SARRAY/" statement must be modified in the following three routines:

ØRBIT - (Main program)

MØRBIT

RSTART

TYPE MOLECULES - The first dimension statement in ØRBIT (main program) must be consistent with the dimension on the load sheet regarding the following four arrayed variables:

ITP

NTSC

NBC

NBCT

INTERNAL ENERGY - In the second dimension statement in ØRBIT (main program), ER must be dimensioned MNM if IØPT = 2. In the third dimension statement TER and TRA must be dimensioned NBX if IØPT = 2. In the sixth dimension statement HTRØT must be dimensioned ND if IØPT = 2. If IØPT = 0 these may be set at (1).

7.4 ORBITER PROGRAM OUTPUT DESCRIPTION

The following is a description of the ØRBITER program output after the establishment of steady flow. As the molecules move in the flow field, a record is kept of collisions with the body surface. With each collision, appropriate amounts are added to the counters for the total flux, drag, and heat transfer. The variables for the appropriate surface segment on the body are also modified. The rates of increase of these quantities with time after the establishment of steady flow give the required flux, drag, and heat transfer coefficients and the distribution of flux, pressure, skin friction, and heat transfer around the surface.

All physical quantities are non-dimensionalized. Distances are referenced to the free stream mean free path. Velocities are normalized to the most probable molecular peculiar velocity in the freestream (i.e., $\sqrt{2RT_\infty}$). Densities and temperatures are also referenced to the freestream values.

Flux, drag, and heat transfer are output in coefficient form. Quantities refer to the entire cross section (i.e., including the half of the body below the centerline).

The total number flux coefficient is defined by,

$$\frac{\text{NUMBER/UNIT TIME}}{n_\infty U_\infty A}$$

where:

n_∞ is the freestream number density

U_∞ is the freestream velocity

A is the reference area taken to be the diameter of the cylinder portion times a unit length in the z direction (i.e., magnitude is that of the body cylinder diameter).

The total drag coefficient is defined by:

$$\frac{\text{DRAG}}{\frac{1}{2}\rho_\infty U_\infty^2 A}$$

where ρ_∞ is the freestream density. The total drag is broken up into a component due to the incident molecules and one due to the reflected molecules. Also the axial drag or drag in the z direction is calculated and normalized as above. It too is broken up into components due to the incident and the reflected molecules.

The total heat transfer coefficient is defined by:

$$\frac{\text{HEAT TRANSFER/UNIT TIME}}{\frac{1}{2}\rho_\infty U_\infty^3 A}$$

The heat transfer is broken up into components along the slab surfaces where the coefficient in these cases is redefined as:

$$\frac{\text{HEAT TRANSFER/UNIT TIME}}{\frac{1}{2}\rho_\infty U_\infty^3 A_{ref}}$$

where A_{ref} is the area of the segment being considered and has a magnitude equal to the length of that segment.

7.4.1 Distribution Around Surface

The next block of output is the distribution of physical quantities at each division around the surface of the body. The following quantities are output for each division.

WETTED LENGTH (denoted "ANGLE" in some program versions) -- Location of that division around the body perimeter in units of cylinder radius. It is assumed zero on the centerline at the leading edge and increases clockwise around the body. The value for any division is taken at the intersection of that division and the next clockwise division.

TOTAL NUMBER Number of molecules to have hit body along the division since the beginning of steady state time.

NUMBER FLUX Defined in coefficient form as:

$$\frac{\text{WEIGHTED NUMBER/UNIT TIME}}{n_\infty U_\infty A_{div}}$$

where A_{div} is the reference area of that division and has magnitude equal to the length of that division.

SHEAR STRESS -- (denoted "THETA STRESS" in some program versions) -- defined in coefficient form per unit area as

$$\frac{\text{SHEAR STRESS/UNIT AREA}}{\frac{1}{2}\rho_\infty U_\infty^2 A_{div}}$$

Z STRESS -- component of shear stress in the z direction defined as

$$\frac{\gamma_Z\text{/UNIT AREA}}{\frac{1}{2}\rho_\infty U_\infty^2 A_{div}}$$

where γ_Z is that component of the shear stress in the z direction.

PRESSURE -- defined as pressure per unit area in coefficient form as:

$$\frac{\text{p/UNIT AREA}}{\frac{1}{2}\rho_\infty U_\infty^2 A_{div}}$$

where p is the pressure on that division.

TRANSLATIONAL HEAT TRANSFER -- the heat transfer imparted to the body from the kinetic energy of impinging molecules along each division - defined as:

$$\frac{\text{TRANSLATIONAL H. T./UNIT TIME}}{\frac{1}{2}\rho_\infty U_\infty^3 A_{div}}$$

ROTATIONAL HEAT TRANSFER -- the heat transfer imparted to the body from the internal energy of impinging molecules along each division - defined as:

$$\frac{\text{ROTATIONAL H. T./UNIT TIME}}{\frac{1}{2}\rho_\infty U_\infty^3 A_{div}}$$

TYPE 1 -- (applicable only with "type molecule" option) --

this is the percentage of the actual number of molecules hitting that division subject to these restrictions:

1) molecules cannot have hit the body previously
2) molecules have had a molecular collision with either a molecule that has hit the body, or a collision with another type 1 molecule.

TYPE 2 -- (applicable only with "type molecule" option --

this is the percentage of the actual number of molecules hitting that division which have hit the body previously.

7.4.2 Flow Field Information

The flow field is divided into cells for which the following information is printed:

NUMBER	- cell number
X	- x coordinate of the cell center. The center of the cylinder corresponds to x = 0.
Y	- y coordinate of the cell center. The body centerline corresponds to y = 0.
SAMPLE	- actual number of molecules in the cell.
NUMBER DENSITY	- cell density normalized to the freestream density.
X VEL	- average x velocity of molecules in the cell normalized to the most probable molecular peculiar velocity in the freestream
Y VEL	- as above for y velocity
Z VEL	- as above for z velocity
TEMP	- cell temperature normalized to the freestream value. It is the average of x, y and z temperatures below.
X TEMP	- cell temperature associated with the x component of the kinetic energy. It is normalized to 1 in freestream.
Y TEMP	- as above for y component.
Z TEMP	- as above for z component.
ROTATIONAL TEMP	- cell temperature associated with the internal energy of molecules in the cell.
TYPE 1	- density of type 1 molecules normalized to cell density.
TYPE 2	- density of type 2 molecules normalized to cell density.

8. DRUM ORBITER I AND II PROGRAMS

8.1 DRUM ORBITER I PROGRAM INPUT FORM

CARD 1 (11I6)

ISTART	6
NSA	12
L1	18
L2	24
LS1	30
LS2	36
IPLØT	42
NSR	48
IØPT	54

CARD 2 (6F10.4)

AKN	10
S	20
TR	30
CR	40
YAW	50

CARD 3(12I6)

NC	6
NF	12
NR	18
NH	24
ND	30
INM	36
MNM	42
KCØL	48
INBX	54
NPR	60

CARD 4 (12I6)

NL	6
NFA	12
NCA	18
NHA	24
MW	30
MH	36
NFB	42
NCB	48
NHB	54
LW	60
LH	66

CARD 5 (12I6)

NBLK	6
MNQ	12

CARD 6 (12I6)

LD(1)	6
LD(2)	12
LD(3)	18
LD(4)	24
LD(5)	30
LD(6)	36
LD(7)	42
LD(8)	48
LD(9)	54
LD(10)	60
LD(11)	66
LDL	72

CARD 7 (12F6.0)

WF(1) 6
WF(2) 12
WF(3) 18
WF(4) 24
WF(5) 30
WF(6) 36
WF(7) 42
WF(8) 48
WF(9) 54
WF(10) 60
WF(11) 66
WFL 72

CARD 8 (6F10.4)

DTM 10
DTS 20
DTP 30
TST 40
TLIM 50
TMAX 60

CARD 9 (6F10.4)

PSPR 10
WAM 20
AMDX 30
AMDY 40
ALENR 50

CARD 10 (12I6)

NDF 6

NDS 12

NDC 18

CARD 11 (6F10.4)

NI 10

TFF 10

Dimension

ITP(N)

NTSC(2,ND)

NBC(2,LS1)

NBCT(2,LS1)

BN1(MNM,7)

BN2(NBX,26)

BN3(1,12)

BN4(ND,9)

BN5(1,5)

$$NBX = (NH)(NC+NF+NR) + MW(MH) + LW(LH)$$

$$ND = NDF + NDS + NDC$$

$$LS1 = \begin{cases} NBX; & \text{for type molecule option} \\ 1\ ; & \text{otherwise} \end{cases}$$

$$N = \begin{cases} MNM; & \text{for type molecule option} \\ 1\ ; & \text{otherwise} \end{cases}$$

$$IOPT = 2 \begin{cases} ER(MNM) \\ TRA(NBX) \\ TER(NBX) \end{cases}$$

$$IOPT \neq 2 \begin{cases} ER(1) \\ TRA(1) \\ TER(1) \end{cases}$$

Q Array Dimensioning

Permanent
- QPAX
- QPAY
- QPAU
- QPAV
- QPAW
- LAMQ
- LPRQ

Optional
- ITPQ
- QER
- QWX
- QXY
- QWZ

Permanent Q Arrays Must Be Dimensioned (NBLK,MNQ)

SET ITPQ(1,1) QER(1,1) QWX(1,1) QWY(1,1) QWZ(1,1)
IF TYPE OPTION, ENERGY SINK, OR ROUGH SPHERES ARE NOT CALLED FOR

TOTAL
STORAGE

NBX*

MNM*

ND*

NBLK*MNQ*

INSTRUCTIONS

8.2 DRUM ORBITER I PROGRAM DIMENSION STATEMENTS

Four FØRTRAN dimension statements must be changed with each run as follows:

BN ARRAYS - These must be consistent with the dimensions on the input variable load sheet. The "CØMMØN /SARRAY/" statement must be modified in the following three routines:

MAIN PROGRAM

SUBROUTINE MORBIT

SUBROUTINE RSTART

TYPE MOLECULES - The second dimension statement in MAIN PROGRAM must be consistent with the dimension on the load sheet regarding the following four arrayed variables:

ITP

NTSC

NBC

NBCT

Q ARRAYS - The third dimension statement in MAIN PROGRAM must be consistent with the dimension on the load sheet regarding the following arrayed variables:

QPAX

QPAY

QPAU

QPAV

QPAW

LAMQ

ITPQ

LPFQ

QER

QWX

QWY

QWZ

INTERNAL ENERGY - In the fifth dimension statement in MAIN PROGRAM, HTROT must be dimensioned ND if IOPT = 2

INTERNAL ENERGY (contd.) - In the sixth dimension statement in MAIN PROGRAM, ER must be dimensioned MNM if IØPT = 2.

In the seventh dimension statement in MAIN PROGRAM, TER and TRA must be dimensioned NBX if IØPT = 2

If IØPT = 0, all these may be dimensioned (1).

8.3 DRUM ORBITER II PROGRAM INPUT FORM*

CARD 1 (11I6)

ISTART	6
NSA	12
L1	18
L2	24
LS1	30
LS2	36
IPLØT	42
NSR	48
IØPT	54

CARD 2 (6F10.4)

AKN	10
S	20
TR	30
CR	40
YAW	50

CARD 3 (12I6)

NC	6
NF	12
NR	18
INM	24
MNM	30
KCØL	36
INBX	42
NPR	48

CARD 4 (12I6)

NBLK	6
MNQ	12
YM	22

* NOTE: Program not yet operational

CARD 4+NBLK (12I6)

NL(i)	6
NH(i)	12
NFA(i)	18
NCA(i)	24
NHA(i)	30
MW(i)	36
MH(i)	42
NFB(i)	48
NCB(i)	54
NHB(i)	60
LW(i)	66
LH(i)	72
NL(i)	6
NH(i)	12
NFA(i)	18
NCA(i)	24
NHA(i)	30
MW(i)	36
MH(i)	42
NFB(i)	48
NCB(i)	54
NHB(i)	60
LW(i)	66
LH(i)	72
NL(i)	6
NH(i)	12
NFA(i)	18
NCA(i)	24
NHA(i)	30
MW(i)	36
MH(i)	42
NFB(i)	48
NCB(i)	54

CARD 4+NBLK (12I6) (contd.)

NHB(i)	60
LW(i)	66
LH(i)	72

CARD 5+NBLK (12I6)

LD(1)	6
LD(2)	12
LD(3)	18
LD(4)	24
LD(5)	30
LD(6)	36
⋮	
LD(NUBLK)	

CARD 6+NBLK (12I6)

WF(1)	6
WF(2)	12
WF(3)	18
WF(4)	24
WF(5)	30
WF(6)	36
⋮	
WF(NUBLK)	

CARD 7+NBLK (7F10.4)

DTM	10
DTS	20
DTP	30
TST	40
TLIM	50
TMAX	60
DTM2	70

CARD 8+NBLK (6F10.4)

PSPR 10

WAM 20

AMDX 30

AMDY 40

ALENR 50

CARD 9+NBLK (6F10.4)

AMDXL 10

AMDXR 20

AMDYB 30

AMDYT 40

CARD 10+NBLK (12I6)

NDF 6

NDS 12

NDC 18

CARD 11+NBLK (6I0.4)

NI 10

TFF 20

CØMMØN
/CELL/

NBC(2,NBX)

NBCT(2,NBX)

NTSC(2,ND)

ITP(MNM)

TER(NBX)

TRA(NBX)

CØMMØN
/MARRAY/

BN1(MNM,7)

BN3(1,12)

BN4(ND,9)

BN5(1,5)

CØMMØN

/CARRAY/

BN2(NBX,25)

DIMENSION

ER(MNM)

WX(MNM)

WY(MNM)

WZ(MNM)

Q Array Dimensioning

Permanent:
- QPAX
- QPAY
- QPAU
- QPAV
- QPAW
- LAMQ
- LPRQ

Optional:
- ITPQ
- QER
- QWX
- QWY
- QWZ

Permanent Q Arrays Must Be Dimensioned (NBLK,MNQ)

SET ITPQ(1,1) QER(1,1) QWX(1,1) QWY(1,1) QWZ(1,1)

IF TYPE OPTION, ENGERY SINK, OR ROUGH SPHERES ARE NOT CALLED FOR

TOTAL STORAGE

NDX*

MNM*

ND *

NBLK*MNQX

INSTRUCTIONS

8.4 DRUM ORBITER II PROGRAM DIMENSION STATEMENTS

Four FØRTRAN dimension statements must be changed with each run as follows:

BN ARRAYS	- These must be consistent with the dimensions on the input variable load sheet. The "CØMMØN /SARRAY/" statement must be modified in the following three routines:
	MAIN PROGRAM
Subroutine	MORBIT
"	RSTART
TYPE MOLECULES	- The second dimension statement in MAIN PROGRAM must be consistent with the dimension on the load sheet regarding the following four arrayed variables:
	ITP
	NTSC
	NBC
	NBCT
Q Arrays:	The third dimension statement in MAIN PROGRAM must be consistent with the dimension on the load sheet regarding the following arrayed variables:
	QPAX QPAY QPAU QPAV QPAW LAMQ ITPQ LPFQ QER QWX QWY QWZ
Internal Energy:	In the fifth dimension statement in MAIN PROGRAM, HTROT must be dimensioned ND if IOPT = 2.
	In the sixth dimension statement in MAIN PROGRAM, ER must be dimensioned MNM if IOPT = 2.
	In the seventh dimension statement in MAIN PROGRAM, TER and TRA must be dimensioned NBX if IOPT = 2.
	If IOPT = 0 all these may be dimensioned (1).

9. 3-D PROGRAM

9.1 GENERAL DESCRIPTION

This program describes the simulation of flow past three dimensional bodies of arbitrary shape. The flow field is divided into hexahedral regions, the six faces of which are numbered as shown in Figure 9, and define either a surface (or plane of symmetry), and outer boundary or an interface with another region. The flow field consists of an arbitrary number of regions. Orientation of regions is arbitrary and one face may interface with faces of more than one adjacent region.

The X, Y, and Z coordinates of the 'O' points on faces 1 and 3 are read in as data. Faces 1 and 3 may therefore have double curvature. Points on face 1 are joined to the corresponding points on face 3 by straight lines. These lines are divided in set ratios to give the 'X' points. Faces 2, 4, 5 and 6 can only have single curvature. The resulting network of 'O' and 'X' points define the 'orignial point grid', the points forming the vertices of the hexahedral 'Interior Cells'. Each hexahedral cell is divided into five tetrahedral elements numbered 1 to 5. Each element 1 to 4 has two faces on the exterior of the hexahedron and one interior face, the four interior faces define tetrahedral element 5. Each of the six Quadrilateral faces of a hexahedral cell is comprised of two triangular faces of tetrahedral elements. The planes of the triangular faces form the surfaces and boundaries. The centroids of the tetrahedral elements are the reference points for the molecular motion. However the molecular properties are averaged over the hexahedral cells. 'Exterior Cells' are located on the outside of the surfaces, boundaries and interfaces. The exterior reference points are the reflections of the interior reference points in the plane of the appropriate triangular boundary element. When a molecule is closer to an exterior reference point than to any interior point, it has crossed the appropriate boundary.

The 3-D body configuration and hexagonal region arrangement for a finite length orbiter cross section with a flat plate for a wing is shown in Figure 10.

HEXAHEDRAL REGION

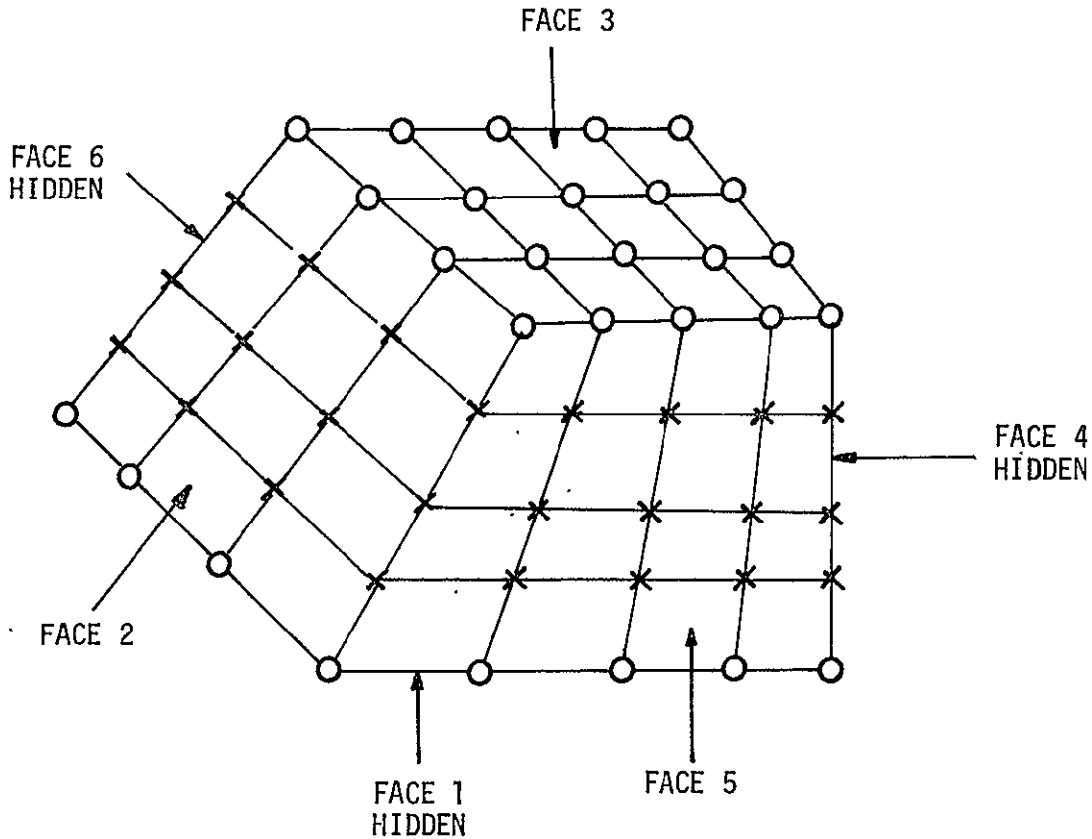
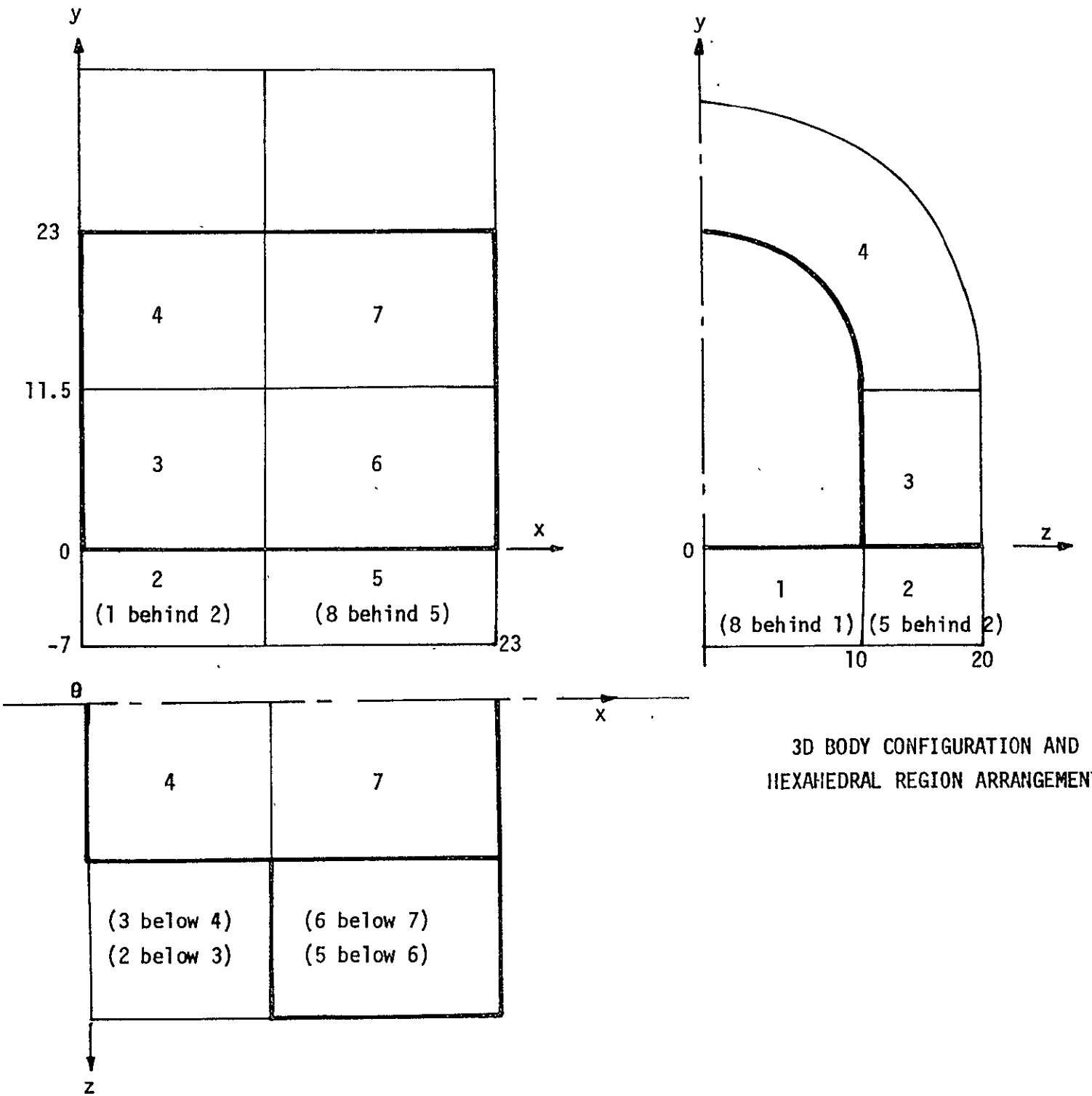


FIGURE 9



3D BODY CONFIGURATION AND
HEXAHEDRAL REGION ARRANGEMENT

FIGURE 10

9.2 3-D PROGRAM VARIABLES DESCRIPTION

CARD 1 - Speed ratio (stream in X-Y plane), direction cosine of stream with X-axis (+VE) direction cosine of stream with Y-axis.

CARD 2 - Speed ratio (stream in +VE X direction), freestream mean free path. Time interval for moving molecules, interval for sampling, interval for printing, steady flow time, time to stop computation, reference area for coefficients, reference length for coefficients.

CARD 3 - Number of regions, initial number of molecules, maximum number of molecules in each region, maximum number of molecules in the buffer storage, indicator 'NPD' for diagnostic printout, starting integer for random number generator (if required)

NPD=0 If no diagnostic required
NPD=1 Provides indication of major operations
NPD=2 Provides complete details of molecular motion (to avoid excessive output, use only when INM is unusually small)

CARDS with R following their number are repeated for each region:

CARD 4R - Number of points along one of the rows along faces 1 and 3 parallel to faces 5 and 6, number of divisions in a line joining a point on face 1 to the corresponding point on face 3, number of layers' of points in planes parallel to faces 5 and 6, code for face 1, code for face 2, code for face 3, code for face 4, code for face 5, code for face 6.

(Code Number =1 For surface or plane of symmetry
=2 For outer boundary
=3 For interface with another region)

CARDS with F following their number are repeated for each face

CARD 5RF (delete unless the face is a surface) surface temperature of face, fraction of molecules reflected diffusely (remainder is reflected specularly, therefore set =0 when face is surface of symmetry)

CARD 6RF (delete unless the face is an interface) number of regions adjacent to the interface

The following card is repeated for each of these regions.

CARD 7RF Number of the adjoining region, number of its adjoining face.

The following card is repeated for each pair of points on faces 1 and 3 (the first pair are at the intersection of faces 2 and 5, then proceed along the intersections of face 5 with 1 and 3, the pair at the intersection of faces 4 and 5 mark the end of the first layer (I.E. the points in layer one all lie along the intersection of face 5 with faces 1 and 3), the process is then repeated for all layers (working from face 2 to face 4, and ending with the layer on the intersection of face 6 with faces 1 and 3).

CARD 8RF -X, Y and Z for point on face 1, X, Y and Z for point on face 3.

The following card is repeated for each interval along the lines joining corresponding points on faces 1 and 3 (starting with the interval nearest face 1)

CARD 9RF -Relative length of interval, the weighting factor for the interval (the weighting factor is proportional to the number of real molecules represented by each simulated molecule).

Dimension Statements

List of variables (identical with or related to data variables)

NBLK Number of blocks (or regions)
MCELL= (N13+1)*(N24+2)*(N56+1) maximum number of cells in a block
MNM Maximum number of molecules in a block
MSRF Maximum number of surface elements in a block (two triangular elements for each interior cells on surface face of block)
MBND Maximum number of outer boundary elements in a block
MINT Maximum number of interface elements in a block
MIRG Maximum number of blocks bounding a single interface face of a block
MC1, MC2, MC3 Maximum number of original grid points along directions C1, C2, C3
(MC1=N13,MC2=N24+1,MC3=N56)
MN24 Maximum value of N24 in any block
MNMT Maximum number of molecules in buffer store
Use of numbers indicates that dimensions are fixed

P(6,MNM),IP(3,MNM),CN(3,MCELL,5),C(14,MCELL),IC(6,MCELL),W(33,MSRF),
IW(2,MSRF),B(22,MBND),IB(2,MBND),II(3,MINT),FI(1,MINT),
CTN(3,MCELL,5),CT(14,MCELL),ICT(6,MCELL),WT(33,MSRF),IWT(2,MSRF),
BT(22,MBND),IBT(2,MBND),IIT(3,MINT),FIT(1,MINT),
(It is essential that 'CN,C' etc. and 'CTN,CT' etc. have identical dimensions)
QX,QY,QZ(MC1,MC2,MC3),QP,QWF(MN24),
PB(6,MNMT),IPB(4,MNMT),NTBLK(NBLK),
LR(6),ST(6),FD(6),KB(6,NBLK),KR(MIRG,6,NBLK),KS(MIRG,6,NBLK),NBC1(N13+1),
NBC2(N24+2),NBC3(N56+1),NBCT(NBLK),VCC(3,8),VTC(3,8,5),NINT(NBLK),NSRF(NBLK),
NBND(NBLK),COTV(3,3),NV(4),NBCEL(8,4,3),NM(NBLK),FNM(NBLK),CLW(3),AA1(3),
AA2(4),CF(16),NCOL(MBLK)

Defintion of Subscripted Variables

P(6,MNM),IP(3,MNM) Contain information on up to MNM molecules in each block

P(1,M) X Co-ordinate of molecule M
P(2,M) Y Co-ordinate
P(3,M) Z Co-ordinate
P(4,M) U Velocity of molecule M

P(5,M) V Velocity
P(6,M) W Velocity

IP(1,M) Cell cross reference array
IP(2,M) Cell number for molecule M
IP(3,N) Tetrahedron number in this cell

CN(3,NC,5) Contains information on the five tetrahedral elements of each of up to NC cells in each region

CN(1,M,N) X Co-ordinate of the N-TH tetrahedral element of cell M
CN(2,M,N) Y Co-ordinate
CN(3,M,N) Z Co-ordinate

C(11,NC),IC(6,NC) Contain Information on up to NC cells in each block

IC(1,M) Type of cell M, =0 For interior cell,
=1 For surface cell
=2 For boundary cell
=3 For interface cell.

For interior (type 0) cells,

C(1,M) X Co-ordinate of cell M
C(2,M) Y Co-ordinate
C(3,M) Z Co-ordinate
IC(2,M) Code (1, to 8) for orientation of cell (interior cells only)

Cell Orientation Code	Tetrahedral Element 1 Has Apex	2 at cell	3 vertex	4 number
1	1	4	6	7
2	2	3	5	8
3	3	2	8	5
4	4	1	7	6
5	5	8	2	3
6	6	7	1	4
7	7	6	4	1
8	8	5	3	2

Tetrahedron with vertex at 1 has other corners at 2,3,5
2 1,4,6
3 1,4,7
4 2,3,8
5 1,6,7
6 2,5,8
7 3,5,8
8 4,6,7

C(4,M) Volume of cell M
C(5,M) Sum of number in cell M
C(6,M) Sum of U velocities in cell M
C(8,M) Sum of W velocities
C(7,M) Sum of V velocities

C(9,M) Sum of squares of U velocities in cell M
C(10,M) Sum of squares of V velocities
C(11,M) Sum of squares of W velocities
C(12,M) Maximum probable value of relative velocity of collision pair
C(13,M) Time in cell M
C(14,M) Weighting factor for cell M

IC(3,M) Number of molecules in cell M
IC(4,M)+1 Is the address in IP(1,N) of the first molecule in cell M

For all outer cells (Type 1, Type 2 or Type 3)

IC(3,M) or IC(4,M) Will correspond with the previous tetrahedron code
If IC(3,M) The molecule transfers to triangle or tetrahedron IC(5,M)
If IC(4,M) The molecule transfers to triangle or tetrahedron IC(6,M)
IC(5,M) and IC(6,M) Therefore contain 'N' for W(31,N), B(22,N) or II(,N)

W(33,NSC) CONTAINS INFORMATION ON UP TO NSC TRIANGULAR SURFACE ELEMENTS

W(1,M),W(2,M),W(3,M) X, Y, Z CO-ORDINATES OF FIRST VERTEX OF ELEMENT M
W(4,M),W(5,M),W(6,M) X, Y, Z OF SECOND VERTEX
W(7,M),W(8,M),W(9,M) X, Y, Z OF THIRD VERTEX
W(10,M),W(11,M),W(12,M) X, Y, Z CO-ORDINATES OF CENTROID OF ELEMENT M
W(13,M) DIRECTION COSINE WITH X AXIS OF NORMAL TO ELEMENT (DIRECTED TO FLOW)
W(14,M) DIRECTION COSINE WITH Y AXIS OF NORMAL
W(15,M) DIRECTION COSINE WITH Z AXIS OF NORMAL
W(16,M) DISTANCE OF ORIGIN FROM PLANE OF ELEMENT
W(17,M) SQUARE ROOT OF SURFACE TEMPERATURE
W(18,M) FRACTION OF MOLECULES REFLECTED DIFFUSELY (REMAINDER SPECULARLY)
W(19,M) DIRECTION COSINE WITH X AXIS OF DIRECTION LYING IN THE PLANE OF THE SURFACE AND IN THE PLANE OF THE SURFACE NORMAL AND A LINE PARALLEL TO THE X-AXIS (ALWAYS +VE, CALLED X-WISE SHEAR DIRECTION)
W(20,M) DIRECTION COSINE WITH Y AXIS OF THIS DIRECTION
W(21,M) DIRECTION COSINE WITH Z AXIS OF THIS DIRECTION
W(22,M) DIRECTION COSINE WITH Y AXIS OF SURFACE DIRECTION NORMAL TO BOTH THE SURFACE NORMAL AND THE X WISE SHEAR DIRECTION (ALWAYS +VE, CALL NORMAL SHEAR DIRECTION)
W(23,M) DIRECTION COSINE WITH Z AXIS OF THIS DIRECTION (IT IS NORMAL TO THE X AXIS)
W(24,M) SUM OF INCIDENT NORMAL VELOCITY COMPONENTS (+VE TO SURFACE)
W(25,M) SUM OF REFLECTED NORMAL VELOCITY COMPONENTS (+VE FROM SURFACE)
W(26,M) SUM OF INCIDENT STREAMWISE SHEAR VEL. COMPS. (+VE IN +VE DIRECTION)
W(27,M) SUM OF REFLECTED STREAMWISE SHEAR VEL. COMPS. (+VE IN -VE DIRECTION)
W(28,M) SUM OF INCIDENT NORMAL SHEAR VEL. COMPS. (+VE IN +VE DIRECTION)
W(29,M) SUM OF REFLECTED NORMAL SHEAR VEL. COMPS. (+VE IN -VE DIRECTION)
W(30,M) SUM OF INCIDENT ENERGY TO SURFACE ELEMENT M
W(31,M) SUM OF REFLECTED ENERGY FROM SURFACE ELEMENT M
W(32,M) AREA OF ELEMENT M
W(33,M) SUM OF FACTORED INCIDENT MOLECULES

IW(1,M) SUM OF INCIDENT MOLECULES
IW(2,M) CELL NUMBER OF ADJACENT CELL

B(22,NBC) CONTAINS INFORMATION ON UP TO NBC OUTER BOUNDARY ELEMENTS

B(1,M),B(2,M),B(3,M) X, Y, Z CO-ORDINATES OF FIRST VERTEX OF ELEMENT M
B(4,M),B(5,M),B(6,M) X, Y, Z OF SECOND VERTEX
B(7,M),B(8,M),B(9,M) X, Y, Z OF THIRD VERTEX
B(10,M) NUMBER OF FREESTREAM MOLECULES ENTERING ACROSS ELEMENT M IN TIME DTM
B(11,M) REMAINDER WHEN ENTERING NUMBER IS ROUNDED TO AN INTEGER
B(12,M),B(13,M) CONSTANTS USED IN SETTING THE ENTERING DISTRIBUTION
B(14,M) DIRECTION COSINE WITH X AXIS OF NORMAL TO ELEMENT (DIRECTED TO FLOW)
B(15,M) DIRECTION COSINE WITH Y AXIS OF NORMAL
B(16,M) DIRECTION COSINE WITH Z AXIS OF NORMAL
B(17,M) DIRECTION COSINE WITH X AXIS OF FIRST PARALLEL AXIS
B(18,M) DIRECTION COSINE WITH Y AXIS OF FIRST PARALLEL AXIS
B(19,M) DIRECTION COSINE WITH Z AXIS OF FIRST PARALLEL AXIS
B(21,M) DIRECTION COSINE WITH Y AXIS OF SECOND PARALLEL AXIS (NORMAL TO)
B(22,M) DIRECTION COSINE WITH Z AXIS OF SECOND PARALLEL AXIS (X AXIS)

IB(1,M) CELL FOR ENTERING MOLECULE
IB(2,M) TETRAHEDRON FOR ENTERING MOLECULE
II(3,40) CONTAINS INFORMATION ON INTERFACE ELEMENTS

II(1,M) CONTAINS BLOCK INTO WHICH THE MOLECULE TRANSFERS
II(2,M) CONTAINS CELL INTO WHICH THE MOLECULE TRANSFERS
II(3,M) CONTAINS TETRAHEDRAL ELEMENT OF THIS CELL

FI(1,M) WEIGHTING FACTOR OF THE CELL INTO WHICH THE MOLECULE TRANSFERS

PB(6,MNMT), IPB(3,MNMT) ARE BUFFER ARRAYS FOR TRANSFER OF MOLECULES TO OTHER BLOCKS, CORRESPOND WITH P,IP EXCEPT THAT -
IPB(1,M) CONTAINS THE NUMBER OF THE NEW BLOCK OF TRANSFER MOL. M
IPB(2,M), IPB(3,M) ARE THE NEW VALUES

NTBLK(NBLK) NUMBER OF MOLECULES IN BUFFER STORAGE TO BE TRANSFERRED TO NBLK
LR(M) IS CODE FOR THE TYPE OF CELL FACES
ST(M) IS THE TEMPERATURE OF THE CELL FACE IF IT IS A SURFACE
FD(M) IS THE FRACTION OF DIFFUSE REFLECTION
KB(M,N) IS THE NUMBER OF BLOCKS ADJACENT TO FACE M OF BLOCK N
KS(L,M,N) ARE THE RELEVANT FACES OF THE ADJACENT BLOCKS
KR(L,M,N) ARE THE L ADJACENT BLOCKS OF FACE M OF BLOCK N
QX(K,L,M),QY(K,L,M),QZ(K,L,M) CO-ORDINATES OF KTH POINT ALONG DIRECTION C1, LTH POINT ALONG C2 AND MTH ALONG C3 IN ORIGINAL POINT GRID
QP(L) PROPORTIONS OF SEGMENTS ALONG LINES JOINING FACE 1 TO FACE 3 (1 TO 31
QWF(L) WEIGHTING FACTORS IN THESE SEGMENTS
NBC1(N),NBC2(N),NBC3(N) ARE THE NUMBER OF CELLS IN DIRECTIONS C1,C2,C3,BLOCK N
NBCT(N) TOTAL NUMBER OF CELLS IN BLOCK N
VCC(3,8) ARE THE 3 CO-ORDINATES OF THE EIGHT VERTICES OF A CELL
VTC(3,4,5) ARE THE 3 CO-ORDS. OF THE 4 VERTICES OF THE FIVE TETRAHEDRAL ELMNTS
NINT(N) NUMBER OF INTERFACE TRIANGLES IN BLOCK N
NSRF(N) NUMBER OF SURFACE TRIANGLES
NBND(N) NUMBER OF OUTER BOUNDARY TRIANGLES
COTV(3,3) USED IN SETTING TRIANGLE VERTICES (X,Y,Z, 3 VERTICES)
NV(4) USED IN SETTING TETRAHEDRA VERTICES (4 VERTICES)
NBCEL(N,M,L) L TH. (OF 3) FACE IS ONE FACE OF M TH. (OF 4) TETRAHEDRON IN CELL OF ORIENTATION (1 to 8) N.

```
AA4(4) WORKING ARRAY
AA3(4) WORKING ARRAY
NCOL(N) THE NUMBER OF COLLISIONS IN REGION N
NM(N) THE NUMBER OF MOLECULES IN REGION N (NMT IS TOTAL NUMBER)
FNM(N) THE FACTORED NUMBER IN REGION N
CLW(3) ARE A MEASURE OF THE SIZE OF A CELL
AA1(3) A WORKING ARRAY
AA2(4) ALSO A WORKING ARRAY
CF IS FOR COEFFICIENT SAMPLING
CF(1) SUM OF INCIDENT S MOMENTUM (DRAG)
CF(2) SUM OF REFLECTED S MOMENTUM
CF(3) SUM OF INCIDENT N MOMENTUM (LIFT)
CF(4) SUM OF REFLECTED N MOMENTUM
CF(5) SUM OF INCIDENT Z MOMENTUM (SIDE FORCE)
CF(6) SUM OF REFLECTED Z MOMENTUM

 CF(7) SUM OF INCIDENT ANGULAR MOM. ABOUT S AXIS (ROLL)
 CF(8) SUM OF REFLECTED ANG. MOM. ABOUT S AXIS
 CF(9) SUM OF INCIDENT ANGULAR MOM. ABOUT N AXIS (YAW)
 CF(10) SUM OF REFLECTED ANG. MOM. ABOUT N AXIS
 CF(11) SUM OF INCIDENT ANGULAR MOM. ABOUT Z AXIS (PITCH)
 CF(12) SUM OF REFLECTED ANG. MOM. ABOUT Z AXIS
 CF(13) SUM OF INCIDENT ENERGY
 CF(14) SUM OF REFLECTED ENERGY
 CF(15) INCIDENT NUMBER SUM
 CF(16) FACTORED INCIDENT NUMBER SUM
 DIMENSION P(6,200),IP(3,200),CN(3,64,5),C(14,64),IC(6,64),W(3
 13,24),B(22,16),II(3,8),IW(2,24),FI(1,8),IB(2,16),
 ARRAYS LISTED ABOVE REFER TO SINGLE BLOCK AND FORM THE BLOCK TRANSFER LIST'
 3CTN (3,64,5)CT(14,64),ICT(6,64),WT(33,24),BT(22,16),
 4IIT(3,8),IWT(2,24),
 2IBT(2,16),FIT(1,8),
 ARRAYS LISTED ABOVE ARE TEMPORARILY (EQUIVALENCE WITH P(N,M)) USED IN THE
 SETTING UP OF ALL BLOCK TRANSFER LISTS
 5QX(3,3,3),QY(3,3,3),QZ(3,3,3),QP(2),QWF(2),
 ARRAYS LISTED ABOVE ARE TEMPORARILY (EQUIVALENCE WITH C(N,M) USED FOR THE
 STORAGE OF DATA ETC. ON THE ORIGINAL POINT GRID
 7PB(6,100),IPB(4,100),NTBLD(2),LR(6),ST(6),FD(6),KB(6,2
 8),KR(1,6,2),KS(1,6,2),NBC1(2),NBC2(2),NBC3(2),NBCT(2),VCC(3,8),VTC
 9(3,8,5),NINT(2),NSRF(2),NBND(2),COTV(3,3),NV(4),NBCEL(8,4,3),
 ANM(2),FNM(2),CLW(3),AA1(3),AA2(4),CF(16),NCOL(2),AA3(4),AA4(4)
 EQUIVALENCE (P(1,1),CTN(1,1,1))
 ARRAYS LISTED ABOVE ARE PERMANENTLY IN THE CORE
 WRITE (6,1)
 1 FORMAT (35H1 THREE-DIMENSIONAL FLOW SIMULATION ///)
 READ GENERAL DATA
 READ (5,2) S,DCSX,DCSY
 THE STREAM DIRECTION LIES IN THE X-Y PLANE (AND DCSX ALWAYS +VE)
 WRITE (6,3) S
 3 FORMAT (14TH SPEED RATIO =,F8.3)
 WRITE (6,141) DCSX,DCSY
 141 FORMAT (43H STREAM DIRECTION MAKES DIRECTION COSINE OF,F10.5,16HW
 IITH X-AXIS AND,F10.5,12H WITH Y-AXIS)
 READ (5,2) R,DTM,DTS,DTP,TST,TLIM,CDIA,CDIM
```

```
2 FORMAT (8F10.5)
DTS SHOULD BE MULTIPLE OF DTM,DTP OF DTS,TST AND TLIM OF DTP
WRITE (6,4) R
4 FORMAT (28H FREESTREAM MEAN FREE PATH =,F10.5)
WRITE (6,5) DTM,DTS,DTP
5 FORMAT (27H TIME INTERVAL FOR MOVING =,F10.5,11H,SAMPLING =,F10.5,
111H,PRINTING =,F10.5)
WRITE (6,6) TST,TLIM
6 FORMAT (29H STEADY FLOW ASSUMED AT TIME =,F10.5,33H and COMPUTATION
ICEASES AT TIME =,F10.5)
WRITE (6,7) CDIA,CDIM
7 FORMAT (56H CHARACTERISTIC DIMENSION FOR NORMALISED COEFFICIENTS I
IS, F10.5,9H FOR AREA, F10.5, 11H FOR LENGTH)
LIFT AND DRAG COEFFICIENTS NORMALISED BY 1/2*FDN*V**2*CDIA
MOMENT COEFFICIENT NORMALISED BY 1/2*FDN*V***2*CDIM*CDIA
HEAT TRANSFER COEFFICIENT NORMALISED BY 1/2*FDN*CDIA*V**3
NUMBER FLUX COEFFICIENT NORMALISED BY FDN*V*CDIA
```

9.3 3-D PROGRAM INPUT DESCRIPTION

INPUT DESCRIPTION

CARD	1	FØRMAT (8F10.5)
	S	Speed ratio
	DCSX	Direction cosine of stream with X-Axis
	DCSY	Direction cosine of stream with Y-Axis
CARD	2	FØRMAT (8F10.5)
	R	Freestream mean free path
	DTM	Movement interval for molecules
	DTS	Interval for sampling
	DTP	Interval for printing
	TST	Steady state time
	TLIM	Time to terminate execution
	CDIA	Reference area
	CDIM	Reference length
CARD	3	FØRMAT (12I6)
	NBLK	Number of regions
	INM	Initial number of molecules (total in all regions)
	MNM	Maximum number of molecules in a region
	MNMT	Maximum number of molecules in buffer region
	NPD	0, no debug print
		1, slight amount of debug print
		2, extensive debug print
	NSR	Initial multiplier for random number generator

The following cards are repeated for each region in turn (there are NBLK regions).

REGION	1	
CARD	4R	FØRMAT (12I6)
	N13	Number of points along a line of the doubly curved boundary face

N24	Number of divisions along lines joining the N13 points
N56	Number of layers of N24-N13 grid

LR(1) (2) (3) (4) (5) (6)	Type code for each face	= 1, surface or symmetry plane = 2, boundary = 3, interface

(Consult "Notes on Cell Structure" at end of this input description for further information on the variables on this card.)

Cards are now inserted for faces 1 thru 6 in order, with the exception that if a face is not a surface or an interface, no card is inserted.

For I running 1 thru 6

If LR(I) = L	Card 5RF Format (8F10.5)
and face is	ST(I) = surface temperature
a surface	FD(I) = fraction of diffuse reflection
If LR(I) = 2	delete card
If LR(I) = 3	Card 6RF Format (12I6)
	KB(I,N) = number of regions adjacent to face I of region N (N = 1 at the moment)

There are KB such cards, L = 1 thru KB

Card 7RF Format (12I6)

KR(L,I,N) = number of Lth region adjacent to face I of region N

KS(L,I,N) = number of the face of region (KR(L,I,N) which is adjacent to face I of region N

The following cards are repeated for each layer in Region 1. In each layer there will be N13 cards. (There are N56 layers. For a particular layer the coordinates (x, y, z) on face 1 will connect with (x, y, z) on face 3 and may have a double curvature.)

CARD	8RF	FØRMAT (8F10.5)	
	Qx Qy Qz	Coordinates on face 1	N13 times per layer
	Qx Qy Qz	Coordinates on face 3	

There will thus be N56 sets of above cards.

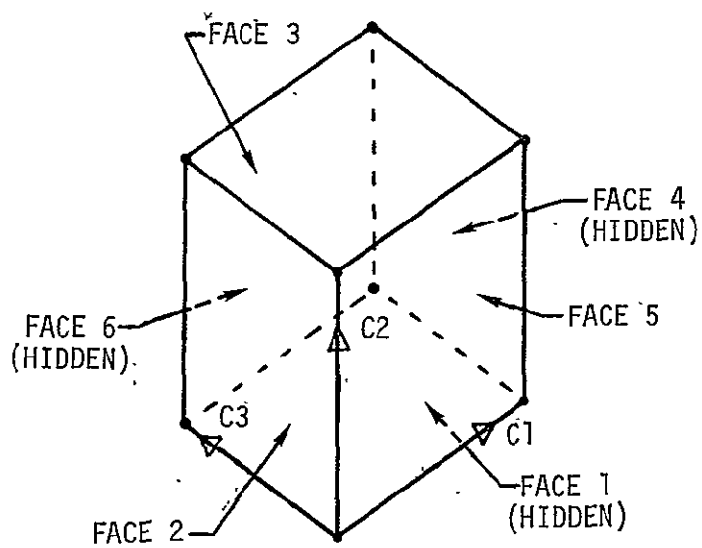
CARD 9RF FØRMAT (8F10.5)

The following card is repeated N24 times

QP(I)	relative length	I = 1, N24
QWF(I)	weighting factor	

The entire set of cards 4R thru 9RF is then repeated for the next region, and so on.

NOTES ON CELL STRUCTURE WITHIN HEXAHEDRAL REGION



Input variables:

N13 = number of points on axis C1

N24 = number of intervals (number of points less one) on axis C2

N56 = number of points on axis C3

NC1 = (N13-1) interior cells + 2 exterior cells

NC2 = N24 interior cells + 2 exterior cells

NC3 = (N56-1) interior cells + 2 exterior cells

Figure 11

Example:

For sample case described in final report, for all 8 regions:

N13 = 3 N24 = 2 N56 = 3

The resulting cell numbering and arrangement typical for all regions is as shown below: (Cell shape and size will vary from region to region.)

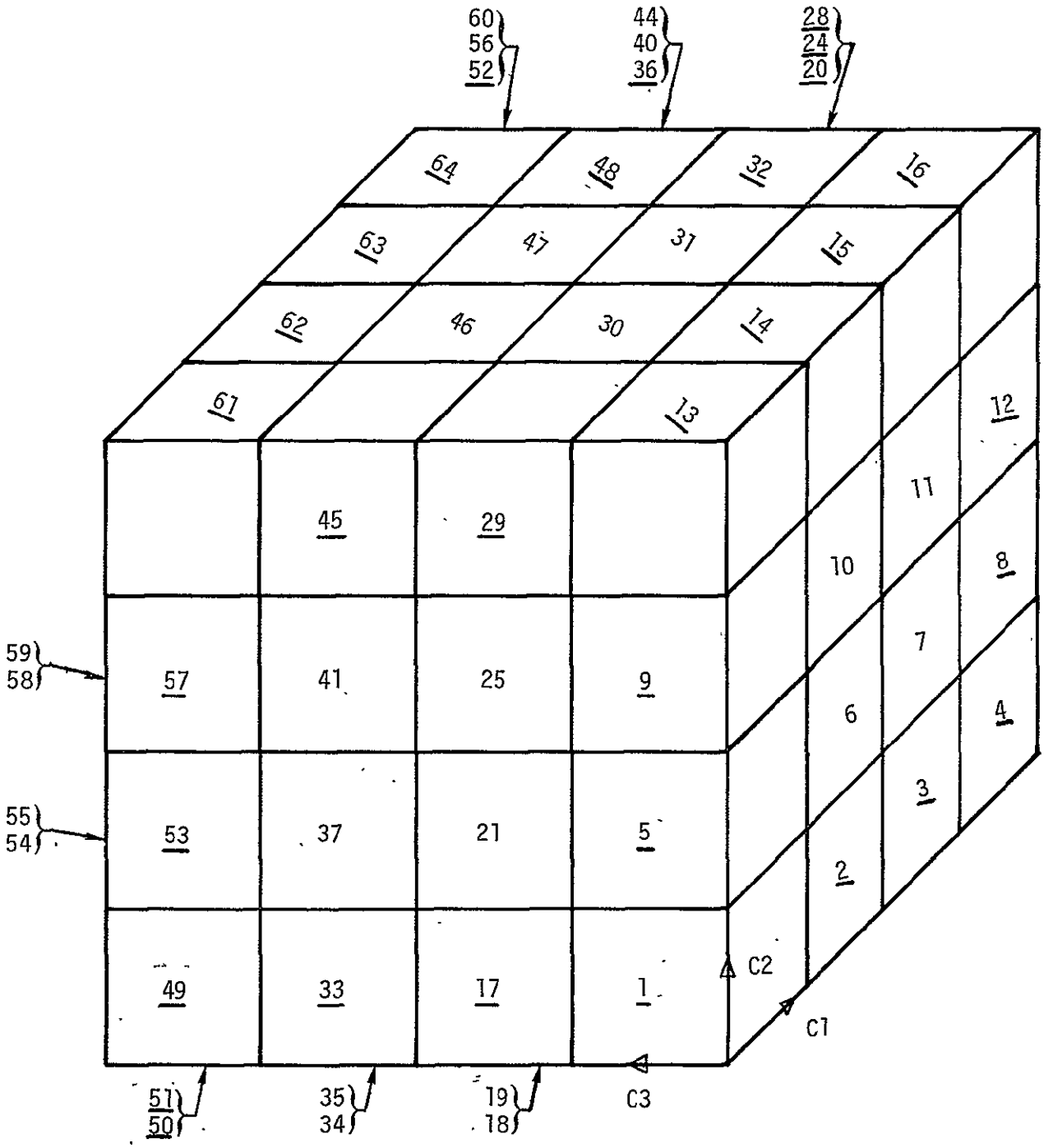


Figure 12

The numbers of cells which are not used are typically shown 13.

The numbers of cells which are exterior control cells are typically shown 21

All other cell numbers between 1 and 64 represent cells in the interior of the region.

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