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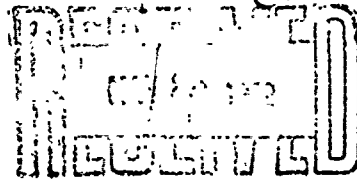
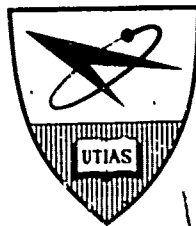
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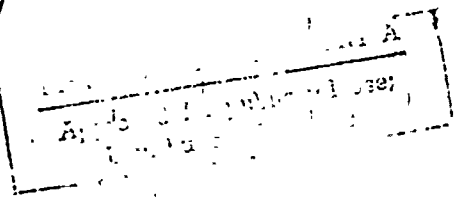
NEAR-FREE-MOLECULE FLOW CALCULATIONS-  
MONTE CARLO STUDY OF SKIMMER INTERACTIONS

by

N.A. Derzko



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October, 1971.

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SUMMARY

The Monte Carlo simulation method of G. A. Bird was applied to the study of flow through a skimmer using various geometries, speed ratios, and Knudsen numbers. The computer program followed a sample of 3500 hard sphere molecules, accumulating distribution function profiles in each of 25 regions of the flowfield, the beam profile at the downstream end of the flowfield, and the mass flow through the skimmer orifice.

The results show beam intensities of the order of .3 of the no skimmer interaction value at Knudsen numbers of 01 and demonstrate clearly that most of the interaction occurs from 0 to 4 mean free paths upstream of the orifice.

TABLE OF CONTENTS

	<u>PAGE</u>
Acknowledgements	
INTRODUCTION	1
Description of Program	2
1. Method	2
2. Initial Conditions	2
3. One Iteration	2
4. Geometry	2
5. Stock Splitting	3
6. TCONS	3
7. Incoming Distribution	4
8. Boundary Conditions	5
9. Referencing Molecule List	6
10. Simulating an Actual Experiment	6
11. Output Format	7
RESULTS	7
TABLE 1	9
TABLE 2	10
FIGURES	
Appendix 1. Program Listing	
2. Typical Output	
3. No Interaction Beam Intensity	

## INTRODUCTION

This report deals with part of the work we have been doing during the past three summers on the development and testing of a number of computer programs designed to simulate molecular flow problems in the transition regime. The simulation is done with hard sphere model using the Monte Carlo method developed by G. A. Bird (2).

We describe here its application to the study of the flow through a skimmer under conditions similar to those involved in the production of molecular beams of high intensity and speed ratio. We simulate the flow which occurs in a cylindrical region reaching upstream and downstream of the skimmer but not including the nozzle.

Since its proposal by Kantrowitz and Grey in 1951, the free jet-skimmer combination has proved far superior to the older methods using the effusive flow from an orifice in an oven source. Nevertheless, in practice the intensity of a beam produced in this way is substantially lower than that one would obtain if the skimmer just removed the portion of the free jet around the beam region - that is, did a perfect job. Considerable experimental work has gone into studying the nature and causes of this effect. Recently Govers, LeRoy and Deckers (6) have studied the effects of background scattering on skimmer interaction; Bossel, Huribut, and Sherman (3) have done experiments to study the magnitude of the skimmer interaction for various geometries and jets.

The effect of the skimmer interaction, whatever its nature, is quite clear. If one plots beam intensity in particles per sec. per steradian vs nozzle skimmer separation, the graph starts at a low value for small separation, increases to a maximum and then drops rapidly as the separation exceeds the distance to the Mach disc (Fig. 4, p. 994, 6). More or less successful attempts have been made to correlate the large amount of experimental data available to enable one to describe a given situation with a fairly small number of parameters. With skimmers of similar geometry, the ratio of mean free path to skimmer orifice diameter appears to be significant. Roger Campargue (4) has discussed a number of dimensionless quantities relevant to the nozzle beam apparatus.

The theory associated with a nozzle beam divides naturally into three areas:

- (a) Description of the free jet - that is the density, velocity, and speed ratio at every point downstream of the nozzle.
- (b) Skimmer interaction.
- (c) Development of the beam downstream of the skimmer (assuming that any molecules involved in skimmer interaction leave the beam).

A satisfactory theory for (a) was published by Ashkenas and Sherman in 1956 (1). A number of authors have also adequately studied (a), e.g. Zapata et al in 1960 (8). A summary appears in Hagena and Morton (7). Thus far (b) has eluded a satisfactory theoretical discussion. It is the purpose of this work to shed some light on this dark area in the theory of nozzle beams.



## DESCRIPTION OF THE PROGRAM

### §1. METHOD USED

The Monte Carlo method used in this study of skimmer interaction is basically the method of G. A. Bird which has been described by him in a number of publications, for example (2). We include a short description here for sake of completeness and to enable us to explain the changes we have introduced to accommodate the peculiarities of this problem.

Bird's method is a Monte Carlo Algorithm for constructing a statistical sample of given size  $N$  of the the molecular paths occurring in some finite regions of an actual flow. The construction process is an imitation of what occurs in nature, at least insofar as probability distributions are concerned. The particle paths are functions of time, so that at any instant only the  $N$  coordinates in phase space (position, velocity-space) appear in computer memory. A time counter  $T$  is also kept in memory.

During each iterate of the calculations  $T$  is advanced by a preset quantity  $DTM$  (actually a number  $DT$  approximately equal to  $DTM$ ) and the coordinates in the molecule list are updated.

### §2. INITIAL CONDITIONS

The initial sample is from a distribution based on what we would have if the skimmer absorbed every molecule which hit it. Actually, the initial distribution is of secondary importance since experience has shown that the molecule list approaches the correct steady state distribution in relatively few iterations.

As soon as  $T$  reaches a preset value  $TEQ$  (time at which steady flow is assumed to have been achieved) data collection for subsequent output is begun and continues until  $T$  reaches  $TEND$ . Following output the program automatically stops or does the next case.

### §3. ONE ITERATION

Each iteration has two components:

- (a) Changes to molecule list due to collision.
- (b) Changes to molecule list due to convection.

The computation of (a) requires that the flow region be divided into cells (Fig. 2) in such a way that the distribution function remains fairly constant over each cell. At any moment the molecules residing in a given cell constitute a sample from the distribution for that cell. If these molecules are allowed to collide among themselves then these collisions are representatives of the collisions actually taking place in the given cell. The theory backing this procedure is stronger than the above suggests. We refer to Bird's original papers on the subject.

The details of the collision process are as follows: A pair of molecules is chosen in such a way that the probability of being chosen is proportional to the relative velocity. If  $\vec{v}_a$  and  $\vec{v}_b$  are the velocities of the pair chosen, they are replaced according to the hard sphere collision law with  $\vec{v}'_a$ ,  $\vec{v}'_b$ , where

$$\bar{v}_a = 1/2[\bar{v}_a + \bar{v}_b - |\bar{v}_b - \bar{v}_a| \bar{n}]$$

$$\bar{v}_b = 1/2[\bar{v}_a + \bar{v}_b + |\bar{v}_a - \bar{v}_b| \bar{n}],$$

where  $\bar{n}$  is chosen from the uniform distribution on the unit sphere.

The position coordinates remain unchanged and a time parameter DT is advanced by

$$DDT = \frac{TCONS}{n^2 |\bar{v}_b - \bar{v}_a|}$$

The number TCONS is fixed for each cell and is explained in §6. Collisions are computed for a given cell until

$$DT + DDT > DTM.$$

The last collision is kept with probability

$$\frac{DTM - DT}{DDT}$$

and ignored otherwise. This last refinement is essential here because some cells have such low collision frequencies that no collisions at all should be computed during some intervals DTM.

The computation of (b) is basically simple. The position coordinates are translated on the basis of the time interval DTM and velocities. The computation involves some work because we use cylindrical coordinates in the program in which the translation equations are nonlinear. We have had to introduce two additional complications which do not appear necessary at first sight - referencing the molecule list §9 - and stock splitting §5. At the end of the collision convection cycle T is incremented appropriately and the whole process is repeated.

#### §4. GEOMETRY

Since the skimmer problem has cylindrical symmetry about the common axis of the free jet and the skimmer, two coordinates suffice to specify position - the axial and radial. They are denoted by (x,y) in the program (rather than (z,r) as is customary because essentially the same program with a few changed subroutines can be used in Cartesian coordinates). The velocity coordinates (u,v,w) are with respect to the Cartesian frame  $\bar{i}, \bar{j}, \bar{k}$  where  $\bar{i}$  is in the axial direction,  $\bar{j}$  is in the radial direction and  $\bar{k}$  is in the direction of increasing  $\theta$ . The actual region of the flow under study is the solid of revolution generated by the shape in Fig. 1.

The flow region is subdivided into cells as required in the collision calculation. The 25 cells and the parameters necessary to specify the geometry are marked in Fig. 1. These parameters are kept in common area (GEOM) (see Appendix 1). Some of them must be specified initially (see Block Data subprogram) and the rest are computed in subroutine SETUP.

#### §5. STOCK SPLITTING

If the coordinates in computer memory simply constituted a sample of the molecular coordinates in an actual flow, we should find that their density in the x,y-plane increased linearly with x. This would be unsatisfactory because then most of the computation would be done for the region far from the axis while

the statistical scatter for the beam region containing only a small number of molecules would render these results almost useless.

The solution we have adopted to this difficulty involves subdividing the flow region into a number of subregions, using the streamlines of the flow to construct the boundary surfaces whenever possible. The subregions are then assigned weights in such a way that a simulator molecule in a subregion far from the axis "represents" several times as many "real" molecules as one in an axial region. For programming reasons we have found it convenient to make the weights inversely proportional to the representation multiples, so that the subregions farthest from the axis have the lowest weights.

Such an arrangement calls for a special strategy when a molecule happens to move between subregions of different weights. The strategy is this: When a molecule moves from a weight  $w_1$  region to a weight  $w_2$  region, it is replaced with

$$\text{INTR}(w_2/w_1)$$

identical molecules. The random variable INTR is defined as follows:

$$\text{INTR}(\alpha) = \begin{array}{l} [\alpha] \quad \text{with probability } 1-\alpha+[\alpha] \\ [\alpha] + 1 \quad \text{with probability } \alpha-[\alpha] \end{array}$$

where  $[\alpha]$  denotes the greatest integer less than or equal to  $\alpha$  as is customary. We have called this process "stock splitting".

#### §6. TCONS CALCULATION

The original formula of G. A. Bird for the time advance per collision is  $\text{DDT} = 2\Omega_k / (a_k n_k v)$  where  $\Omega_k$ ,  $n_k$ ,  $a_k$  are respectively the volume, total number of simulator molecules, and cross-section per simulator molecule for cell  $k$ , and  $v$  is the relative velocity of the collision pair. When the cells are weighted then  $a_k$  must be inversely proportional to the weight. That is if the weights are  $w_k$ , then

$$a_k w_k = \text{const} = \lambda.$$

The additional requirements on  $a_k$  in an actual calculation are

- (1) The cross-section density in a specified region of the flow is given (see §10).
- (2) The total number of molecules must be in the vicinity of some  $N_0$  smaller than the capacity of the molecule list.

Let us say  $N_0$  is the number of molecules obtained in the flowfield if the skimmer caused no disturbance, i.e. absorbed everything that hit it. Let  $A_k$  be the total cross-section ((cross-section/molecule) x number of molecules) in cell  $k$ .  $A_k$  can be computed from the free jet structure and the cross section density  $A_0$  at the skimmer orifice (subroutine VPOL). Then

$$N_k = \frac{A_k}{a_k} = \frac{A_0 w_k}{\lambda}$$

and

$$N_0 = \frac{1}{\lambda} \sum_k A_k w_k,$$

so that

$$\lambda = \frac{1}{N_0} \sum_k A_k w_k$$

and

$$TCONS(\kappa) = 2\Omega_k / a_k = 2\Omega_k w_k N_0 / \Sigma A w, \quad DDT = \frac{TCONS(\kappa)}{n_k^2 v}.$$

### §7. THE INCOMING DISTRIBUTION

First the total influx rate CU to the flow region from the jet is computed from the jet cross-section density  $A_e$  at the entry point, its velocity  $v$  (taken = 1 in our units) and the weights of the cells receiving the molecules. The total entering cell  $\kappa$  (assuming all  $\kappa$  borders on the entry plane) is

$$\frac{A_e v}{a_\kappa} \times \text{area of entry surface element.}$$

CU is the sum of all such quantities.

The number entering the flow region during time DT is CU x DT. Each entering molecule has its position coordinates chosen at random in accordance with the Ashkenas-Sherman formula [1] for variation of jet density with distance from the axis

$$\frac{\rho(R, \theta)}{\rho(R, 0)} = \cos^2 \left( \frac{T \theta}{2\phi} \right)$$

and the weight of the cell about to receive the molecule. The details of this calculation appear in subroutine INPUT (Appendix 1).

### §8. BOUNDARY CONDITIONS

The boundaries in question are the skimmer walls and the artificial boundaries introduced to enclose the flow field. A molecule colliding with a skimmer has a choice of being reflected or reemitted from a cosine distribution at a specified temperature CR. The probability of reemission is a specified accommodation coefficient ACCOM.

The artificial boundaries are:

- (1) The entry plane,
- (2) The upstream outer boundary,
- (3) The downstream boundary.

Molecules which collide with (1) and (3) are deleted. If a molecule collides with (2) its velocity vector is reflected and augmented by the vector  $2pn$  where  $n$  is the outward normal to the wall the  $p$  is a specified constant. If the resulting velocity vector points out of the region the molecule is deleted; otherwise it

is allowed to reenter. When  $p$  is roughly equal to the normal component of the average velocity of the molecules crossing the wall, its net effect is to simulate no discontinuity in the flow due to the boundary.

#### §9. REFERENCING THE MOLECULE LIST

We discuss here the actual arrangement of the molecule coordinates  $C_d = 1, 2, \dots$  in computer memory consistent with a fast method for referring to the coordinates corresponding to a given cell.

The list is arranged in such a way that

$$C_1 \quad \dots \quad C_{N1}$$

are in cell 1,

$$C_{N1+1} \quad \dots \quad C_{N2}$$

are in cell 2, etc. The numbers  $N_i$  are stored in an auxiliary list called MAP. The basic operations which must be performed on this list are

- (1) Removal of a molecule, and
- (2) Addition of a molecule.

(1) To remove  $C_\alpha$  where  $N_{i-1} < \alpha \leq N_i$ , store  $C_{N_i}$  in place of  $C_\alpha$ ,  $C_{N_{i-1}}$  in place of  $C_{N_i}$ , etc. until the end of the list is reached.

(2) To insert coordinates  $C$  into cell  $i$  we make room for it by storing the first molecule of each cell in the location following the last molecule, starting from the end and going up to cell  $i + 1$ . This leaves location  $N_i + 1$  for  $C$ .

Of course, in each case MAP is updated to reflect the new configuration.

It is clear that a simple transfer of molecule from one cell to another does not require the operations to go to the end of the coordinate list. A time saving procedure to accomplish this task is incorporated into the program.

#### §10. SIMULATING AN ACTUAL EXPERIMENT

The program takes the limiting mean centreline jet velocity to be 1. All other velocities are given in terms of it. The simulator geometry must be similar (in the geometric sense) to the real geometry, but the units are arbitrary. Once the velocity and the distance unit are fixed, the time unit is automatically determined. Since we are mostly concerned with the steady state we do not even need to compare computed times with real times except in the initial approach to the steady state.

The remaining parameter that must be assigned is the cross section density  $A$  at some reference point: the flow which we have chosen to be the skimmer orifice assuming perfect skimming.  $A$  has units of reciprocal length, in fact it is just a multiple of  $1/\text{mean free path}$ . Thus  $Ad$ , where  $d$  is the skimmer orifice diameter is dimensionless, and we give it the same value in the simulator as it has in the experiment.

Though this prescription is simple, it has its problems, not the least

being that the hard sphere cross section of real molecules depends on their relative velocity. The best we can do is to use some sort of average relative velocity. The relative velocity of the beam and the molecules coming off the skimmer wall is a good candidate because this is when most of the collisions take place.

#### §11. OUTPUT FORMAT

The output from each run contains the following information (see Appendix 2).

- (1) A printout of DT and MAP for each interval DTM for checking purposes.
- (2) A flow density profile at the skimmer orifice as well as a total particle flow rate.
- (3) A flow density profile at the far downstream end of the flowfield as well as the total particle flow rate through the geometrical beam area. This last figure is useful in estimating the centreline beam intensity.
- (4) Histograms for the integrated distribution function profiles  $\int fdvdw$ ,  $\int fdvdu$ ,  $\int fdvduv$  for each cell.

The distribution function is broken down into the distribution function of the molecules which have not undergone collision in the flowfield and the remainder. The mean velocity, mean square velocity, and mean number of molecules are also given along with a theoretical comparison number for no skimmer interaction. The histograms are obtained by time averaging regular observations of the flowfield for the duration of the computation after equilibrium is reached.

#### RESULTS

A simulator program such as this one should be viewed rather like an experimental facility suitable for investigating a range of problems connected with the skimmer. We describe here the results of a study of skimmer interaction.

A preliminary study was done to check a model proposed by French (5) suggesting a significant interaction downstream of the skimmer orifice. This was done in a program which preceded the present one by making the downstream skimmer wall absorbing. No downstream effect was observed. A check of the distribution functions in the present study supports this conclusion.

In fact this study shows that the skimmer interaction is caused by a screen of molecules originating from the wall and from collisions extending approximately one mean free path upstream of the skimmer orifice. The supporting material for this conclusion is contained in the following graphs and tables.

Table 1 shows the cases computed in this study.

Fig. 1 defines the geometric variables in the program and Figs 2 - 4 give the specific geometries used in the calculations.

Table 2 shows condition near the skimmer wall for an assortment of cases. It is most significant that for all but the sharpest skimmer (angles  $50^\circ$ ,  $45^\circ$ ) the flow is subsonic. We suspect there is always a subsonic region close to

the skimmer wall which is very thin for small angles but grows rapidly as the angle increases. Also the surface interaction with the skimmer plays a significant role, since case 23 (ACCOM = 0) gives a high Mach number even for a blunt skimmer.

Fig. 5 shows the mass flow rate through the skimmer orifice vs A in terms of the theoretical no interaction value. The mass flow is less than one in all cases computed but shows a tendency to go to 1 in the cold skimmer and no lip cases.

Fig. 6 shows beam intensity vs A. The importance of the skimmer lip sharpness is here clearly indicated. The skimmer angle seems to have less effect than the skimmer temperature. Though the general shape of the experimental beam intensity vs Knudsen number curves is evident, our results do not show decreases in intensity as strong as those in [3] for instance.

Figs. 7, 8 show mass flow and beam intensity vs various parameters. It is most interesting that an increase in PRES which leads to a decrease in the number of molecules entering the flowfield through the outer upstream boundary leads to a decreased mass flow but no significant change in beam intensity. Furthermore, a low accommodation coefficient gives high values in both graphs.

Figs. 9, 10 were obtained by smoothing the histograms produced by the program. It is clear that a Knudsen number of  $1/2$  ( $A = 4$ ) leads to more or less complete destruction of the beam by skimmer interaction.

Figs. 11, 12 show clearly a sharp increase of molecules having a broad distribution function and infiltrating the beam region between Knudsen numbers  $1/2$  and 1.

Finally a note on the standard deviation of the results. The beam intensity and mass flow curves have a relative standard deviation of between 3% and 5%. It follows from the theory of Monte Carlo simulators that the probability distribution of each value obtained is normal. Accuracy is expensive in these calculations. A fourfold increase in computing time would cut the standard deviation in half.

TABLE 1

CASES COMPUTED

	CHARACTERISING PARAMETERS							COMMENTS
	A	SIA	CR	PRES	ACCOM	THLIP	GEOM	
1	0.5	0.1	1.	1.	0.5	0.1	3	Sharp skimmer
2	1.	0.1	1.	1.	0.5	0.1	3	
3	2.	0.1	1.	1.	0.5	0.1	3	
4	4.	0.1	1.	1.	0.5	0.1	3	
5	2.	0.1	1.	2.	0.5	0.1	1	Effect of PRES
6	2.	0.1	1.	1.5	0.5	0.1	1	
7	2.	0.1	1.	0.75	0.5	0.1	1	
8	2.	0.1	1.	0.5	0.5	0.1	1	
9	2.	0.0546	1.	1.	0.5	0.1	1	High mach number Absorbing walls
10	1.	0.1	1.	2.	0.5	0.1	1	
11	0.5	0.1	0.5	1.	0.5	0.1	1	Cold skimmer series
12	1.	0.1	0.5	1.	0.5	0.1	1	
13	2.	0.1	0.5	1.	0.5	0.1	1	
14	4.	0.1	0.5	1.	0.5	0.1	1	
15	0.5	0.1	1.	1.	0.5	0.1	1	Standard series blunt skimmer
16	1.0	0.1	1.	1.	0.5	0.1	1	
17	2.0	0.1	1.	1.	0.5	0.1	1	
18	4.0	0.1	1.	1.	0.5	0.1	1	
19	0.5	0.1	1.	1.	0.5	0.0	1	Perfect edge
20	1.0	0.1	1.	1.	0.5	0.0	1	
21	2.0	0.1	1.	1.	0.5	0.0	1	
22	4.0	0.1	1.	1.	0.5	0.0	1	
23	2.	0.1	1.	1.	0.	0.1	1	Effects of surface interaction
24	2.	0.1	1.	1.	1.	0.1	1	
25	0.5	0.1	1.	1.	0.5	0.1	2	Intermediate angle
26	1.	0.1	1.	1.	0.5	0.1	2	
27	2.	0.1	1.	1.	0.5	0.1	2	
28	4.	0.1	1.	1.	0.5	0.1	2	

Notes

A vs Knudsen number Kn

A	0.5	1	2	4
Kn	4	2	1	0.5

SIA, CR, PRES, ACCOM, THLIP are explained in Appendix 1.

GEOM 1, 2, 3 are shown in Figs. 1, 2, 3 respectively.



TABLE 2

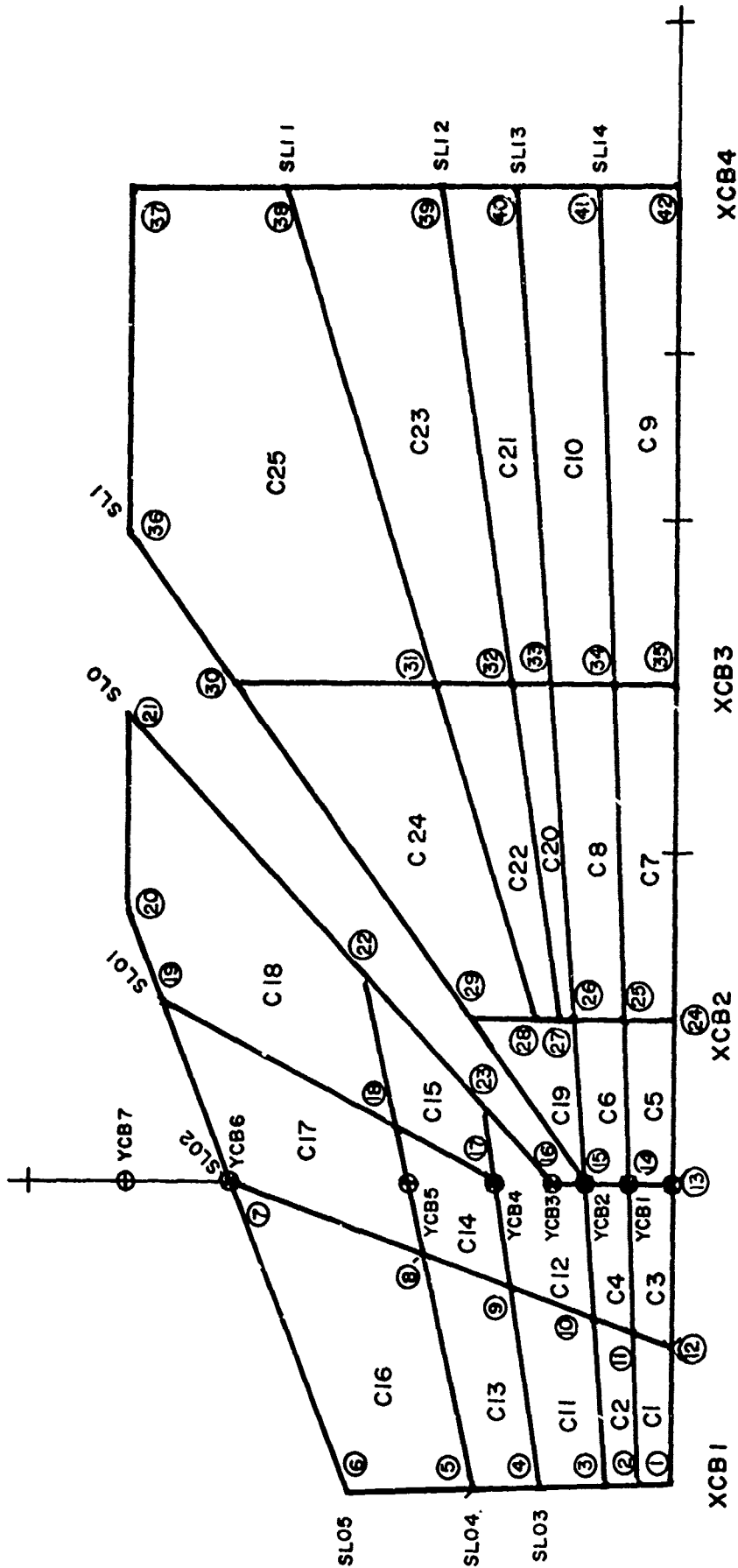
CONDITIONS IN FRONT OF SKIMMER

<u>Case</u>	<u>CELL 14</u>		<u>CELL 15</u>		
	<u>Mean Speed</u>	<u>Mach #</u>	<u>Mean Speed</u>	<u>Mach #</u>	<u>Inclination</u>
15	0.55	0.64	0.51	0.55	0.83
18	0.52	0.79	0.34	0.44	0.69
5	0.62	0.88	0.48	0.57	0.52
8	0.33	0.44	0.28	0.34	0.73
1	0.80	1.4	0.72	1.2	0.28
4	0.86	2.1	0.71	1.	0.32
23	0.87	2.2	0.75	2.3	0.62
25	0.68	1.0	0.60	0.82	0.43
28	0.71	1.3	0.53	0.73	0.47

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FIG. 1 DEFINITION OF GEOMETRICAL PARAMETERS



KEY: SLO, . . . . . SLO5 SLOPES  
 XCB1, . . . . . XCB4 X & Y INTERCEPTS RESP.  
 ①, . . . . . ④② VERTEX NUMBERS  
 C1, . . . . . C25 CELL NUMBERS

FIG. 2 FLOWFIELD FOR GEOM = 1, SKIMMER ANGLES  $96^\circ$ ,  $70^\circ$

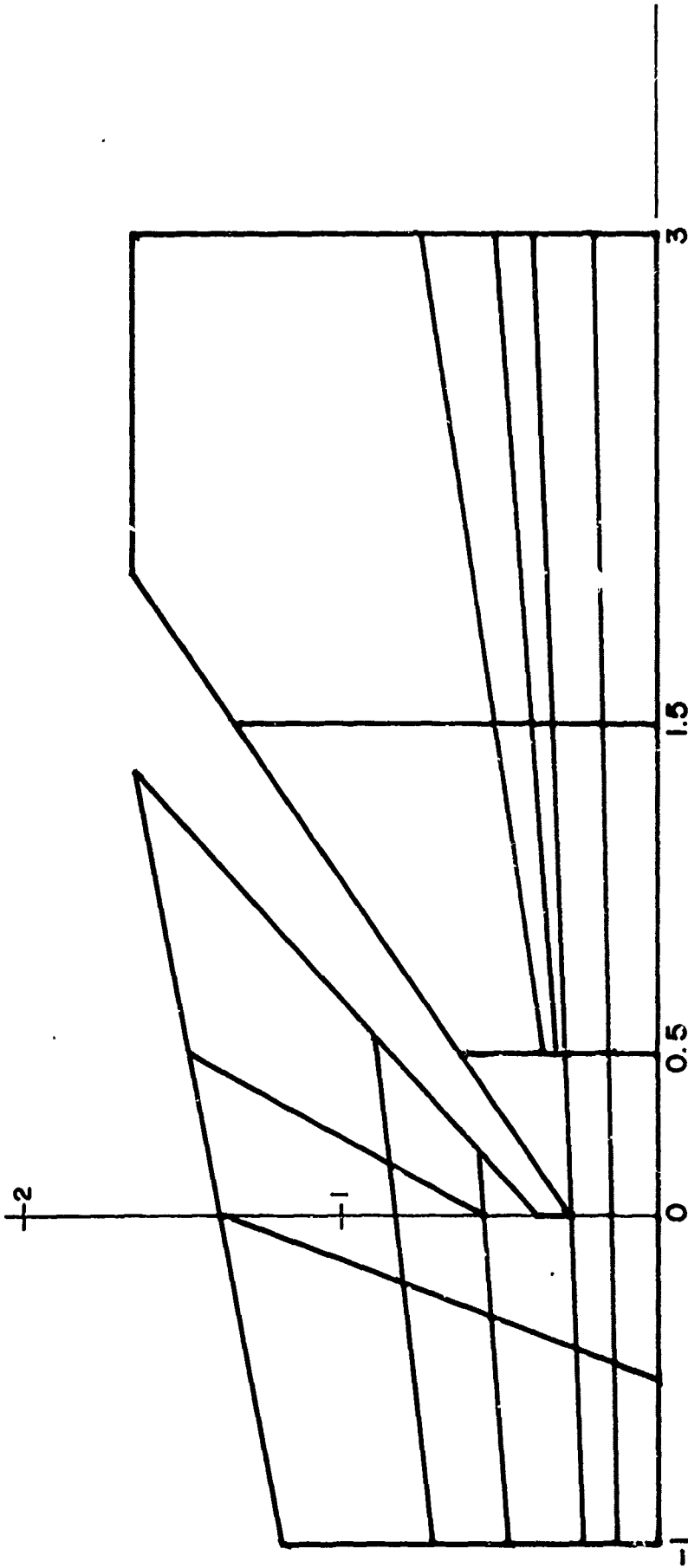


FIG. 3 FLOWFIELD FOR GEOM = 2, SKIMMER ANGLES 68°, 53°

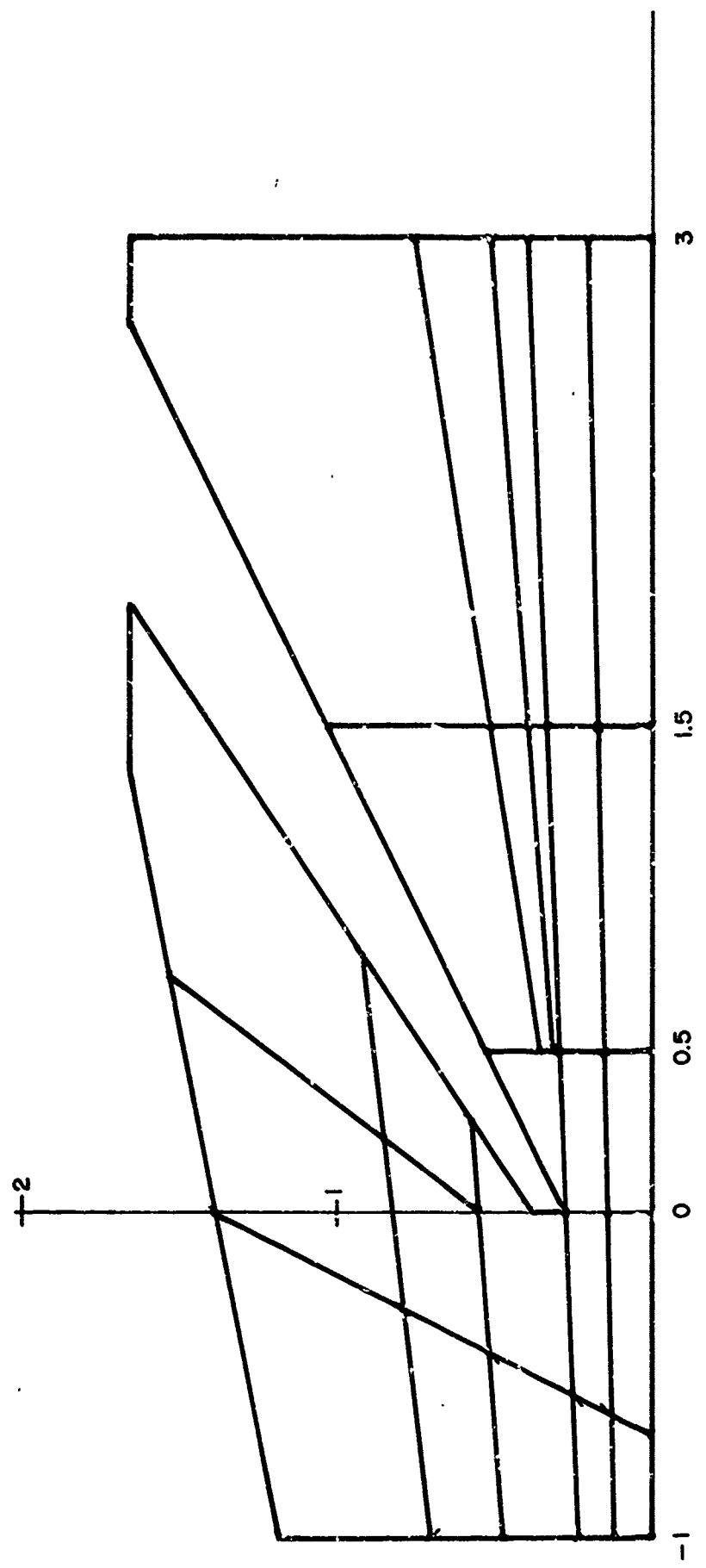


FIG. 4 FLOWFIELD FOR GEOM = 3, SKIMMER ANGLES 50°, 40°

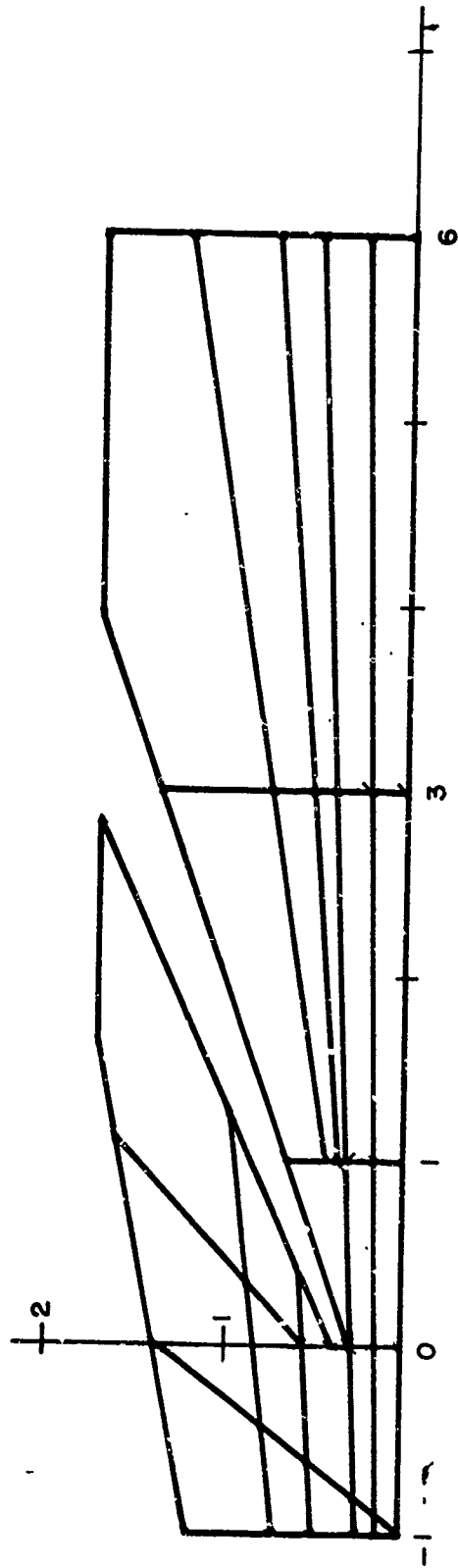


FIG. 5 MASS FLOW THROUGH SKIMMER UNDER VARIOUS CONDITIONS

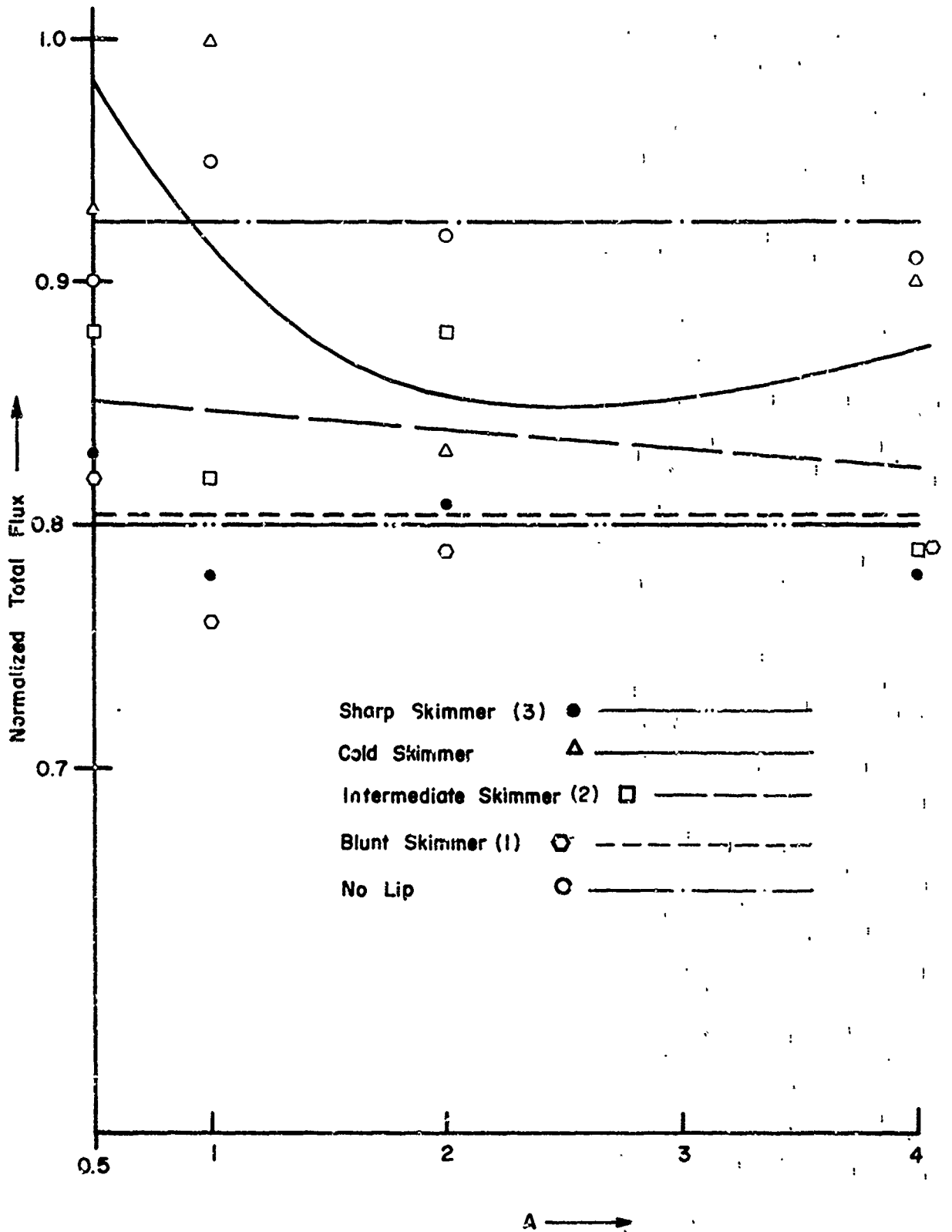


FIG. 6 BEAM INTENSITY UNDER VARIOUS CONDITIONS

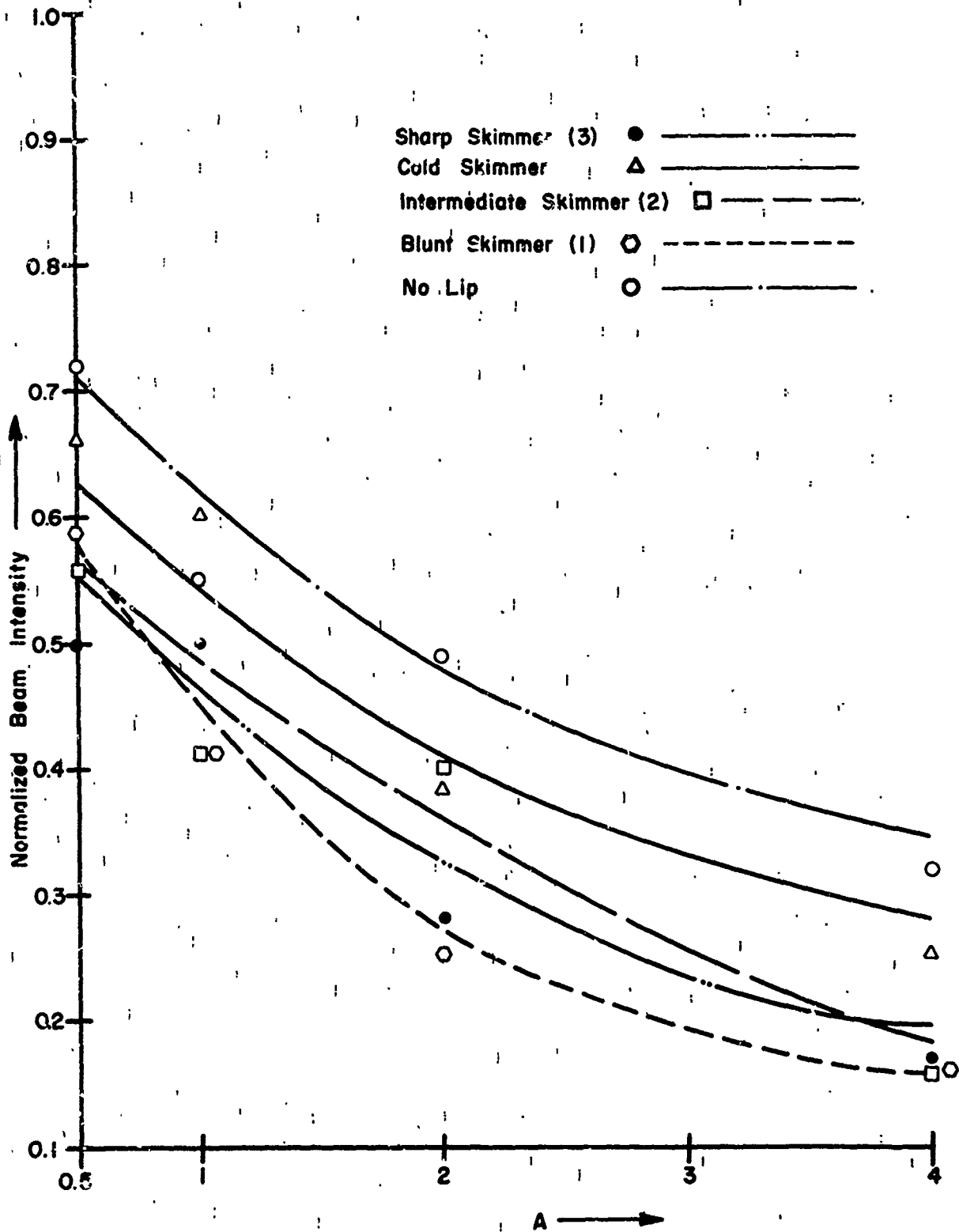




FIG. 7 MASS FLOW THROUGH SKIMMER VS OTHER PARAMETERS

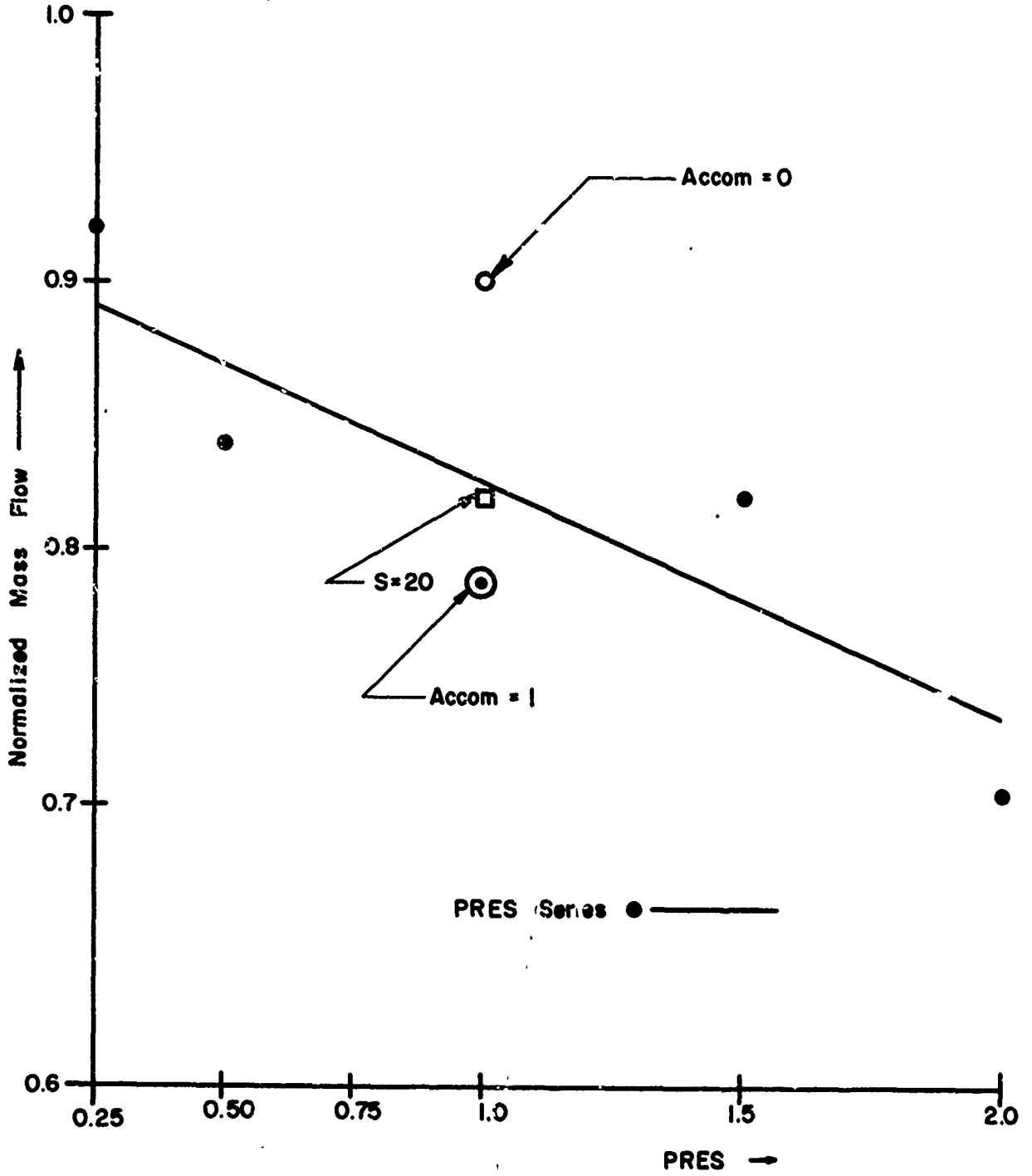


FIG. 8 BEAM INTENSITY VS OTHER PARAMETERS

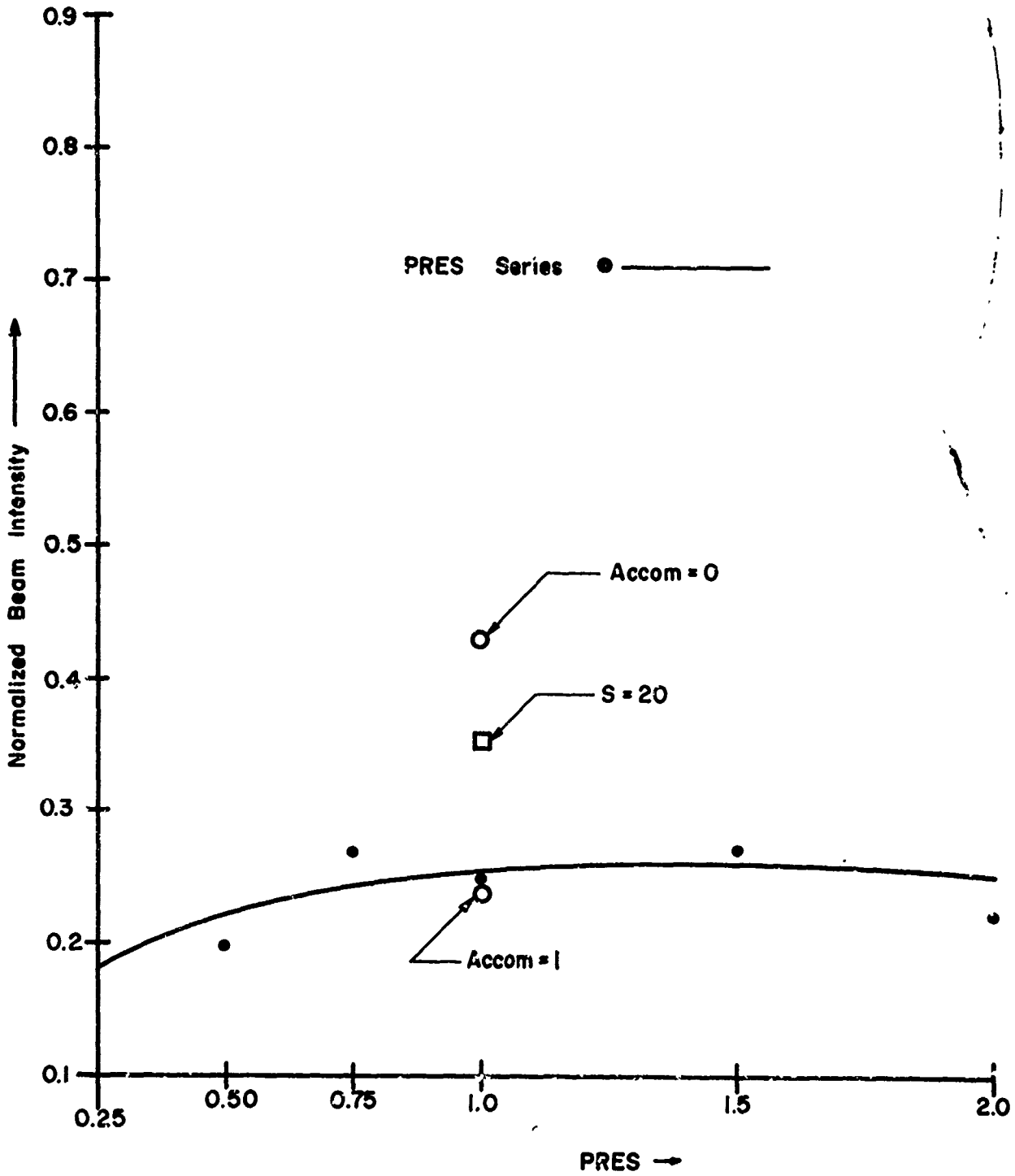


FIG. 9 FLUX DENSITY AT SKIMMER ORIFICE (GEOM=2)

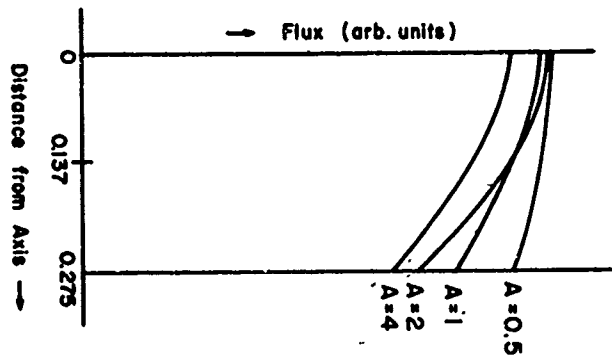


FIG. 10 BEAM PROFILES (GEOM=2)

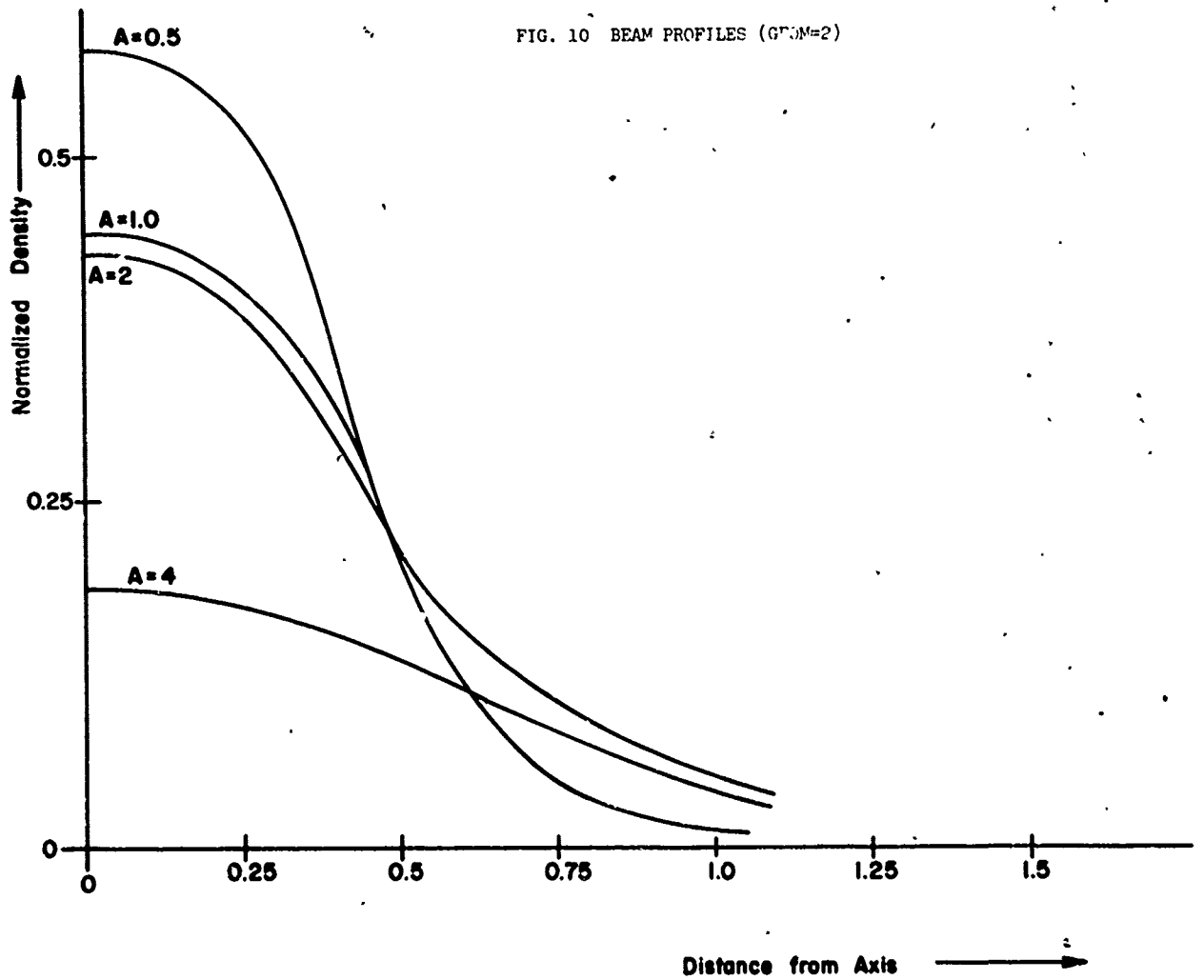
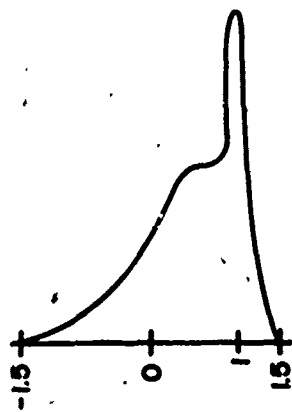


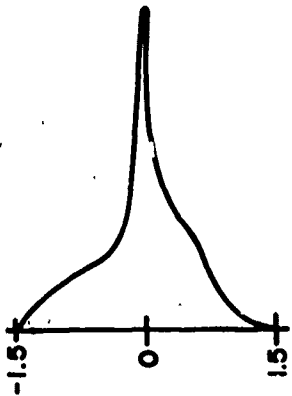
FIG. 11 DISTRIBUTION FUNCTION IN CELL 4 (GEOM=2)

BACKGROUND MOLECULES (A=2)

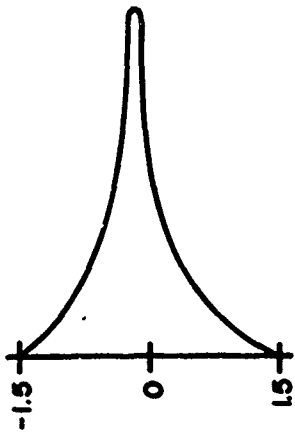
AXIAL



RADIAL



ANGULAR



ALL MOLECULES

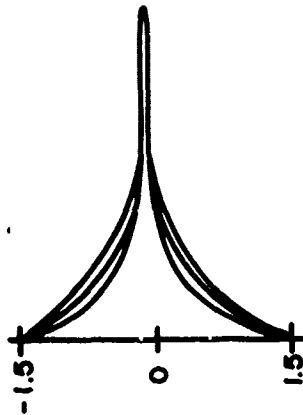
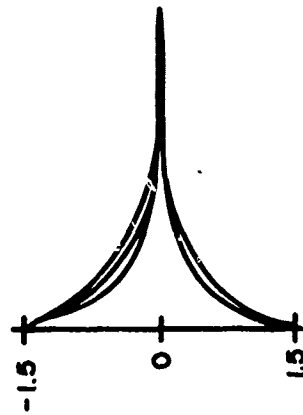
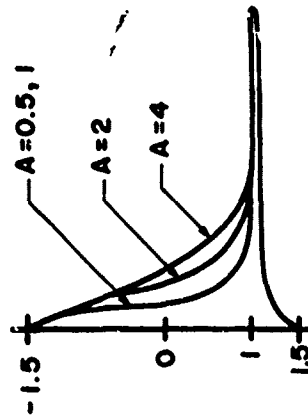
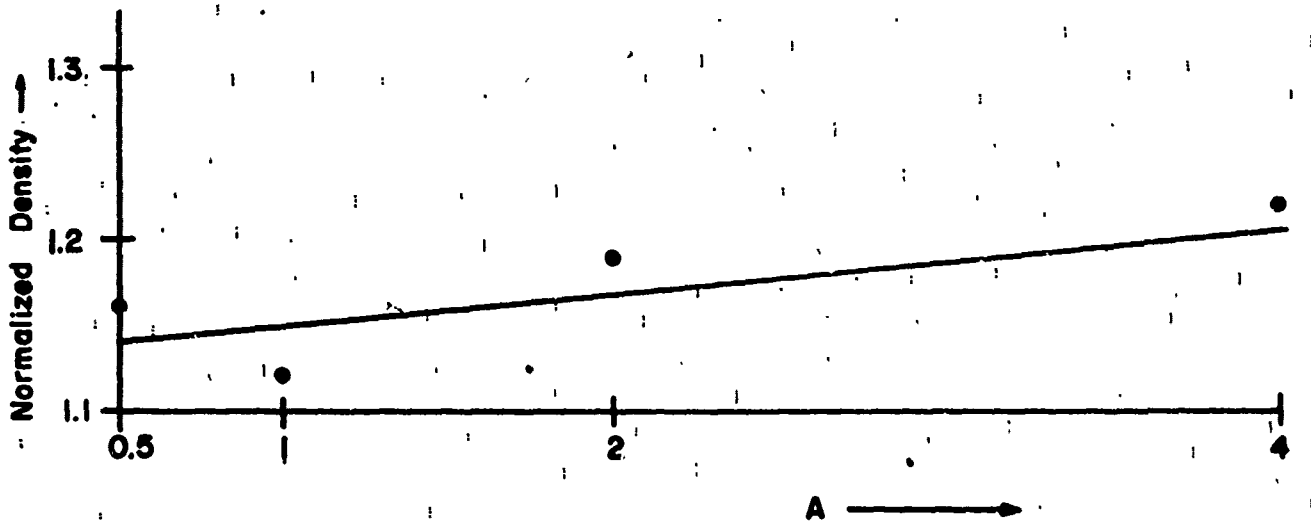
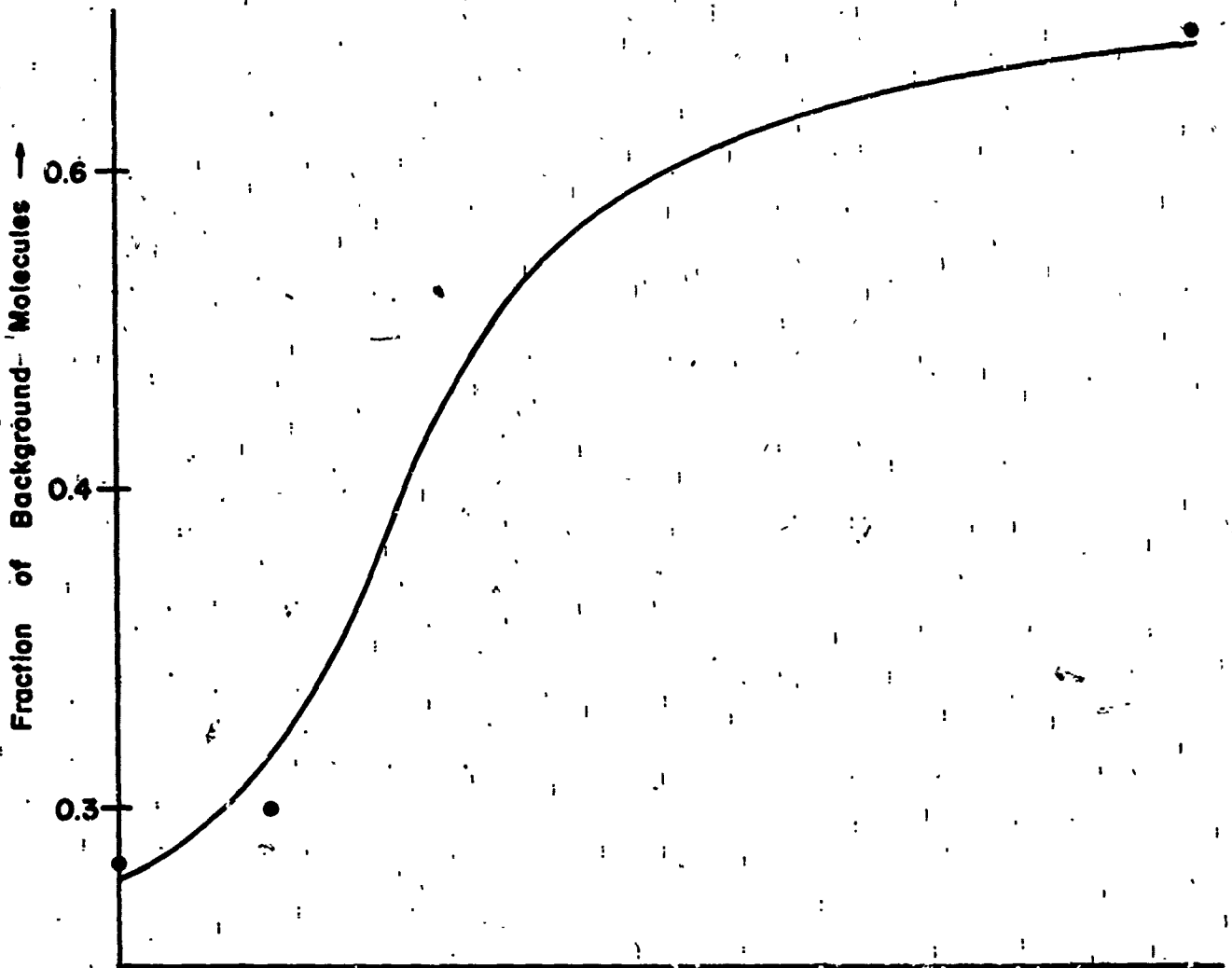


FIG. 12 CONDITIONS JUST UPSTREAM OF ORIFICE (GEOM=2)



COMMENTSA. The Variables

<u>Common Area</u>	<u>Purpose</u>
/RCRD/	Storage area for beam and orifice profile histograms. BPRFL and HPRFL resp. DBPR and DHPR are the widths of the histogram cells in each case.
/GEOM/	Geometrical definition of the flow field - see Fig.
/NPRFL/	For internal use in the program to save computer time in the introduction of molecules through the input plane.
/CONS/	CU is the total number of molecules entering the flow field through the input plane per unit time, SIA is the speed ratio, in the jet, CR is a speed defining the temperature of the skimmer walls, ACCOM is the accommodation coefficient, PRES is related to the pressure on the upstream outer boundary, CLWT is the list containing the cell weights, TCONS is the list of time advance per collision constants for the cells. The remaining variables are for internal use of the program to save recomputing frequently used numbers. They are initially computed in SETUP.
/BEGIN/	BE and BG are initial values for the sequencing variables of the random number generators. A is the cross section density at the orifice, and NST is starting number of simulator molecules in the flow field.
/TIME/	T - Accumulated time variable for the program. DT - Weighted time per iteration (DT ~ DTM). DTM - Preset time allowance per iteration. TEQ - Value of T for which equilibrium is assumed to have been achieved. TEND - Value of T at which computation ceases and output is begun.
	The remaining variables were not actually used in this program.
/STORE/	NCL is the number of cells, MCP = 5000, and MAP is for purposes of referencing the list of molecules. The remaining variables in this common area constitute the molecular list.
/HIST/	Storage area for the histograms FU etc; CFU etc; the mean velocity vectors for each cell - UB etc. and the mean square velocity vector for each cell UUB - CORC counts the number of molecules in each cell which have undergone more than one collision.
/SW/	Contains control parameters for the data collection operation.

## A1-2

- /RAND/ Contains the sequencing parameters for the random number generators.
- /VARS/ Temporary storage area for one molecule to save address computation time while the molecule is being processed.

### B. Subroutines

- MAIN This program is used to set up the cases. Each call to PROG constitutes the computation of one case.
- BLOCK DATA Used to assign values to variables which are common to the computation of many cases.
- PROG Control program for the computation of one case.
- SETUP Computes variables not assigned in MAIN or BLOCK DATA and performs all the initialization necessary to begin computation of a case.
- VPOL Computes cell volumes and cell masses for the undisturbed free jet.
- INPR Sets up an array used to obtain the input profile by interpolation.
- LOC Function which computes the cell containing the coordinates (x,y). LOC works by computing a word IX which has 0 or 1 in the k-th bit depending on which side of the k-th boundary (x,y) is found. Then IX is compared with a standard ordered list (MASK, LDFR).
- COLI Collision increment for cell L.
- SQM Estimates the maximum relative velocity in a given cell.
- TRBKP "Translate and Book-keep". This subroutine essentially controls computation of the convection increment.
- INVRs Computes the cell number L of the M-Th molecule in the molecule list.
- UP, DOWN Used in inserting, deleting or moving molecules in the molecule list.
- TRS, TR Transfer of coordinates.
- FRP Checks a given molecule for collision with boundaries and it moves it a distance appropriate to the time DT.
- TRANS Changes coordinates of a given molecule appropriate to the time interval DT.
- LCHK Checks whether collision occurs with a given boundary.
- EMIT Emits a fully accommodated molecule in the direction C,S.
- REFL Reflects a molecule in the direction C,S.
- INPUT Introduces CU and DT molecules through the input plane on the basis of the input profile defined by FNPR, DFNPR.

Al-3

CBSFL Cubic Spline interpolation subroutine.

TABU Controls the accumulation of histograms and moments of the distribution function.

FIT Inserts molecule at cell L.

SIFT Auxiliary subroutine to accumulate histograms.

INTR See §5.

RANDG Standard normal random number generator.

RANDL Uniform on [0,1] random number generator.

RANDR Uniform on [-1,1].

UMAX Finds the maximum element in an array.

ISGN 
$$\text{ISGN}(X) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

DUMP Controls the output function of the program.

BAR Sets up one histogram bar for printing.

HIST1 Sets up one histogram for printing.

HIST3 Sets up and prints the 3 x 3 histogram describing the distribution function in cell L.











```

A
YFL=LY
YFI=YFI+.4656A13 F=9
IX=LY
RANFL=YFI
RETURN
END
71
FUNCTION RANR(X)
RANR = 2.*RANR(X)-1.
RETURN
END
72
FUNCTION DMAT(X,L)
DIMENSION X(L)
DO J=1,L
Y=X(J)
IF(Y<0) Y=1.-Y
CONTINUE
IMAX=Y
RETURN
END
73
FUNCTION ISGM(X)
ISGM=0
IF(X<F.O.) ISGM=1
RETURN
END
74
SUBROUTINE DIMR
COMMON /STORE/ NCL,MCP,P(120,50)
COMMON /RCRD/ DRPR,DHPR,NPREL(50),MPL(10)
COMMON /CFD/ PFI,DISMS,DIAMS,THI,IP,SL0,SL1,XCR1,XCR2,XCR3,XCR4,
X SL1,SL2,XCR0,XCR1,XCR5,YCR1,YCR2,YCR3,YCR4,YCR5,YCR6,YCR7,
X XN0,YN0,XMS,YMS, VOL(25),VMD(25)
COMMON /CONS/ CU,STA,SIR,CR,CT,AC,COM,PRES,CLMT(26),TCMS(25)
COMMON /RG/ RR,RG,R,G
COMMON /TIME/ T,DT,DTM,TEO,DTSM,TFND,DTAP,TREP
COMMON /HIST/ FU(10,25),EV(10,25),FW(10,25),CEV(10,25),
ICF(10,25),IUR(25),VVR(25),WR(25),IHR(25),VVH(25),WVR(25),CFW(25)
COMMON /RAND/ R,G
IMIEGR RR,RG,R,G
NAMELIST/CFD/ PFI,DISMS,DIAMS,THI,IP,SL0,SL1,XCR1,XCR2,XCR3,XCR4,
X SL1,SL2,XCR0,XCR1,XCR5,YCR1,YCR2,YCR3,YCR4,YCR5,YCR6,YCR7,
X XN0,YN0, XMS,YMS, VOL(25),VMD(25), RADIN,DTSM, XN1,YN1
NAMELIST/CONS/ CU,STA,SIR,CR,CT,AC,COM,PRES,CLMT,TCMS
NAMELIST/RG/ RR,RG,R,G
NAMELIST/TIME/ T,DT,DTM,TEO,DTSM,TFND,DTAP,TREP
WRITE(6,1)
FORMAT(1,'4X,'SKINNEK 1071'//)
WRITE(6,CF)
WRITE(6,COM)
WRITE(6,REG)
WRITE(6,TIM)
FLT=1-TEO
C PREPARATION OF HISTOGRAMS FOR OUTPUT
IMPR=0
DO 21 I=1,50
I=LDC(XCR4,I*DRPR)
IF(I<1,1) TPRR=APREL(I)/FLT+TPRR
21
APREL(I)=APREL(I)/(CMT(L)*F1T6,2831*(I-0,5)*DRPR)
IMPR=0
DO 22 J=1,10
I=LDC(I,IMPR)
IMPR=IMPR+APREL(I)/CMT(L)/F1T
22
APREL(I)=APREL(I)/(CMT(L)*F1T6,2831*(I-0,5)*DRPR)
TNI=1.57079*XCR2*YCR2+A*TCMS(I)/VMD(I)/CMT(I)
DO 24 I=1,NCL
FTWI=LT*CMT(I)
DO 23 J=1,10
FHI(L)=FHI(L)/FTWI
FVI(L)=FVI(L)/FTWI
FMI(L)=FMI(L)/FTWI
CFVI(L)=CFVI(L)/FTWI
CFMI(L)=CFMI(L)/FTWI
CORGI(L)=CORGI(L)/FTWI
UR(L)=UR(L)/FLT
VR(L)=VR(L)/FLT
WR(L)=WR(L)/FLT
IHR(L)=IHR(L)/FLT
VVR(L)=VVR(L)/FLT
WVR(L)=WVR(L)/FLT
24
C PRINTING OF HISTOGRAMS
WRITE(6,41)
41
FORMAT(1,'30X,'FLUX PROFILE AT ORIFICE'//,' DISTANCE FROM AXIS',
X 45X,' NUMBER PER UNIT TIME'//)
CALL HIST(HPREL,10,P,2,40,TOTM)
DO 42 J=1,10
P(L,J)=IMPR
WRITE(6,43) (P(L,J),J=1,10)
43
FORMAT(10,F10.5,5X,40A1,F10.5//)
WRITE(6,44) TOTM,IMPR,TM
44
FORMAT(1,'TOTAL',4X,F10.5//,' NUMBER/TIME THRU ORIFICE',F10.5,
X 4,' THEORETICAL FIGURE FOR NO SKINNEK INTERACTION',F10.5)
WRITE(6,45)
45
FORMAT(1M,'30X,'FRESH FLUX PROFILE AT CM OF FLOWFIELD'//,
X 4,' DISTANCE FROM AXIS',40X,' NUMBER PER UNIT TIME'//)
CALL HIST(HPREL,50,P,2,100,TOTR)
DO 46 J=1,50
P(L,J)=*DRPR
WRITE(6,47) (P(L,J),J=1,102),J=1,50
47
FORMAT(50,F10.5,10A1,F10.5//)
WRITE(6,48) TPRR,TOTR
48
FORMAT(1,' NUMBER/TIME IN REAM',F10.5,75X,' TOTAL',F10.5)
C DISTRIBUTION FUNCTION PART
DO 72 I=1,NCL
WRITE(6,81)
72
A
FORMAT
X 41M,45X,'VELOCITY HISTOGRAMS FOR CELL',14,' THE FIRST HISTOGR
AM TRIPLE REFERS TO MOLECULES WHICH HAVE UNDERGONE NO COLLISIONS I
N THE FLOWFIELD,' THE SECOND TO MOLECULES WHICH HAVE UNDE
R GONE AT LEAST ONE COLLISION, AND THE THIRD GIVES THE SUM OF THE F
IRST TWO,' LOWER CELL BOUNDARY VALUES APPEAR DOWN THE
LEFT. TIME AVERAGED NUMBER OF MOLECULES APPEARS AT THE RIGHT OF EA
CH BAR.'//)
CALL HIST3(P,FI,FV,FW,I)

```

APPENDIX 2

Typical Output

Note: The "Histograms for cell - " is done for each of the 25 cells.



SKIMMER 1971

```

CGED 1.1499996 ,DISNS= 7.0000000 ,DIANS= 0.5499995 ,THLP= 0.0099996E-01,SLN= 0.2200095 ,SLI= 0.6999999 ,XCBI=
-1.0000000 ,XC2= 0.5000000 ,XC83= 1.5000000 ,XC84= 3.0000000 ,SLI1= 0.15714276 ,SLI2= 0.7857137E-01,XC8D=
1.3631897 ,XCBI= 1.9530518 ,XC85= 1.3631916 ,XC81= 0.1374999 ,YCR1= 0.2745998 ,YCR2= 0.3749994 ,YCR3=
0.5499995 ,YCR3= 0.8229993 ,YCR6= 1.3745990 ,YCR7= 1.6577670 ,YCR1= 1.8589997 ,YCR2= 2.7499990 ,YCR3=
0.7857137E-01,SL04= 0.11785710 ,SL05= 0.19042842 ,SL13= 0.39285708E-01,SL14= 0.19642452E-01,PADIN= 1.1785698 ,DISNI=
0.0000000 ,XNI= 0.76188570 ,YNI= 0.81923199 ,YNO= 0.68101281 ,YND= 0.73227185 ,XNS= 0.19274509 ,YNS=
-0.98124856 ,VDI= 0.25639997E-01, 0.8392024E-01, 0.25675233E-01, 0.70551922E-01, 0.31860690E-01, 0.95608950F-01, 0.77679157E-01,
0.23303765 , 0.15591383 , 0.46774197 , 0.3805275 , 0.20136091 , 0.73771054 , 0.38943589 , 0.38877684 ,
2.9284039 , 1.7104807 , 2.9427347 , 0.20664322 , 0.8363806E-01, 0.34364694 , 0.19970407 , 0.91639000 ,
2.5210074 , 10.137089

```

```

SEND
SCON
CU= 404.85156 ,SIA= 0.9999996E-01,SIB= 0.70699930E-01,CS= 1.0000000 ,CT= 0.70699986 ,ACOM= 1.0000000 ,PRFS=
1.0000000 ,CLMT= 1.0000000 , 1.0000000 , 1.0000000 , 1.0000000 , 1.0000000 , 1.0000000 , 1.0000000 ,
1.0000000 , 1.0000000 , 1.0000000 , 0.25000000 , 0.25000000 , 0.62500000E-01, 0.62500000E-01,
0.25000000E-01, 0.15625000E-01, 0.15625000E-01, 1.0000000 , 1.0000000 , 1.0000000 , 1.0000000 ,
1.0000000 , 1.0000000 , 0.0 , 1.0000000 , 1.0000000 , 1.0000000 , 1.0000000 , 1.0000000 ,
51.988815 , 23.484360 , 70.453018 , 57.240784 , 171.72246 , 114.80091 , 344.67310 , 70.111633 ,
53.675018 , 33.975586 , 17.935638 , 17.905273 , 33.717224 , 19.694229 , 33.882233 , 152.27275 ,
61.632446 , 253.22893 , 146.48874 , 675.27612 , 1858.1342 , 7469.8906

```

```

SEND
BR= 1795.8G= 1795.A= 2.0000000 ,NST= 1000.R= 8537182R.G= 972226277
SEND
CTIM T= 12.303652 ,DT= 0.34669107 ,DTM= 0.33333331 ,TEQ= 4.0000000 ,DTSM= 1.0000000 ,TENN= 12.000000 ,DTRP=
1.0000000 ,TREP= 12.000000

```

FLUX PROFILE AT ORIFICE

DISTANCE FROM AXIS	NUMBER PER UNIT TIME
0.02750	19.51538
0.05500	22.30128
0.08250	18.67900
0.11000	18.51970
0.13750	21.52887
0.16500	15.84042
0.19250	17.47406
0.22000	17.28504
0.24750	14.51355
0.27500	9.63750
TOTAL	175.20087

NUMBER/TIME THRU ORIFICE = 137.62980. THEORETICAL FIGURE FOR NO SKINNER INTERACTION = 17.07062



BEAM FLUX PROFILE AT END OF FLOWFIELD

DISTANCE FROM AXIS	NUMBER PER UNIT TIME
0.03206	1.16574
0.06571	1.55566
0.09857	2.56682
0.13142	2.93352
0.16428	2.98168
0.19713	2.75776
0.22999	2.33349
0.26284	1.94457
0.29570	2.60902
0.32855	2.45630
0.36141	1.64454
0.39425	2.07985
0.42712	1.68011
0.45997	1.38281
0.49283	0.68395
0.52569	0.97856
0.55854	0.70712
0.59140	1.16674
0.62425	0.75681
0.65711	0.98775
0.68996	0.22766
0.72282	0.43414
0.75567	0.44077
0.78853	0.25789
0.82138	0.50003
0.85424	0.49042
0.88709	0.41877
0.91995	0.31920
0.95280	0.74563
0.98566	0.23730
1.01851	0.16341
1.05137	0.42595
1.08423	0.21940
1.11708	0.36570
1.14994	0.27055
1.18279	0.23006
1.21565	0.29749
1.24850	0.19668
1.28136	0.31020
1.31421	0.14769
1.34707	0.37451
1.37992	0.18274
1.41278	0.13170
1.44563	0.14752
1.47849	0.13664
1.51134	0.16668
1.54420	0.21328
1.57706	0.09825
1.60991	0.20448
1.64277	0.64319
TOTAL 43.4531P	

A2-3

UNIVERSITY OF TORONTO

VELOCITY HISTOGRAMS FOR CELL 4

THE FIRST HISTOGRAM VECTILE OFFERS TO MOLECULES WHICH HAVE UNDERGONE NO COLLISIONS IN THE FLOWFIELD, THE SECOND TO MOLECULES WHICH HAVE UNDERGONE AT LEAST ONE COLLISION, AND THE THIRD GIVES THE SUM OF THE FIRST TWO. LOWER CELL BOUNDARY VALUES APPEAR ON THE LEFT, TIME AVERAGED NUMBER OF MOLECULES APPEARS AT THE RIGHT OF EACH BAR.

-1.50000	0.70648	0.94152	0.27461
-1.20000	0.79896	1.31512	0.51806
-0.90000	2.88463	0.95511	0.47028
-0.60000	1.75585	1.39375	0.84047
-0.30000	0.62503	0.81504	12.36533
0.0	0.0	0.52901	14.70052
0.30000	0.0	0.08213	0.74295
0.60000	2.19485	0.04804	0.98111
0.90000	23.98384	0.49769	0.28260
1.20000	0.0	0.37321	0.37541
TOTALS	33.14963	33.14960	33.14961
-1.50000	0.51958	0.0	0.14307
-1.20000	0.0	0.26665	0.61572
-0.90000	0.67336	4.97926	7.00127
-0.60000	0.96652	5.33958	3.97033
-0.30000	3.67065	11.95767	14.43795
0.0	4.58103	14.99689	14.58814
0.30000	10.14162	6.87838	9.04415
0.60000	12.34117	3.06251	2.77678
0.90000	11.70164	0.86544	0.78821
1.20000	1.54171	0.22189	0.65171
TOTALS	48.51729	48.51721	48.51730
-1.50000	1.22606	0.94152	1.11748
-1.20000	0.79896	1.27877	0.87431
-0.90000	3.55799	5.93437	2.38055
-0.60000	2.90247	7.23333	4.81079
-0.30000	4.29568	20.77269	27.40327
0.0	6.98103	33.62590	29.29765
0.30000	10.14162	6.91051	9.12709
0.60000	14.53602	3.11058	3.15789
0.90000	35.68552	1.36412	1.07082
1.20000	1.54171	0.59510	1.52712
TOTALS	91.66693	91.66685	91.66689

THEORETICAL NO INTERACTION TOTAL = 55.20851

MEAN VELOCITY VECTOR 0.52728 -0.00041 0.00086 MEAN SQUARE VELOCITY VECTOR 3.68413 0.17106 0.18060  
 TIME AVERAGED NUMBER OF MOLECULES WHICH HAVE UNDERGONE MORE THAN ONE COLLISION IN THE FLOWFIELD 31.45020

APPENDIX 3No Interaction Beam Intensity

We derive here a formula for the beam intensity at points close to the skimmer.

Let  $D$  be the nozzle skimmer distance,  $L$  be the skimmer-observation point distance and  $b$  be the skimmer radius. Consider a particle in the skimmer orifice plane at position  $(r \cos \theta, r \sin \theta)$  whose velocity has a probability density function proportional to

$$\exp[-(u-1)^2 + (v-r \cos \theta/D)^2 + (w-r \sin \theta/D)^2]/c^2$$

That is, the mean velocity vector points in the direction

$$(1, \frac{r \cos \theta}{D}, \frac{r \sin \theta}{D})$$

The impact position of the particle on the plane normal to the axis distance  $L$  downstream of the skimmer then has probability distribution

$$\frac{1}{L^2 d^2} e^{-\frac{1}{Lc}} [(x-\alpha r \cos \theta)^2 + (y-\alpha r \sin \theta)^2]$$

where

$$\alpha = \frac{L+D}{D}$$

If the flux through the orifice is  $\phi$  particles per unit area then the flux through the point  $x, y$  is

$$\phi_L(x, y) = \phi \int_0^b r dr \int_0^{2\pi} d\theta \frac{1}{L^2 c^2 \pi} e^{-\frac{1}{Lc}} [(x-dr \cos \theta)^2 + (y-dr \sin \theta)^2]$$

This integral is messy in general, but if we ask only for the centreline flux ( $x = y = 0$ ) we obtain

$$\phi_{Lo} = \int_0^b r dr \int_0^{2\pi} d\theta \frac{1}{Lc^2 \pi} e^{-\frac{1}{Lc}} \alpha^2 r^2$$

which one can easily evaluate to obtain

$$\phi_{Lo} = \left(\frac{D}{L+D}\right)^2 (1 - e^{-[\frac{b}{c}(\frac{1}{L} + \frac{1}{D})]^2})$$