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The work reported herein was carried out for the Naval Postgraduate School by Dr. Shaul Abramovich under Contract Number N62271-83-M-1939. The work presented in this report is in support of DARPA project. The work is based on general publications and theory and provides specific means for solving the exhaust flow from a spacecraft laser. Computer programs have been developed to calculate the flowfield in the continuum region as well as in the molecular region. It provides the means to calculate the flux of the exhausted gas towards the walls of the spacecraft. The project on LASER EXHAUST is funded by Defense Advanced Research Projects Agency and is under the cognizance of Distinguished Professor A. E. Fuhs.

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#### 20. Abstract (continued)

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The axisymmetric Monte Carlo Simulation begins outside the nozzle, where the breakdown parameter has a value of approximately 0.05. The actual shape of this breakdown limit is a closed lobe surface which starts at the nozzle lips, approximately follows a specific Mach wave in the Prandtl/Meyer fan and closes back to the axis far downstream. Because our interest is limited to the close vicinity of the corners, there the shape of this limit may be approximated to a straight line (for an axisymmetric flow making a cone).

For the simulation purposes, the domain between the breakdown limit and the wall is divided into sectors, each sector divided into radial regions and each region into simulation cells. Each cell is filled with a number of simulated molecules relative to the cell volume and local number density.

The simulation is performed for each region separately and contains:

- \* molecular motions
- \* generation of new molecules to simulate input flows
- \* deactivation of molecules to simulate output flows
- \* molecular collisions

Because there is no apriori information about the flow interaction between different regions, the whole simulation is done on an iterative basis. A first run will supply the output flux from each region. These results are used as input data for consecutive runs.

`The program runs as far as the collision frequency is still high and the mean free path is low compared with the size of the cells. Beyond this limit the flow may be regarded as collisionless, and the flux towards the solid wall may be computed directly.

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#### ABSTRACT

Some procedures have been developed to analyze the flowfield of highly underexpanded axisymmetric ring jets operated at high altitudes. The Method of Characteristics (NOC) was used to compute the Prandtl-Meyer expansion fan and the flow parameters in that region. The MOC may also be used to obtain some indications about the repetitive expansion — compression behavior of the jet as well as the divergent shape of the expansion part downstream, when the ambient pressure goes below certain limits.

The continuum methods may be used as far as the limit where translational equilibrium ceases to exist. The breakdown of the continuum theory may be evaluated using the experimental breakdown parameter as proposed by G. A. Bird. Beyond this limit, the molecular Direct-Simulation-Monte-Carlo method (DSMC) is applied.

The axisymmetric Monte Carlo Simulation begins outside the nozzle, where the breakdown parameter has a value of approximately 0.05. The actual shape of this breakdown limit is a closed lobe surface which starts at the nozzle lips, approximately follows a specific Nach wave in the Prandtl-Neyer fan and closes back to the axis far downstream. Because our interest is limited to the close vicinity of the corners, there the shape of this surface may be approximated by a straight line (making a cone in an axisymmetric flow).

For the simulation purposes, the domain between the breakdown surface and the wall is divided into sectors, each sector divided into radial regions and each region into simulation cells. Each cell is filled with a number of simulated molecules relative to the cell volume and local number density.

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The simulation is performed for each region separately and contains:

- \* molecular motions
- \* generation of new molecules to simulate input flows
- \* deactivation of molecules to simulate output flows
- \* molecular collisions

Because there is no apriori information about the flow interaction between different regions, the whole simulation is done on an iterative basis. A first run will supply the output flux from each region. These results are used as input data for consecutive runs.

The program runs as far as the collision frequency is still high and the mean free path is low compared with the size of the cells. Beyond this limit the flow may be regarded as collisionless, and the flux towards the solid wall may be computed directly.

#### I. INTRODUCTION

Gas jets released from spacecrafts and external flows about vehicles at high altitudes have a renewed interest in particular with regard to two main aspects:

a. contamination of the spacecraft walls

b. optical disturbances caused by the plume.

A spacecraft gas dynamics laser releasing a large quantity of gas is highly affected by these two factors and the interest in analyzing them and being able to control them have a unique importance in further development.

A spacecraft laser is assumed to have a long cylindrical shape with the optical power output devices installed at one of its bases as shown in Figure 1.

The output gas is released through a ring nozzle, undergoes a fast three dimensional axisymmetric expansion, and forms a plume covering the whole meridian plane of the vehicle. It widens to large angles of expansion so that it may intersect the laser beam. Back scattered molecules may return to the wall of the spacecraft causing contamination and degradation of surfaces and vehicle parts.

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Figure 1. The Spacecraft Laser.  $M_0$  - Mach number at the exit surface ~ 4 the jet gas is composed of two species

heavy molecules  $M_{G1} = 19$ light molecules  $M_{G2} = 4$ 

Altitudes between 200 to 1000 km.

Continuum flow theory may be used to solve the flowfield and flow parameters as far as there is translational equilibrium, it means that intermolecular interactions are fast enough to maintain expansion rates. Wherever these interactions are too slow, the continuum flow becomes invalid and the molecular flow theory should be employed.

The solution for the continuum regime is computed here by means of the Method of Characteristics (MOC) [1,2,3]. The limit where continuum breakdown occurs was estimated by the experimental breakdown parameter as proposed by G. A. Bird [4]. Beyond this limit, it is proposed to compute the molecular flow by means of the Direct Simulation Monte Carlo technique as described in detail by Bird [4].

For moderate and low pressure ratios (static pressure at the nozzle exit to the ambient pressure), an underexpanded jet exhibits a repetitive expansion - compression behavior with a geometry depending on the initial Hach angle, on the Prandtl-Meyer fan angle, and on the gas specific heats ratio. For lower ambient pressure which occurs at higher altitudes, the first compression region is pushed out to the envelope of the jet forming the barrel shock. If the ambient pressure is low enough, this compression region may disappear due to the molecular behavior of the flow [6,11].

The breakdown of the continuum theory occurs in a region where the gas density and pressure are high compared with the density and pressure in the ambient gas. At high altitudes the ratios between these parameters may reach 10<sup>6</sup> or more. Considering this range of variations, computational validity dictates the use of the Direct Simulation Monte Carlo method. In the higher density range the jet will be considered as consisting of two species of gas, their molecular model will be "the hard sphere molecule" model and

ambient gas is not allowed to protrude. In the lower density region the flow will be regarded as collisionless.

**I** 

In the following chapters we bring the detailed description of the computer programs which solve the different parts of the flowfield.

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#### II. THE CONTINUUM REGIME

A. THE TWO DIMENSIONAL ISENTROPIC UNDEREXPANDED JET

The results brought here are based on the supersonic steady isentropic flow theory as described in literature (see for example, Shapiro [1], Liepman and Roshko [2], and Owczarek [3]).

The ranges of paremeters of a jet emerging from a gas dynamics spacecraft laser are:

a. The Mach number at the exit surface  $M_0 = 4$ . The static pressure at the exit plane  $P_0 = 136$  pa. Ambient pressure  $(P_{amb})$ , temperature  $(T_{amb})$  and other thermodynamic properties of ambient gas depend on the altitude as shown in Table 1. The jet gas may consist of DF, HF, Helium and other species. In the programs we limit the compositon to two species: Air and He. (The program allows changes in the composition and types of gas.)

. b. The pressure ratio  $\frac{P_o}{P_{amb}}$  for the minimum required altitude (200

km) assures that the jet is highly underexpanded (we show later the influence of this ratio on the shape of the jet).

The following thermodynamic relations are valid as long as the compessible flow is isentropic

$$T_{T} = T(1 + \frac{\gamma - 1}{2} N^{2})$$
 (1)

$$P_{\rm T} = P(1 + \frac{\gamma - 1}{2} \, {\rm M}^2)^{\frac{1}{\gamma - 1}}$$
(2)

$$\rho_{\rm T} = \rho (1 - \frac{\gamma - 1}{2} M^2)^{\frac{1}{\gamma - 1}}$$
(3)

TABLE 1

ACAM MANYAY TETTING SAMANA

# ATMOSPHERIC WATA (Abstracted from U.S. Standard Atmosphere 1976)

Altitude	Pressu	re	numbe		particle	colli	sion	mean		molecular	dens 1	ty	temperature
_			densi	ty	speed	frequ	ency	free pa	th	weight			
ka	m ba	1	B-3		tu/sec	sec.	-	a		kg/kmol	kg/m	e	۰k
100	3.2011	-4	1.189	+19	381.4	2.68	 F	1.42		28.4	5.604	7	195.08
200	8.4736	-	7.182	+15	921.6	3.9		2.4	+7	21.3	2.541	-10	854.56
300	8.7704	30 I	6.5()9	+14	1079.7	4.2	 ī	2.6		17.73	1.916	-11	976.01
400	1.4518	20 1	1.056	+14	1148.5	7.2	-2	1.6	+4	15.98	2.803	-12	995.83
200	3.0236	6-	2.192	+13	1215.0	1.6	-2	7.7		14.33	5.215	-13	999.24
600	8.2130	-10	5.950	+12	1356.4	4.8		2.8		11.51	1.137	-13	58.999
700	3.1908	-10	2.311	+12	1627.0	2.2		7.3	- <u>-</u> -	8.00	3.070	-14	76.999
800	1.7036	-10	1.234	+12	1954.3	1.4	ñ	1.4	 \$	5.54	1.136	-14	66*666
006	1.0873	-10	7.876	+11	2192.6	1.0	<del></del> -	2.1		4.40	5.759	-15	1000.00
1000	7.5138	-11	5.442	+11	2318.1	7.5	 -	3.1	- <u>-</u> -	3.94	3.561	-15	1000.00
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where  $T_T$ ,  $P_T$ , and  $\rho_T$  are the total temperature, pressure and density (constant for isentropic field). T, P, and  $\rho$  are local temperature, pressure and density  $\gamma$  is the specific heat ratio of the gas (considered here as constant), M is the local Mach number.

The partial differential equation of motion for supersonic 2-D irrotational and isentropic flow is a hyperbolic equation having solutions obtained from invariants along characteristic lines. Physical interpretation of these lines are the compression or expansion waves which are oriented at Mach angles relative to the streamlines.

Once the directions of the characteristics (waves) are determined everywhere in the field, all other parameters may be calculated.

#### B. THE TWO DIMENSIONAL PLANAR JET

The compressible supersonic jet flow is characterized by two families of characteristics (pressure waves) starting at each corner of the nozzle lips. Each of these families of waves forms a Prandtl-Meyer fan. The streamlines crossing the characteristic waves bend outwards resulting in an increase in the flow area. The angle  $\mu$  between the streamline and the pressure wave is a function of the local Mach number as

#### $\mu = \arcsin (1/M)$ (4)

The symbol  $\mu$  is the Mach angle.

Using the isentropic relations, we can find the relation between the turning angle ( $\theta$ ) and the local Mach number (H) as

$$d\theta = - \frac{(M^2 - 1)}{M(1 + \frac{\gamma - 1}{2}M^2)} dM$$
 (5)

Integration between the conditions M=1 and M gives the total turning angle starting at the throat (where M=1) up to a point with given M. The result gives the Prandtl-Meyer function (angle) as

$$\nu(M) = \frac{\gamma+1}{\gamma-1} \quad \arctan \frac{\gamma-1}{\gamma+1} (M^2-1) - \arctan (M^2-1)$$
 (6)

In the close vicinity of the nozzle lips where the two families of characteristics do not intersect with each other there is a "simple region" of expansion. There the flow parameters are defined by v and  $\theta$  of each characteristic line. Further downstream the waves intersect each other. In this part of the flow parameters are defined by the two intersecting characteristics. A singularity occurs when the initial Mach number is unity and a special treatment is required to start the calculations at that point (this special treatment has not been brought here). A particular importance of the Prandtl-Meyer function is when analyzing the two dimensional flow using the hodograph plane.

#### C. THE HODOGRAPH PLANE FOR A TWO DIMENSIONAL JET

The hodograph plane is a representation of the flow parameters in the velocity plane. Figure 2 shows a hodograph plane calculated for a simple gas ( $\gamma$ =1.4). The circles represent constant Mach numbers and constant





1-2-3-4-1 defines a jet with  $M_0>1$  expanding into  $P_{amb1} < P_0$ , resulting simple repetitive expansion-compression.  $1^*-2^*-3^*-3^{**}-4^*-1^*$  defines a jet with  $M_0=1$  expanding into  $P_{amb2} << P_0$ , resulting in a highly underexpanded jet. pressure ratios  $(\frac{P}{P_T})$ . The epicycloids are the two families of characteristics. The angles  $\theta$  are the turning angles due to expansion or compression (which are both present in supersonic jets).

To define an isentropic supersonic jet on the hodograph plane it is necessary to define the Mach number at the exit plane, the pressure ratios  $(\frac{P}{P_T})$  and  $(\frac{P_{amb}}{P_T})$ , and the specific heat ratio ( $\gamma$ ) of the gas.

Investigating the shapes of the jet as a function of ranges of parameters we may get:

a. simple underexpanded jets for which  $\frac{P_{amb}}{P_{T}}$  is high enough so that

the two families of characteristics intersect each other.

b. a critical underexpanded jet for which  $\frac{P_{amb}}{P_{T}}$  is low enough so that

the intersection between the outer characteristic lines of the two familes occur on the outer hodograph circle.

c. highly underexpanded jets for which a part of characteristics do not intersect at all.

d. expansion into complete vacuum so that there are no reflections from the jet boundaries and therefore the compression region disappears.

D. THE SHAPES OF TWO DIMENSIONAL JETS

The following paragraphs further detail the different shapes.

#### 1. Simple Underexpanded Jets

Figure 3 shows the physical plane and the hodograph plane of a simple underexpanded jet. If  $l_0>1$ , an initial turn of the flow  $\theta_0$  is made within the nozzle. An aditional turn of  $\theta$  is due to the underexpansion.  $\theta$  is found by the intersection of characteristics (1-2) with the circle defined by  $P_{amb}/P_T$ .

When  $M_0>1$ , the characteristic line 1-2 is described in the physical plane by a region in which only one family of expansion waves are present (simple region, see transverse line between 1 to 2 in the physical plane). A different family of expansion waves forms a second simple region when moving between 2 to 3. At a larger distance from the exit plane, reflected waves from the free streamline (jet boundary) cause compression. An ideal representation of such a jet is a repetitive pattern of expansion and compression.

For  $M_0=1$ , the tail waves of both families are perpendicular to the flow, thus, both lie on line AB. That means that if  $N_0=1$  there is no simple region near the exit plane of the jet. The characteristic line 1-2 on the hodograph plane becomes a single point A (or B) when located in the physical plane.

#### 2. Critical Underexpanded Jets

We define a critical underexpanded jet when point (3) (see Figure 4) lies on the limiting circle  $H_{\infty}$  or  $P/P_{\infty}=0$ . This means that there is a core within the jet where the pressure approaches zero and Hach approaches infinity. This core is theoretically bounded at its upstream side by expansion waves and downstream by compression waves.



(b) Hodograph Plane

Using the theoretical expressions for isentropic ideal flow one

may derive the values of  $\frac{P_{amb}}{P_{T}}$  or  $\frac{P_{amb}}{P_{o}}$  as function of M which causes a jet

to be critical underexpanded.

Figure 5 shows results of  $\frac{P_{amb}}{P_{o}}$  as functions of M<sub>o</sub> for gases with different specific heat ratio.

#### 3. Highly Underexpanded Jets

When  $P_{amb}$  is lower than the critical values as shown in figure 4, point 3 does not exist (there is no intersection between lines 2-3 2'-3'). This means that the repetitive reversible expansion/compression shapes ceases to exist. The envelope of the jet starts at an angle defined by  $\theta$  at the nozzle exit plane and approaches an asymptotic angle defined by  $\theta_{lim}$  (see Figure 6).

In this case we get two (symmetric) groups of characteristics  $C_1-C_2$  and  $C'_1-C'_2$  (Figure 6) with no intersection between them.  $C_1$  and  $C_1'$  define the inner limit for reflected characteristics,  $C_2$  and  $C_2'$  define the outer limit. As the rest of reflected waves lie between  $C_2$  or  $C'_2$  and the jet boundary, we may conclude that a compression region may exist only in a layer along the jet boundary.

Because of irreversible effects such as shear stresses, heat transfer due to high temperature gradients, or condensation effects in real gases, the compression layer may be interpreted as the "barrel shock".



(1-2-3-4-1), (Y=1.4)



Figure 5. Dependence of critical values of  $P_{amb}/P_o$ on the Mach number at the exit plane  $(M_o)$  for different values of specific heat ratio  $(\gamma)$ .



Figure 6. The Hodograph Plane for a Highly Underexpanded Jet

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 $(\gamma = 1.4)$   $\theta_{max} - maximum turning angle$   $\theta - total turning angle in the specific jet <math>\theta > \theta_{max}/2$  $\theta_{lim} - limiting angle of compression region.$  Figure (7) shows the hodograph plane for an air jet ( $\gamma$ =1.4) expanding into an ambient pressure 105 times lower than the static pressure at the exit plane. Figure (8) is a schematic description of the jet (the data for this jet is given in Table 2). The shape shown in Figure (8) may be compared with the barrel shock photograph in page 208 Reference [3].

#### 4. EXPANSION INTO A COMPLETE VACUUM - Pamb=0

This is an extreme situation in which the maximum turn angle of streamlines occur near the nozzle exit plane. The theoretical free stream is defined only by the theoretical turning angles. All streamlines in the flow expanded monotonically towards  $P \approx 0$  without being reflected by the jet boundaries.

State	θ <b>*</b> +	θ <b>*</b>	θ	v(M)	M	μ	<del>0+</del> μ	θ <del>-</del> μ	P/P <sub>t</sub>
					I	008	00°	_00°	
	U	10	10	10	1 / 35	90   44 15	90 54 15	-36 15	0.5205
2	0	20	20	20	1.775	34.3	54.3	-14.3	.2990
4	0	40	30	30	2,135	27.93	57.93	2.07	.1810
5	0	60	40	40	2.54	23.18	63.18	16.82	.1035
6	Ő	80	50	50	3.013	19.38	69.38	30.62	.55 -1
7	Ō	100	60	60	3.595	16.15	76.15	43.85	.2672 -1
8	Ō	120	67.7	67.7	4.145	13.96	88.7	53.74	.1146 -1
9	20	135.4	0	20	1.775	34.3	34.3	-34.3	.5437 -2
10	20	20	10	30	2.135	27.93	37.93	-17.93	.1810
11	20	40	20	40	2.54	23.18	43.18	- 3.18	.135
12	20	60	30	50	3.013	19.38	49.38	10.62	.55 -1
13	20	80	40	60	3.595	16.15	56.15	23.85	.2672 -1
14	20	100	50	70	4.339	13.315	63.32	36.69	.1146 -1
15	20	120	57.7	77.7	5.085	11.34	69.04	46.4	.425 -2
16	40	135.4	0	40	2.54	23.18	23.18	-23.18	
17	40	40	10	50	3.013	19.38	29.38	- 9.38	.55 -1
18	40	60	20	60	3.595	16.15	36.15	3.85	.26/2 -1
19	40	80	30		4.339		43.32	10.09	.1146 -1
20	40	120	40	80	5.34/9	10.///	50.78	29.23	.4215 -2
	40	135.4	4/./	8/./	0.433	0.943	20.04	30.70	11/6 -1
22	60	80	10	70	3.373	10.15	23 32	-10.13	.1140 -1
1 24			20	80	4.335	1 10 777	30.78	9.22	•4215 -2
24		100	30	1 90 I	6.8190	8 433	38 43	21.57	
26	60	135.4°	37.7	97.7	9,2105	6.2330	43.93	31.5	
27	80	80	0	80	5.3479	10.777	10.777	-10.77	1
28	80	100	10	90	6.8190	8.433	18.433	1.57	
29	80	120	20	100	9.2105	6.233	26.23	13.8	
30	80	135.4	27.7	107.7	12.45	4.61	32.3	23.1	
31	100	100	0	100	9.2105	6.233	+ 6.233	- 6.233	
32	100	120	10	110	13.874	4.1331	14.13	5.9	
33	100	135.4	17.7	117.7	21.4	2.678	20.37	15.0	
34	120	120	0	120	27.335	2 097	2.097	- 2.097	
35	120	135.4	7.7	127.7	104	0.546	8.2	7.2	
36	-	-	11°	-	C10	0	-	-	0
51	20	115.4	47.7	67.7°	4.145	13.96		33.7	.5437 -2
52	40	115.4	37.7	77.7	5.085	11.34		26.36	
53	40	95.4	+27.7	67.7°	4.145	13.96		13.7	.5437 -2
54	60	75.4	÷ 7.7	67.7°	4.145	13.96	ļ	- 6.26	.5437 -2
55	60	95.4		77.7	5.085	11.34	ļ	6.4	ļ
56	60	115.4	2/./	87.7	6.433	8.943	1	1 18*8	

# TABLE 2

CALCULATION OF CHARACTERISTICS ON PHYSICAL PLANE



Figure 7. Hodograph plane showing the points on the mesh of characteristics. (Related to physical plan Figure 8).



# E. THE METHOD OF CHARACTERISTICS; COMPUTATION OF PLANAR AND AXISYMMETRIC TWO-DIMENSIONAL FLOWS

For a planar two dimensional flow, the Prandtl-Meyer function v and flow direction  $\theta$  at any point (3) in the field may be calculated using data of two other points (1) and (2) located on characteristic lines that intersect at (3) (see Fig. (9))

$$\nu_3 = \frac{1}{2} (\nu_1 + \nu_2) + \frac{1}{2} (\theta_1 - \theta_2)$$
 (7)



Figure 9. The calculation of v and  $\theta$  for point (3) is based on data for points 1 and 2.

For axisymmetric, two-dimensional flow, Liepmann and Roshko [2] developed expressions for finding the Prandtl-Meyer function ( $\nu$ ) and the flow direction ( $\theta$ ) which are given by: 
$$v_{3} = \frac{1}{2} (v_{1} + v_{2}) + \frac{1}{2} (\theta_{1} - \theta_{2}) + \frac{1}{2} [\sin \mu_{1} \frac{\sin \theta_{1}}{r_{1}} \Delta \xi_{13} + \sin \mu_{2} \frac{\sin \theta_{2}}{r_{2}} \Delta n_{23}]$$
(9)

$$\theta_{3} = \frac{1}{2} (\nu_{1} - \nu_{2}) + \frac{1}{2} (\theta_{1} + \theta_{2}) + \frac{1}{2} [\sin \mu_{1} \frac{\sin \theta_{1}}{r_{1}} \Delta \xi_{13} - \sin \mu_{2} \frac{\sin \theta_{2}}{r_{2}} \Delta \eta_{23}]$$
(10)

The angles and subscripts are shown in Figure (10).

-



Figure 10. Calculation of  $\theta$  and v for axisymmetric flow.

It is obvious that for the axially symmetric flows the increase in the radius causes the increase in the flow cross section and influences the flow direction and the Prandtl-Meyer function. These facts have been taken into account when developing the "compatibility equations" (9,10).

Using equations (9,10) we have developed a computer program which enables the calculation of the jet flow for a two dimensional and for an axially symmetric geometry (ring jet).

The listing of the program, the program description and some results are given in Appendix A.

#### III. THE BREAKDOWN OF THE CONTINUUM THEORY

#### A. GENERAL CRITERIA

As described in detail by Bird (Chapter 1 Keference [4]), the validity of the continuum approach has been identified with the validity of the Navier Stokes equations. This requires that the Knudsen number  $K_n = \lambda/L$  should be small compared with unity ( $\lambda$  is the mean free path and L is a scale length for the specific flow field). For  $K_n$  larger than a certain limit (between 0.01 to 0.1 depending on the required accuracy) a microscopic approach is necessary.

For small values of L , the microscopic approach may lead to statistical fluctuations of the results due to the small number of molecules participating in the flow processes. In figure (11) which was reproduced from Bird's book [4, figure 1.6], the regimes of rarefied flow and high fluctuations are depicted. The flow around the jet-air boundaries near a spacecraft is generally rarefied (high Knudsen number), but has insignificant fluctuations.



Figure 11. Limits for continuum approach and microscopic approach  $(d=3.7 \times 10^{-10} m)$ .
#### B. THE EMPIRICAL CRITERION

The Method of Characteristics (MOC) was used to compute the jet flow and the results obtained from the computer program "AXSYM" are valid as long as the continuum flow theory is valid.

The continuum flow requires that the mean free path should be negligibly small in comparison with the scale length of the macroscopic flow variations. The classical theory for Prandtl-Meyer expansion may therefore be expected to fail at progressively larger distances from the nozzle lips as the gas density decreases with the increasing flow angle and Mach number. The empirical criterion for the breakdown of continuum flow in steady expansion flow [4] is that

$$P \equiv \frac{q}{\rho v} \left| \frac{d\rho}{dS} \right| \simeq 0.05 \tag{11}$$

where

q = stream velocity

$$\rho = density$$

v = molecular collision frequency

 $\left|\frac{d\rho}{dS}\right|$  = absolute change in density while moving a distance dS along a streamline

Introducing the breakdown parameter P into the program, gives the aefinition of the boundary where the flow should be calculated by means of the molecular flow theory, i.e., by solving the Boltzmann equation.

For an underexpanded jet with a high initial Mach number,

the breakdown surface is nearly a streamline. Furthermore, the range of flow parameters for the present problem are such that the simple region extends to very large distances and near the nozzle lip the breakdown limit may be approximated by a straight line.

For the axisymmetric jet there is no simple region, however, for the region of interest it may be regarded as linear.

The method proposed in the present work for solving the flow behind the breakdown boundary is the Direct Simulation Monte Carlo (DSMC). For this purpose, a computer program "SIMUL" was developed. In the following chapter we describe the algorithms required for the specific problem, the geometry and the data organization. Detailed program description is given in Appendix (B).

## IV. THE MOLECULAR FLOW IN AN AXISYMMETRIC RING JET

## A. GENERAL CONSIDERATIONS

The part of the field in which the jet may be calculated by means of the continuum theory was described in Chapter II. There we calculated also the boundaries where continuum theory becomes invalid and molecular calculation should be employed. In fact, the molecular theory and the molecular Boltzmann equations are universal and hold for the entire flowfield. However, computational requirements make the Boltzmann equation impractical for the upstream flows. Therefore we limit our solution only to the part of the flow beyond the region where continuum breakdown occurs.

As a result obtained from MOC solution the "breakdown", i.e., the locus where the breakdown parameter p has values between 0.03 to 0.06, for the region close to the nozzle lips this boundary may be approximated by a straight line (for axisymmetric flow this line is the envelope of a cone, see Figure (12)).

For the specific jet and gas, the breakdown occurs in a region where the number density is in a range of  $10^{21}$  molecules/m<sup>3</sup>. For ambient gas at an altitude of 200 km the number density is  $10^{15}$  and decreases to a range of  $10^{11}$  at 1000 km. In order to be able to express this vast change in a simulation, we would need to have an extremely large number of cells which would be impossible to store in a computer. To overcome this problem we are required to make a less exact formulation which enables the production of results, having to pay the penalty of "smearing" the steep gradients and obtaining averages within layers of simulated cells. Unfortunately it is impossible to





predict how far the simulated results will be from the exact solutions. These comparisons have to be made after getting final results of this simulation.

# 1. The Direct Simulation Monte Carlo Method

The direct simulation Nonte Carlo Method is a technique for a computer modeling of a real gas by some thousands of simulated molecules. The velocity components and the coordinates of the simulated molecules are stored in the computer and are modified with time as a result of collisions and boundary interactions. A detailed description of some problems and their solutions by means of direct simulation is given in [4].

To follow the molecular motion it is necessary to divide the simulated domain into a network of cells. <u>The size of a cell must be such that the</u> <u>change in flow properties across each cell is small</u>. The time is advanced in discrete steps DTM, <u>such that DTM is small compared with the mean collision</u> <u>time per molecule</u>. If there is a flow going through the domain, DTM should be small compared with the mean time required for the mean flow to cross the cells.\* Both cell size ((DR),(DDALFA) - radial size and angular size as they appear in the program) and DTM may vary in the simulation with position and time.

Applications such as free jet expansion in which large gradients of flow properties are expected, may require a very large number of cells for the simulation. In these cases the computer memory requirements to store cells' data and molecules' data may exceed the available computer storage. A

<sup>\*</sup>If DTM is chosen to be very small compared with the mean time between collisions then the simulation will require a very large number of runs such that the number of collisions will be sufficient. If DTM is large the molecules are washed out by the mean flux and there is no time for the collisions to influence the flow.

solution for this problem is to divide the simulation space into smaller regions and to run the simulation for each region separately. If there is an interaction between different regions, which apriori is undefined, the solution should be found iteratively. (That means that each run will provide data for consecutive runs and the procedure should be repeated until the results converge to a steady solution.

The computation of a representative set of collisions based on mean collision time per molecule is invalid for a computerized simulation because of the large computer time and computer memory requirements. Instead, the method proposed by Derzko which is described in details by Bird [4] may be employed. Following this method, an averaged mean time between collisions of species L with species M for a cell is calculated. The number of collisions of each type (L.M species) is such that the collision time counters are kept concurrent with the overall time parameter. The L.M collision time for a cell containing N<sub>L</sub> and N<sub>M</sub> molecules with collision cross section  $\sigma_{LM}$ , number densities n<sub>L</sub> and n<sub>M</sub> and relative velocity C<sub>r</sub>, is given by

$$\Delta t_{c} = \frac{LP}{N_{L}} \frac{1}{\sigma_{LM} n_{M} C_{r}} + \frac{MP}{N_{M}} \frac{1}{\sigma_{LM} n_{L} C_{r}}$$
(12)

where LP and MP are the probabilities that the collision will be effective for the L and H molecules respectively. B. THE GEOMETRY OF THE SIMULATED DOMAIN, SECTORS, REGIONS AND CELLS

Figure (13) shows a cross section of the simulated domain for the axisymmetric (ring) flow. Points A and A' are the nozzle lips. Starting at "A" and assuming the "breakdown" boundary to be a straight line, we obtain the cross section of the molecular domain as a sector defined by LAM. The solid wall is defined by AL. The arc LM may be assumed to be far enough so that the pressure along it may be assumed to equal the ambient pressure. Molecules originated in the jet cross the breakdown boundary with a velocity, direction, temperature (and other thermodynamic properties) as found from the continuum solution.

The molecular domain LAM is divided into secondary sectors, and each of these are divided into several radial regions making the "simulation regions".

Because we have no apriori information on how the expansion occurs, the angle of each sector (which mainly is in the direction of the expansion gradients) is left to be a result of the internal calculation.

Each region is divided into NRD radial divisions and NAD angular divisions making a network of NAD\*NRD simulation cells. The angle DALFA of all regions in a sector is constant. Taking NAD constant for all regions in a sector, we get the angle of a cell DDALFA constant. Defining the radial size of a cell DR as constant we get a cell cross section area proportional to the radius R measured from the nozzle lip (point A).



Figure 13. Cross section of the simulation domain, definition of sectors, regions, cells and coordinates.

The size of a cell: In order to get accurate simulated results it is recommended to define the size of a cell (DR and R\*DDALFA) small compared with the mean free path of the molecules  $\lambda$  (typical DR= $\lambda/3$ ). However, as we do not expect to get large changes in flow parameters along the radius we may allow DR be much larger than  $\lambda/3$ . The angular size of the largest cell in a sector should comply with this requirement, but because of the computer limitation it is set to be equal to  $5*\lambda$ . This will be the basis for defining DALFA for each sector.

C. INITIAL NUMBER OF MOLECULES IN CELLS

A "reasonable" number of molecules in a simulation is several thousands (a larger number, which is better, may be used for simple problems or when using a single user computer with large user memory space). The initial setting of molecules in cells is usually based on a guess of the number density in the specific cell. (The number of molecules in cells will change during the simulation according to the input/output calculated fluxes to the specific region).

The number density and the size of a cell are specified only in three dimensional flows. When applied to a two dimensional flow the simulation may be regarded as applying to an arbitrary thin slice of the real flow. In the axisymmetric flow we define the width of a cell by the angle DFI as shown in Figure (14), constant within a region.

The initial number density in cells of a given region is set constant. Defining the total number of simulated molecules in the region the number of molecules in each specific cell becomes a function of DFI. For example, assume that we limit the number of molecules in the smallest cell in the region to 15 then:



Figure 14. Variation of the angle DFI.

To maintain the number of simulated molecules within computational limits, the 'width' of each region defined by DFI is such that: MIN = number of molecules in smallest cell in a region MIN = VOLUME (smallest cell) \* number density = f(R, ALFA, DALFA) \* DFI \* number density for flux calculations DFI is a weighting factor.

# DFI\*(contant) \* (number density) = 15

Other cells contain the initial number of molecules proportional to their volumes.

D. DEFINITION OF INPUT AND OUTPUT FLOWS FOR A REGION

The cross sections of all regions (except those regions near the nozzle lips) are quadrilateral. Through the sides of the region molecules are allowed to enter or to leave according with the boundary conditions or as a result of molecular velocity. For the first sector, near the breakdown boundary the input flow (FWP1 and FWP2 see Figure (15)) is defined by the results from the continuum flow. FEN1, FNN1, FSN1, etc. are results of counting and averaging the outgoing molecules (the different vector names will be explained in Appendix B).

For the neighbor regions these output fluxes become inputs and have to be adjusted according to the differences in the angle DF1 of the different regions.

The simulation starts with regions in the sector near the breakdown boundary. At this time there is no data for input flows through faces E and N of the cell. An additional run of the whole program is required in order to take these calculated flows into account. If the accuracy of the results is important we may run this type of iteration several times until the results become stable. (Only after running the program for the whole domain once we shall be able to evaluate the importance of these iterations.)



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Figure 15. Definition of input and output flows of species 1 to a region (KR) in a sector (KS).

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(For species 2 the flux names will change as follows:
    instead FWN1( ) + FWN2( )
    instead FOW1( ) + FOW2( )
    etc.
```

## E. COLLISIONLESS FLOW

In several sectors near the breakdown boundary we may find a high number density and the mean free path small compared with the size of a cell. There the calculated collisions are expected to have an influence on the flow parameters. For wider expansion angles the collisions become rare mainly because of the decrease in the density. In the ambient gas the mean free path (for 200 km altitude) is 240 m. Comparing this number with the size of the simulated domain may lead to the conclusion that there the flow may be regarded as collisionless.

We may define a limiting line in the flow where the collisions become insignificant. Consequently, molecules crossing this limit will in fact continue moving in straight lines; a part of them reach the solid wall.

Introducing this idea of the collisionless flow we may reduce the computation time and the memory requirements.

F. TWO DIMENSIONAL PLANAR FLOW VS. AXISYMMETRIC FLOW

The cell dimensions are completely specified only in three dimensional flow. When applied to two dimensional flow, the simulation may be regarded as applying to an arbitrarily thin slice of the real flow. The thickness of the slice may be chosen such that the number of simulated molecules complies with the cell volume and the physical number density. For the axisymmetric flow we have defined the angle DFI as the third coordinate so that the volume of the cell is completely specified.

Once the geometry is defined, the simulation may be accomplished and there is no difference if doing it for two dimensional or for axisymmetric flows.

#### APPENDIX A - THE AXSYM PROGRAM

#### A.1 DIFFERENT REGIONS IN THE JET

For the two dimensional jet with initial Mach number greater than unity the different regions are shown in Figure (16).



Figure 16. The three regions in an underexpanded jet.

For planar 2-D flow region 1 is a uniform flow core, region 2 is a simple region in which only one family of characteristics define the flow, and region 3 which contains the intersection of the two families of characteristics. Because our intention is to find solutions for highly underexpanded jets with very low ambient pressure, the calculation of further downstream flow is not necessary.

For the axisymmetric ring jet, we use the same definition for the different regions however, in this case none of the three regions has uniform flow and is not a simple region. As shown in Equations (9,10) the PM function (v) and the flow direction ( $\theta$ ) of a point at location I,j may be calculated from the v and  $\theta$  of two upstream points (I-1,j) and (I,j-1). Later, from the PM function at the new point we may derive the local Mach number, the local pressure, temperature, velocity and other thermodynamic parameters as required.

Definition of the mesh of points for the different regions is shown in Figure (17).

#### A.2 PROGRAM FLOWCHART

A simplified flowchart for the NOC program is shown in Figure (18). The program is designed to solve both axisymmetric as well as two dimensional flow

for kD = 2 it solves two dimensional flow

for kD = 3 it solves axisymmetric flow (This is also the default condition)

Initial data such as Mach number and pressure at the exit surface, ambient pressure and jet gas parameters are input data.

Output data contains the following for each mesh point: Mach number, coordinates of mesh point (R,X), flow direction (TETA), pressure, temperature, local velocity, Knudsen number based on the distance between two points along a streamline, mean free path and breakdown parameter as defined by Bird.\*

For each of the three regions, we start with precalculated boundary conditions enabling the calculation of the Hach angles, coordinates of mesh points and distances  $d\xi$  and  $d\eta$  as described in [2].

\*For the exit plane instead the Bird's breakdown parameter, we calculate the ratio between time per three collisions and time of motion. Sometimes this ratio may be regarded as a measure of the breakdown of the continuum theory.



Figure 17. Indexing of mesh points for the different regions in the 'AXSYM' program.



Figure 18. AXSYM Program Flowchart

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The number of characteristics used in the program is arbitrary and depends on the required resolution (it may affect also the accuracy of the results and the amount of computation). We start with 20 characteristics along the exit cross section and with 50 characteristics in the Prandtl-Meyer fan thus a total of 70 characteristics of each family are calculated. In region 1 there are 20 left running and 20 right running characteristics. In region 2 there are 20 right running and 50 left running characteristics. In region 3 there are 50 left running and 50 right running characteristics.

In region 3 we limit the calculation where the two characteristics defining a new mesh point intersect at an angle smaller than the computational accuracy. In fact this occurs far downstream where continuum theory becomes invalid.

After defining the mesh geometry (successively) we calculate the Prandtl-Meyer function and flow direction, using equations (9,10).

The local Mach number is an implicit function of the Pradtl-Neyer angle. It is calculated by iterations with an initial guess of local Mach number set equal to a precalculated Mach number at an adjacent point, and the slope of the function as given by Equation (5). Figure (19) shows the iterative procedure for evaluating the Mach number at each mesh point.





Once the local Mach number has been found all other flow parameters may be defined using the Equation (1,2,3).



Figure 20. The mesh of characteristics in Region 2 and Region 3 Axisymmetric ring jet.  $M_0 = 4$ . Altitude=200km.





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A.3 PROGRAM 'AXSYN' LISTING	
\$J0B	AXS00010
C PROGRAM AXSYM	AXS00020
C THIS PROGRAM CALCULATES THE ISENTROPIC EXPANSION OF A JET BY MEANS OF	AXS00040
C THE METHOD OF CHARACTERISTICS.	AXS00050 AXS00060
C FOR AN AXISYMMETRIC RING JET 'KD' SHOULD BE SET EQUAL TO 3	AXS00070
	AXSOOO80
DIMENSION TETA(20,50), AM(20,50), R(20,50), X(20,50), PM(20,50)	AXS00100
DIMENSION AMCOR(20,20),TETAC(20,20),XC(20,20),RC(20,20),PMC(20,20)	AXS00110 AXS00120
DIMENSION AMX(50,50),TETAX(50,50),XX(50,50),RX(50,50),PMX(50,50)	AXS00130
C C TETA TS THE FLOW ANGLE (PADTANS) MEASURED FROM Y AVIS	AXS09140 AXS00150
C AM IS THE MACH NUMBER	AXS00160
C R IS THE RADIUS (NORMAL TO THE WALL)	AXS00170 Axs00180
C PM IS THE PRANDTL MEYER FUNCTION	AXS00190
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX	AXS00200 AXS00210
PAMB = 8.4736E-5	AXS00220
KD = 3 C FOR TWO DIMENSIONAL FLOW KD=2 .FOR AXISYMMETRICAL FLOW KD=3	AXSUU23U AXS00240
Cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx	AXS00250
C CONSTANTS	AXSUU26U AXSU0270
PI = 3.141593	AXS00280
BOLTZ = 1.38032E-23 AVOG = 6.0225F+26	AXS00290 AXS00300
RG = 8314.3	AXS00310
C EXIT SURFACE Amo = 4.00	AXS00320
TO = 300.0	AXS00340
P0 = 136.0 C	AXS00360
R1 = 2.5	AXS00370
XI = 0.5	AXS00390
C GAS DATA	AXS00400
DIAM = 2.95E-10	AXS00420
GM = 17.0	AXS00430
CXS = PIXDIAMXDIAM	AXS00450
GMM = GM/AVOG	AXS00460
Č MESH DEFINITION	AXS00480
C NI=CHARACTERISTICS FROM THE EXIT PLANE C N2=CHARACTERISTICS FROM THE CORNERS	AXS00490 AXS00500
N1 = 20	AX500510
N2 = 50 C	AXS00520 AXS00530
C CONSTANTS FOR THE ISENTROPIC EXPANSION	AXS00540
Al = (GAMA-1.U)/GAMA Bl = 1.0/Al	AXS00550
	AXS00570
A2 = DSQRI((GAMA+1.))(GAMA-1.)) B2 = 1.0/A2	AXS00580
	AXS00600
AJ - (UAFIA-1.7/2. C	AXS00620
$C \qquad C = MACH \times MACH \times A3 + 1.$	AXS00630
	AXS00650
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX	AXS00660
Č DEFINE STAGNATION PARAMETERS	AXS00680
	AXS00690
C = (1.0+A3*AM0*AM0)	AXS00710
C PRESSURE	AXS00720

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PN = CXXB1	AXS00730
PSTG = POXPN	AXS00740
TSTG = TOXC	AXS00750
C DENSITY	AXS00770
D0 = P0/(RJXT0)	AXS00780
- DSIG = PSIG/(KJ*ISIG)	AX500790 AX500800
ČXXXXXXXXXXXX	AXS00810
WRITE(6,1)PSTG,TSTG,DSTG,DIAM,GM	AXS00820
I FORMAT('0','STAGNATION PRESSURE*',E12.5,' TEMPERATURE*',E1 1! DENSITY=!.E12.5.! MOL DIAM=!.E12.5.! MOL MASS=!.E10.5)	J.5,AX500830 Aysoo840
WRITE (6,2)PO,TO,DO,AMO	AX300850
2 FORMAT('0', 'EXIT PLANE PRESSURE=', E12.5, ' TEMPERATURE=', F1	D.5,AXS00860
1' DENSITY=',El2.5,' MACH=',Fl0.5)	AXS00870
	EXXXAXSO0890
Č	AXS00900
C DEFINE FREE STREAM PARAMETERS AT THE RIGHT CORNER	AXS00910
	AX500920 07900224444
C MACH NUMBER	AXS00940
FSM = DSQRT(((PSTG/PAMB)**A1-1.)/A3)	AXS00950
C TEMPERATURE	AXS00960
C DENSITY	AX500970 AX500980
FSD = PAMB/(RJ*FST)	AXS00990
C MACH ANGLES FOR HEAD AND TAIL OF FAN	AXS01000
AMII = DARSIN(I./AMU) AMIH = DARSIN(I./ESM)	AX501010 AX501020
C PRANDTL MEYER FUNCTION FOR HEAD AND TAIL OF FAN	AXS01030
D1 = DSQRT(AMO*AMO-1.)	AXS01040
D2 =DSQRT(FSM×FSM-1.)	AXS01050
PMT = A2×DATAN(B2×D2)-DATAN(D2) PMT = A2×DATAN(B2×D1)-DATAN(D1)	AXS01060 AXS01070
C EXTERNAL TURNING ANGLE (FREE STREAM ANGLE)=EXTA	AXS01080
EXTA = PMH - PMT	AXS01090
C PRANDIL MEYER FAN ANGLE PMFA DMEA = FYTA - AMTH + AMTT	AXS01100 AXS01110
	AXS01120
CXXXXXXXXXXXX	AXS01130
C WRITE(6,3)PAMB,FST,FSD,FSM	AXSO1140
C 1' DENSITY='.El2.5.' MACH='.Fl0.5///)	AXS01150
Cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx	EXXXAXS01170
C*************************************	KXXXAXSO1180
C DEFINE THE MESH OF CHARACTERISTICS-AND FLOW PARAMETERS	AX501190 AX501200
	AXS01210
	KXXXAXS01220
C THE CURNER PUINT - LEFT RUNNING CHAR. C PMEA IS DEVIDED INTO N2 (=50) NONEQUAL DIVISIONS	AXSU1230 AXS01260
	AXS01250
RAT = (FSM/AM0-1)/0.02	AXS01260
RAT2 = FLOAT(N2-1) Fl - DLOG(PAT)(DLOG(PAT2)	AXS01270
	AXS01280
WRITE(6,4)	AXS01300
4 FORMAT('1', 'PRANDTL MEYER FAN LINE MACH	AXS01310
DO 20 N=2.N2	AXSU1520 AXS01330
EN2 = FLOAT(N-2)	AXS01340
EN1 = FLOAT(N-1)	AXS01350
AMD - AMUX(1,7,UZX(ENZ)XXE1) AMF = AMOX(1,+,O2X(EN1)XXE1)	AXSU1360 AXS01370
DELM = AMF-AMB	AXS01380
AM(1,N) = AMF	AXS01390
DI =DSQKI(AM(I,N)#AM(I,N)=1.) PM(1.N) = A2*DATAN(B2*D1)=DATAN(D1)	AXS01400
AMI = DARSIN(1./AM(1,N))	AXS01420
TETA(1,N) = PI/2 (PM(1,N) - PMT)	AXS01430
C TETA IS THE FLOW ANGLE ON THE CHARACTERISTICS AT THE CORNER	AXS01440

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```
R(1,N) = R1
                                                                  AXS01450
     X(1,N) = X1
ALFAL = TETA(1,N)+AMI
                                                                  AXS01460
                                                                  AXS01470
C ALFAL IS THE ANGLE OF THE LEFT RUNNING CHARACTERISTICS
                                                                  AXS01480
                                                                  AXS01490
C PRESSURE,
          TEMPERATURE AND DENSITY VARIATION AT THE CORNER
                                                                  AXS01500
     C = AM(1, N) \times AM(1, N) \times A3+1.
                                                                  AXS01510
     PRES = PSTG/(C**B1)
TEMP = TSTG/C
                                                                  AXS01520
                                                                  AXS01530
     DENSF(1,N) = PRES/(RJXTEMP)
                                                                  AXS01540
                                                                  AXS01550
CXXXXXXXXX
                                                                  AXS01560
   WRITE (6,5) N,AM(1,N),PM(1,N),TETA(1,N)
5 FORMAT(' ',' ','
                                                                  AXS01570
                                        ,115,3E20.5)
                                                                  AXS01580
CXXXXXXXX
                                                                  AXS01590
  20 CONTINUE
                                                                  AXS01600
                                                                  AXS01610
AXSD1630
WRITE(6,10)
                                                                  AXS01650
  10 FORMAT('0','
                             MACH
                                                         TETA
                                                                  AXS01660
                   I
                                        ₽
                                                  X
                       VELOCITY
                                    KNUDSËN
                                               MFP
    1TEMP
              PRESS
                                                        ND
                                                                  AXS01670
        P1)
                                                                  AXS01680
    1
С
                                                                  AXS01690
C
                                                                  AXS01700
AXS01730
С
 DEFINE THE PARAMETERS AT THE EXIT SURFACE (PLANE)
                                                                  AXS01740
                                                                  AXS01750
DO 25 J = 1,N1
Amcor(1,J) = Amo
                                                                  AXS01770
                                                                  AXS01780
     D = DSQRT(AM0 \times AM0 - 1.)
                                                                  AXS01790
  PMC(1,J) = A2 \times DATAN(B2 \times D) - DATAN(D)
25 TETAC(1,J) = PI/2.
                                                                  AXS01800
                                                                  AXS01810
                                                                  AXS01820
C THE EXIT PLANE IS DIVIDED INTO (N1-1) DIVISIONS (N1 POINTS)
                                                                  AXS01830
     DO 30 J=1,20
                                                                  AXS01840
     SOUND = DSQRT(GAMA*RJ*T0)
                                                                  AXS01850
     VELO = AMCOR(1,J)*SOUND
DNO = PO/(BOLTZ*TO)
                                                                  AXS01860
                                                                  AXS01870
     FP0 = .707/(DN0 \times CXS)
                                                                  AXS01880
     DX = X1 \times 2.7 FLOAT(N1)
                                                                  AXS01890
     AKNO = FPO/DX
                                                                  AXS01900
C
                                                                  AXS01910
     XC(1,J) = X1*(1.-FLOAT(J-1)/FLOAT(N1-1)*2.)
CENTR = DABS(XC(1,J))
                                                                  AXS01920
                                                                  AXS01930
     IF(CENTR.LT.0.001) \times C(1,J) = 0.
                                                                  AXS01940
     RC(1,J) = R1
                                                                  AXS01950
С
                                                                  AXS01960
c.
                                                                   AXS01970
С
     KZ=1**************
                                                                  AXS01980
IF (J.GT.1) GO TO 29
C AT THE EXIT PLANE THE BREAKDOWN PARAMETER IS EVALUATED BY MEANS OF
C THE RATIO OF THE COLLISION TIME AND THE FLOW TIME. LENGTH SCALE IS
                                                                  AXS01990
                                                                  AXS02000
                                                                  AXS02010
 THE MESH DIMENSION.
                                                                  AXS02020
     SCALE = DX*DTAN(DARSIN(1./AMO))/2.
                                                                  AXS02030
     TIME1 = SCALE/VELO
TIME2 = 3./(4.*CXS*DNO*DSQRT(BOLTZ*T0/(PI*GMM)))
                                                                  AXS02040
                                                                  AXS02050
     P =TIME2/TIME1
                                                                  AXS02060
     DENSF(1,1) = DO
                                                                  AXS02070
   29 CONTINUE
                                                                  AXS02080
С
                                                                  AXS02090
     WRITE(6,11)1, J, AMCOR(1, J), R1, XC(1, J), TETAC(1, J), T0, P0, VEL0, AKNO, FPAXS02100
    10, DNO, P
                                                                  AXS02110
  11 FORMAT(' ',214,5F10.3,3E12.3,F9.4,2E12.3)
                                                                  AXS02120
                                                                  AXS02130
   30 CONTINUE
C
                                                                  AXS02140
```

⋒⋬**୷⋎⋏⋺**⋎⋳⋤⋎⋎⋏⋤⋎⋎⋏⋤⋎⋎⋏⋤⋎⋎⋵⋤⋎⋎⋵⋤⋎⋎⋵⋤⋎⋎⋵⋤⋎⋽⋶⋤⋎⋶⋶⋤⋎⋽⋵⋤⋎⋏⋵⋤⋎⋎⋵⋤⋎⋏⋵⋤⋎⋏⋵⋤⋎⋎⋵⋤⋎⋶⋤⋎⋎⋵⋤⋎⋶∊⋎⋵⋤⋎⋶⋳∊⋎⋵

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AXS02170
С
 CALCULATE THE FLOW PARAMETERS IN THE CORE BOUNDED BY THE TWO MACH
Waves starting at the nozzle lips (corner points)
at the exit the flow is assumed to be uniform
                                                                                        AXS02180
AXS02190
C
C
C
C
                                                                                        AXS02200
                                                                                        AXS02210
                                                                                       XAXS02220
WRITE (6,198)
198 FORMAT('1','
                                                                                        AXS02230
                                                                                        AXS02240
                         CORE
                                  1/1
                                                                                        AXS02250
       APM=0.
                                                                                        AXS02260
       BPM=0.
       CPM=0.
                                                                                        AXS02270
                                                                                        AXS02280
C
                                                                                        AXS02290
       DO 199 I = 2,N1
      WRITE (6,10)
DO 199 J = 1,N1
IF ((I+J-1).GT.N1) GO TO 199
                                                                                        AXS02300
                                                                                        AXS02310
                                                                                        AXS02320
                                                                                        AXS02330
       AMIL = DARSIN(1./AMCOR(I-1,J))
       ALFAL = PI-(TETAC(I-1,J)+AMIL)
                                                                                        AXS02340
С
                                                                                        AXS02350
       AMIR = DARSIN(1./AMCOR(I-1,J+1))
                                                                                        AX902360
       ALFAR = TETAC(I-1,J+1)-AMIR
                                                                                        AXS02370
                                                                                        AXS02380
C
       XC(I,J) = (RC(I-1,J)-RC(I-1,J+1)+XC(I-1,J)*DTAN(ALFAL)+XC(I-1,J+1)AXS02390
      1×DTAN(ALFAR))/(DTAN(ALFAL)+DTAN(ALFAR))
                                                                                        AXS02400
       CENTR = DABS(XC(I,J))
IF (CENTR.LT.0.001) XC(I,J) = 0.
                                                                                        AX502410
                                                                                        AXS02420
       RC(I,J) = RC(I-1,J+1)+(XC(I,J)-XC(I-1,J+1))*DTAN(ALFAR)
                                                                                        AXS02430
С
                                                                                        AXS02440
       DKSI = DSQRT((XC(I,J)-XC(I-1,J+1))**2+(RC(I,J)-RC(I-1,J+1))**2)
DETA = DSQRT((XC(I,J)-XC(I-1,J))**2+(RC(I,J)-RC(I-1,J))**2)
                                                                                        AXS02450
                                                                                        AXS02460
С
                                                                                        AXS02470
                                                                                        AXS02480
  CALCULATE NOW THE PRANDTL MEYER FUNCTION AND FLOW ANGLE IN CORE.
                                                                                        AXS02490
       APM = PMC(I-1,J)+PMC(I-1,J+1)+TETAC(I-1,J+1)-TETAC(I-1,J)
                                                                                        AXS02500
                                                                                        AXS02510
       IF (KD.EQ.2) GO TO 151
       BPM = DSIN(AMIR)*DSIN(TETAC(I-1,J+1))/RC(I-1,J+1)*DKSI
CPM = DSIN(AMIL)*DSIN(TETAC(I-1,J))/RC(I-1,J)*DETA
                                                                                        AXS02520
                                                                                        AXS02530
  151 PMC(I,J) = (APM+BPM+CPM)/2.0
                                                                                        AXS02540
C
                                                                                        AXS02550
       APM = PMC(I-1,J+1)-PMC(I-1,J)+TETAC(I-1,J+1)+TETAC(I-1,J)
                                                                                        AXS02560
       TETAC(I,J) = (APM+BPM-CPM)/2.0
                                                                                        AXS02570
                                                                                        AXS02580
  DEFINE MACH NUMBER (BY ITERATIONS)
                                                                                        AXS02590
  INITIAL GUESS AMCOR(I, J)=AMCOR(I-1, J+1)
                                                                                        AXS02600
                                                                                        AXS02610
                                                                                        AXS02620
       AMG = AMCOR(I-1, J+1)
       KZ = 0
                                                                                        AXS02630
  154 IF (KZ.GE.100) GO TO 160
KZ = KZ+1
                                                                                        AXS02640
                                                                                        AXS02650
       C = AMG \times AMG \times A3 + 1
                                                                                        AXS02660
       D = DSQRT(AMG*AMG-1.)
PMCAL = A2*DATAN(B2*D)-DATAN(D)
                                                                                        AXS02670
                                                                                        AXS02680
       DELNI = PMCAL - PMC(I,J)
                                                                                        AXS02690
       DEL = DABS(DELNI)
IF (DEL.LT..000002) GO TO 160
IF (DELNI.LT.0.) GO TO 156
                                                                                        AXS02700
                                                                                        AXS02710
                                                                                        AXS02720
       AMG = AMG*.999
GO TO 154
                                                                                        AXS02730
                                                                                        AXS02740
      AMG = AMG*(1.-DELNI*C/D)
  156
                                                                                        AXS02750
  GO TO 154
160 AMCOR(I,J) = AMG
                                                                                        AXS02760
                                                                                        AXS02770
С......
                                                                                        AXS02780
                                                                                        AXS02790
C CALCULATE FLOW PARAMETERS
                                                                                        AXS02800
       IF (J.GT.1) GO TO 197
                                                                                        AXS02810
       C = AMCOR(I,J)*AMCOR(I,J)*A3+1.
PRES = PSTG/(C**B1)
                                                                                        AXS02820
                                                                                        AXS02830
       TEMP = TSTG/C
                                                                                        AXS02840
             = PRES/(BOLTZ*TEMP)
= .707/(DN*CXS)
       DH
                                                                                        AXS02850
                                                                                        AXS02860
       FP
       SCALE = DKSI × DSIN(ALFAL)
                                                                                        AXS02870
       AKN = FP/SCALE
                                                                                        AXS02880
```

6.8

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SOUND = DSQRT(GAMA×RJ×TEMP)
                                                               AXS02890
                                                               AX502900
     VEL = SOUNDXAMCOR(I,J)
                                                               AXS02910
 BREAKDOWN PARAMETER AS DEFINED BY 'BIRD'.
DENSF(I,J) = PRES/(RJ*TEMP)
                                                               AXS02920
                                                               AXS02930
     DDENS = DENSF(I-1,J) - DENSF(I,J)
COLF = 4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM))
                                                               AXS02940
     COLF = 4.*CXS*DN*DSWRItBULL
P = VEL*DDENS/(SCALE*DENSF(I,J)*COLF)
                                                               AXS02950
                                                               AXS02960
 197 CONTINUE
                                                               AXS02970
С
                                                               AXS02980
С
     TIME1 = SCALE/VEL
                                                               AXS02990
     TIME2 = 3./(4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM)))
Ĉ
                                                               AXS03000
Ĉ
      = TIME2/TIME1
                                                               AXS03010
WRITE(6,11)I, J, AMCOR(I, J), RC(I, J), XC(I, J), TETAC(I, J), TEMP, PRES, VELAXS03050
    1, AKN, FP, DN, P
                                                               AXS03060
                                                               AXS03070
 199 CONTINUE
C
                                                               AXS03080
C MATCH CORE AND FAN POINTS
                                                               AXS03110
     DO 200 I=1,N1
X(I,1) =XC(I,1)
                                                               AXS03120
                                                               AXS03130
     R(I,1) = RC(I,1)
                                                               AXS03140
     AM(I,1) = AMCOR(I,1)
                                                               AXS03150
     PM(I,1) = PMC(I,1)
                                                               AXS03160
 200 \text{ TETA(I,1)} = \text{TETAC(I,1)}
                                                               AXS03170
                                                               AXS03180
AXS03210
 CALCULATE FLOW PARAMETERS IN REGION 2 (SIMPLE PRANDTL MEYER FAN).
                                                                AXS03220
C
                                                                AXS03230
WRITE (6,298)
298 FORMAT ('1','
                                                                AXS03250
                     REGION
                              21/)
                                                                AXS03260
C
                                                               AXS03270
                                                                AXS03280
     KFIN = 51
С
                                                                AXS03290
     DO 299 I = 2,N1
                                                                AXS03300
     WRITE(6,10)
D0 299 J = 2,N2
IF (J.GT.KFIN) G0 T0 299
                                                                AXS03310
                                                                AXS03320
                                                                AXS03330
     \mathbf{k}\mathbf{z} = \mathbf{0}
                                                                AXS03340
     AMIL =DARSIN(1./AM(I-1,J))
                                                                AXS03350
     AMIR = DARSIN(1./AM(I,J-1))
                                                                AXS03360
     ALFAL = PI-(TETA(I-1,J)+AMIL)
                                                                AXS03370
     ALFAR = TETA(I, J-1) - AMIR
                                                                AXS03380
                                                                AXS03390
 CHECK ANGLES AND CALCULATE COORDINATES
Angle1 = PI/2.-.000001
                                                                AXS03400
                                                                AXS03410
     ANGLE2 = PI/2.+.000001
                                                                AXS03420
     IF (ALFAL.LE.ANGLE1.OR.ALFAL.GE.ANGLE2) GO TO 201
                                                                AXS03430
     X(I,J) = X(I-1,J)
                                                               AXS03440
 GO TO 207
201 IF (ALFAR.LE.ANGLE1.OR.ALFAR.GE.ANGLE2) GO TO 205
                                                               AXS03450
                                                               AXS03460
     X(I,J) = X(I,J-1)
                                                               AXS03470
     GO TO 207
                                                                AXS03680
С
                                                                AXS03490
  205 X(I,J) = (R(I~1,J)-R(I,J-1)+X(I,J-1)*DTAN(ALFAR)+X(I-1,J)*DTAN(ALFAXS03500
    1AL))/(DTAN(ALFAL)+DTAN(ALFAR))
                                                               AXS03510
С
                                                               AXS03520
  207 IF (ALFAL.LE.0.000001.GR.ALFAL.GE.0.000001) GO TO 209
                                                               AXS03530
     R(I,J) = R(I-1,J)
                                                               AXS03540
 GO TO 213
209 IF (ALFAR.LE.0.000001.OR.ALFAR.GE.0.000001) GO TO 211
R(I,J) = R(I,J-1)
GO TO 213
                                                               AXS03550
                                                               AXS03560
                                                               AXS03570
                                                               AXS03580
                                                               AXS03590
 211 R(I,J) = (X(I,J)-X(I,J-1)) \times DTAN(ALFAR)+R(I,J-1)
                                                               AXS03600
```

```
213 DKSI = DSQRT((R(I,J)-R(I,J-1))**2+(X(I,J)-X(I,J-1))**2)
DETA = DSQRT((R(I,J)-R(I-1,J))**2+(X(I,J)-X(I-1,J))**2)
                                                                              AXS03610
                                                                              AXS03620
С
                                                                              AXS03630
      IF (R(I,J).GT.0..AND.X(I,J).GT.0.) GO TO 219
                                                                              AXS03640
      KFIN = J-1
                                                                              AXS03650
      WRITE(6,12)
                                                                              AXS03660
   12 FORMAT(
               , FURTHER POINTS ON THE CHARACTERISTICS ARE DIVERGENT )AX503670
  219 CONTINUE
                                                                              AXS03680
 LOCATION OF THE NEW MESH POINT HAS BEEN FOUND
                                                                              AXS03690
č
                                                                              AXS03700
С
                                                                              AX$03710
Ĉ
 CALCULATE NOW PRANDTL MEYER FUNCTION AND FLOW DIRECTION FOR NEW POINT AXS03720
      APM = PM(I,J-1)+PM(I-1,J)-TETA(I-1,J)+TETA(I,J-1)
IF (KD.EQ.2) GO TO 251
                                                                              AXS03730
                                                                              AXS03740
      BPM = DSIN(AMIR)*DSIN(TETA(I,J-1))/R(I,J-1)*DKSI
                                                                              AXS03750
      CPM = DSIN(AMIL)*DSIN(TETA(I-1,J))/R(I-1,J)*DETA
                                                                              AXS03760
  251 PM(I,J) = .5 \times (APM+BPM+CPM)
                                                                              AXS03770
С
                                                                              AXS03780
      APM = PM(I,J-1)-PM(I-1,J)+TETA(I,J-1)+TETA(I-1,J)
                                                                              AXS03790
      TETA(I,J) = .5 \times (APM+BPM-CPM)
                                                                              AXS03800
                                                                              AXS03810
 CALCULATE NOW MACH NUMBER FOR EACH POINT
INITIAL GUESS AM(I,J) = AM(I-1,J)
AMG = AM(I-1,J)
                                                                              AXS03820
                                                                              AXS03830
                                                                              AXS03840
      KZ = 0
                                                                              AXS03850
  254 IF (AMG.GT.200.) GO TO 257
                                                                              AX$03860
      D = DSQRT(AMG \times AMG - 1.)
                                                                              AXS03870
      GO TO 258
                                                                              AXS03880
  257
      D = AMG
                                                                              AXS03890
  258 IF (KZ.GE.100) GO TO 260
                                                                              AXS03900
      KZ = KZ + 1
PMCAL = A2*DATAN(B2*D)-DATAN(D)
                                                                              AXS03910
                                                                              AXS03920
      DELNI = PMCAL - PM(I,J)
DEL = DABS(DELNI)
                                                                              AXS03930
                                                                              AXS03940
      IF (DEL.LT..000002) GO TO 260
IF (DELNI.LT.0.)GO TO 256
                                                                              AXS03950
                                                                              AXS03960
      AMG = AMG \times .999
                                                                              AXS03970
      GO TO 254
                                                                              AXS03980
256 IF (AMG.LT.2000.)GO TO 2560
                                                                              AXS04000
      KFIN = J-1
                                                                              AXS04010
      GO TO 299
                                                                              AXS04020
2560 D1 = (A3*AMG*AMG+1.)
                                                                              AXS04040
      AMG = AMG*(1.-DELNI*D1/D)
                                                                              AXS04050
      GO TO 254
                                                                              AXS04060
С
                                                                              AXS04070
  260 \text{ AM(I,J)} = \text{AMG}
                                                                              AXS04080
C CALCULATE NOW LOCAL TEMPERATURE, PRESSURE, VELOCITY, KNUDSEN NO.
                                                                              AXS04090
      C = AM(I,J)*AM(I,J)*A3+1
PRES = PSTG/(C**B1)
TEMP = TSTG/C
                                                                              AXS04100
                                                                              AXS04110
                                                                              AXS04120
      DN = PRES/(BOLTZ*TEMP)
                                                                              AXS04130
      DENSF(I,J) = PRES/(RJ*TEMP)
                                                                              AXS04140
      DDENS = DENSF(I-1,J-1)-DENSF(I,J)
                                                                              AXS04150
      SCALE = DSQRT((X(I,J)-X(I-1,J-1))**2+(R(I,J)-R(I-1,J-1))**2)
                                                                              AXS04160
AXS04170
С
                                                                              AXS04180
  271 FP = .707/(DN*CXS)
                                                                              AXS04190
С
                                                                              AXS04200
      AKN = FP/SCALE
                                                                              AXS04210
      SOUND = DSQRT(GAMA*RJ*TEMP)
                                                                              AXS04220
      VEL = AM(I,J)*SOUND
                                                                              AXS04230
C
C
                                                                              AXS04240
                                                                              AXS04250
      COLF = 4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM))
                                                                              AXS04260
        = VEL*DDENS/(SCALE*DENSF(I,J)*COLF)
                                                                              AXS04270
                                                                              AXS04280
 PRINT RESULTS FOR MESH POINTS
                                                                              AXS04290
      KL = (-1) \times I
IF (KL.LT.0)
                                                                              AXS04300
         (KL.LT.0) GO TO 299
                                                                              AXS04310
      WRITE(6,11)I, J, AM(I, J), R(I, J), X(I, J), TETA(I, J), TEMP, PRES, VEL, AKN, AXS04320
```

v

. . .

```
1FP, DN, P
                                                                AXS04330
  299 CONTINUE
                                                                AXS04340
С
                                                                AXS04350
AXS04380
Ć
 MATCH 'REGION 2' AND 'REGION 3' POINTS
                                                                AXS04390
                                                                AXS04400
C
L = KFIN - 1
                                                                AX504420
     DO \ 300 \ J =
              1,1
                                                                AXS04430
     XX(1,J)
               = X(20,J)
                                                                AXS04440
     RX(1,J)
               = R(20, J)
                                                                AXS04450
               = AM(20,J)
= PM(20,J)
                                                                AXS04460
     AMX(1,J)
     PMX(1,J)
                                                                AXS04470
  300 TETAX(1, J)
              = TETA(20, J)
                                                                AYS04480
AXS04510
 CACULATE FLOW PARAMETERS FOR REGION 3
                                                                AXS04520
C
                                                                AXS04530
WRITE (6,397)
397 FORMAT ('1','
D0 399 I = 2,L
                                                                AXS04550
                            31/)
                                                                AXS04560
                   REGION
                                                                AXS04570
     DO 399 J = I,L
IF (J.GT.KFIN) GO TO 399
                                                                AXS04580
                                                                AXS04590
     IF (J.GT.I)GO TO 320
                                                                AXS04600
     WRITE (6,10)
                                                                AXS04610
  320 KZ = 0
                                                                AXS04620
C
                                                                AXS04630
     AMIL = DARSIN(1./AMX(I-1,J))
ALFAL = PI-(TETAX(I-1,J)+AMIL)
                                                                AXS04640
                                                                AXS04650
     IF (J.GT.I) GO TO 301
                                                                AXS04660
     ALFAR = ALFAL
                                                                AXS04670
     TETAX(I,J) = PIX.5
                                                                AXS04680
     TETAX(I, J-1) = PI-TETAX(I-1, J)
                                                                AXS04690
     XX(I,J) = 0.
RX(I,J) = RX(I-1,J)+XX(I-1,J)*DTAN(ALFAL)
                                                                AXS04700
                                                                AXS04710
     RX(I,J-1) = RX(I-1,J)
                                                                AXS04720
     XX(I,J-1) = -XX(I-1,J)
                                                                AXS04730
     DKSI = (RX(I,J)-RX(I-1,J))/DSIN(ALFAL)
                                                                AXS04740
     DETA = DKSI
                                                                AXS04750
     PMX(I,J-1) = PMX(I-1,J)
GO TO 316
                                                                AXS04760
                                                                AXS04770
  301 AMIR = DARSIN(1./AMX(I,J-1))
                                                                AXS04780
     ALFAR = TETAX(I, J-1) - AMIR
                                                                AXS04790
С
                                                                AXS04800
     IF (ALFAL.LE.ANGLE1.OR.ALFAL.GE.ANGLE2) GO TO 302
                                                                AXS04810
     XX(I,J) = XX(I-1,J)
                                                                AXS04820
     GO TO 307
                                                                AXS04830
  302 IF(ALFAR.LE.ANGLE1.OR.ALFAR.GE.ANGLE2) GO TO 305
                                                                AXS04840
     XX(I,J) = XX(I,J-1)
                                                                AXS04850
     GO TO 307
                                                                AXS04860
  305 XX(I,J) = (RX(I-1,J)-RX(I,J-1)+XX(I,J-1)*DTAN(ALFAR)+XX(I-1,J)*DTAAXS04870
     1N(ALFAL))/(DTAN(ALFAL)+DTAN(ALFAR))
                                                                AXS04880
С
                                                                AXS04890
  307 IF (ALFAL.LE.0.000001.OR.ALFAL.GE.0.000001) GO TO 309
                                                                AXS04900
     RX(I,J) = RX(I-1,J)
                                                                AXS04910
     GO TO 315
                                                                AXS04920
  309 IF (ALFAR.LE.0.000001.OR.ALFAR.GE.0.000001) GO TO 311
                                                                AXS04930
     RX(I,J) = RX(I,J-1)
                                                                AXS04940
     GO TO 315
                                                                AXS04950
  311 RX(I,J) = RX(I,J-1)+(XX(I,J)-XX(I,J-1))*DTAN(ALFAR)
                                                                AXS04960
С
                                                                AXS04970
  315
     DKSI = DSQRT((RX(I,J)-RX(I,J-1))**2+(XX(I,J)-XX(I,J-1))**2)
                                                                AXS04980
.
     DETA = DSQRT((RX(I,J)~RX(I-1,J))**2+(XX(I,J)~XX(I-1,J))**2)
                                                                AXS04990
  316 CONTINUE
                                                                AXS05000
С
                                                                AXS05010
     IF (RX(I,J).GE.0..AND.XX(I,J).GE.0.)GO TO 319
                                                                AXS05020
     KFIN = J-1
                                                                AXS05030
     WRITE (6,398)
                                                                AXS05040
```

```
398 FORMAT ( ' ', 'FURTHER POINTS ON THE CHARACTERISTICS ARE DIVERGENT')AXS05050
С
                                                                               AXS05060
  LOCATION OF THE NEW POINT HAS BEEN FOUND
                                                                               AXS05070
C
AXS05080
                                                                               AXS05090
C
  CALCULATE NOW P.M. ANGLE AND FLOW DIRECTION

319 APM = PMX(I,J-1)+PMX(I-1,J)-TETAX(I-1,J)+TETAX(I,J-1)

IF(KD.EQ.2) GO TO 351
                                                                               AXS05100
C
                                                                               AXS05110
                                                                               AXS05120
      BPM = DSIN(AMIR)*DSIN(TETAX(I,J-1))/RX(I,J-1)*DKSI
                                                                               AXS05130
      CPM = DSIN(AMIL)*DSIN(TETAX(I-1,J))/RX(I-1,J)*DETA
                                                                               AXS05140
  351 PMX(I,J) = .5*(APM+BPM+CPM)
                                                                               AXS05150
      APM = PMX(I,J-1)-PMX(I-1,J)+TETAX(I,J-1)+TETAX(I-1,J)
TETAX(I,J) = .5*(APM+BPM+CPM)
                                                                               AXS05160
                                                                               AXS05170
                                                                               AXS05180
  CALCULATE NOW THE MACH NUMBER FOR EACH POINT INITIAL GUESS AMX(I,J) = AMX(I-1,J)
                                                                               AXS05190
                                                                               AXS05200
      AMG = AMX(I-1,J)
                                                                               AXS05210
      KZ = 0
                                                                               AXS05220
      KH=0
                                                                               AX$05230
       KL = 0
                                                                               AXS05240
  354 IF (AMG.GT.2000.) GO TO 357
                                                                               AXS05250
       D = DSQRT(AMG \times AMG - 1.)
                                                                               AXS05260
      GO TO 358
                                                                               AXS05270
  357
      D = AMG
                                                                               AXS05280
  357 D = AMG

358 IF (KZ.GE.50)GO TO 360

KZ = KZ +1

PMCAL = A2×DATAN(B2×D)-DATAN(D)

DELNI = PMCAL-PMX(I,J)
                                                                               AXS05290
                                                                               AXS05300
                                                                               AXS05310
                                                                               AXS05320
       DEL = DABS(DELNI)
                                                                               AXS05330
      IF (DEL.LT..000002) GO TO 360
IF (DELNI.LT.0.)GO TO 356
                                                                               AXS05340
                                                                               AXS05350
      AMG = AMG \times .98
                                                                               AXS05360
      GO TO 354
IF (AMG.LT.5000.) GO TO 3560
                                                                               AXS05370
  356
                                                                               AXS05380
      KFIN = J-1
                                                                               AX$05390
 GO TO 399
3560 D1 = A3*AMG*AMG+1.
                                                                               AXS05400
                                                                               AXS05410
C*******************************
                                                                               AXS05420
      DDELNI = DELNI
                                                                               AXS05430
       IF (AMG.GT.20.) DDELNI = DELNI*(.95**KZ)
                                                                               AXS05440
AXS05450
      AMG = AMG*(1.-DDELNI*D1/D)
GO TO 354
                                                                               AXS05460
                                                                               AXS05470
                                                                               AXS05480
  360 \text{ AMX(I,J)} = \text{AMG}
C
                                                                               AXS05490
C CALCULATE NOW THE LOCAL TEMPERATURE, PRESSURE, VELOCITY, KNUDSEN

C = AMX(I,J) * AMX(I,J) * A3+1.
                                                                               AXS05500
                                                                               AXS05510
      PRES = PSTG/(C**B1)
TEMP = TSTG/C
                                                                               AXS05520
                                                                               AXS05530
      DN = PRES/(BOLTZ*TEMP)
                                                                               AXS05540
AXS05550
      DENSF(I,J)=PRES/(RJ*TEMP)
DDENS=DENSF(I-1,J-1)-DENSF(I,J)
                                                                               AXS05560
                                                                               AXS05570
      FP = .707/(DN \times CXS)
                                                                               AXS05580
      SCALE=DSQRT((XX(I,J)-XX(I-1,J-1))**2+(RX(I,J)-RX(I-1,J-1))**2)
                                                                               AXS05590
      AKN=FP/SCALE
                                                                               AXS05600
С
                                                                               AXS05610
Ĉ
                                                                               AXS05620
AXS05630
                                                                               AXS05640
                                                                               AXS05650
                                                                               AXS05660
                                                                               AXS05670
                                                                               AXS05680
      SCALE=BF*(RX(I,J-1)-DTAN(ALFALL)*(XX(I,J-1)-XX(I-1,J))-RX(I-1,J)) AXS05690
      SCALE = DABS(SCALE)
                                                                               AXS05700
CXXXXX
                                      *****
                                                                               AXS05710
      ********
      SOUND = DSQRT(GAMA*RJ*TEMP)
                                                                               AXS05720
      VEL = AMX(1,J)*SOUND
                                                                               AXS05730
С
                                                                               AXS05740
      COLF=4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM))
                                                                               AXS05750
      P=VEL*DDENS/(SCALE*DENSF(I,J)*COLF)
                                                                               AXS05760
```

```
C
C PRINT RESULTS
WRITE(6, 11)I,J,AMX(I,J),RX(I,J),XX(I,J),TETAX(I,J),TEMP,PRES,VEL,AXS05780
1AKN,FP,DN,P
399 CONTINUE
STOP
END
END
$ENTRY
```

j,

1

1.15. 1.1.1

Parameter	T			
Name	Physical Name	Units	Туре	Description
PAMB	ambient pressure	pascals	real	ambient atmosphere
				pressure
KD	K dimensions	-	integer	KD=2 for two dimen-
				sional jet
ĺ				KD=3 for axisymmetric
	l			ring jet
PI	π	-	real	
l			constant	
BOLTZ	Boltzmann constant	Joule	real	1.38032 10-23
		degree		joules/degree
AVOG	Avogadro's constant	molecules	real	6.0225 x 10 <sup>26</sup>
	1	mol		1/kmo1
RG	Universal gas	Joule	real	8314.3
	constant	mol.deg		
AMO	Mach No. (E.P)	-	real	Mach number at exit
<b>T</b>				plane
TO	Temperature (E.P)	°k	real	Temperature at exist
-				plane
PO	Pressure (E.P)	pascals	real	Pressure at exit
-				plane
Rl	Cylinder radius	m	real	Radius of the
Ì				cylindrical vehicle
X1	0.5* nozzle width	m	real	Half width of nozzle
GAMA		-	real	averaged heat
				capacity ratio (jet)
DIAM	Molecule diameter	m	real	averaged molecular
				diameter (jet)
GM	Molecular mass	kg/kmol	real	averaged molecular
ĺ				weight (jet)
RJ	Gas constant	joules	real	gas constant (jet)
		kj.deg		
CXS		m <sup>2</sup>	real	collision cross
				section (hard sphere)
GMM	mass of a molecule	kg	real	averaged mass of a
Ì		Ŭ		molecule
N1	· · · · · · · · · · · · · · · · · · ·		integer	number of divisions
	1		_	(characteristics from
				the exist plane)
N2	· · · · · · · · · · · · · · · · · · ·		integer	number of character-
	ĺ		_	istics in the Prandtl
İ				Meyer fan
Al		1	real	γ - 1
	İ			
B1		1	real	Y
	İ			$\frac{1}{y-1}$

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Parameter	Physical Name	   Unite		Description
	Thysical name		real	$\frac{1}{(x+1)/(x-1)}$
 	• <u> </u>		real	1/A2
<u>A3</u>	·		real	x - 1
				2
C			real	$\frac{M^2}{2} \frac{\gamma - 1}{2} + 1$
D, D1, D2			real	$11^2 - 1$
PSTG		pascals	real	stagnation pressure
TSTG		°k	real	stagnation tempera- ture
DSTG		kg/m <sup>3</sup>	real	stagnation density
FSM			real	free stream Mach number
FST		°k	real	free stream tempera- ture
FSD		kg/m <sup>3</sup>	real	free stream density
AMIT	μ <sub>T</sub>	radius	real	Mach angle (tail of P.M. fan)
AMIH	μΗ	radius	real	Mach angle (head of P.M. fan)
PMT	<u>ਆ</u>	radius	real	P.M. function (tail)
PIH	<u></u>	radius	real	P.M. function (head)
RAT, RAT2,			real	used to define a
E1				loparithmic division
				of the corner char-
		;	]	acteristics (50 lines
				in P.H. fan)(a linear
			i	division would have
	j –	i	İ	resulted in concen-
		1	ĺ	tration of character-
		Ì		istics at high Nach
				numbers)
DELM			real	difference of Mach
			L	numbers
AM(I,J)	11		real 2-D	Mach number at
	1	1	array	location (I,j)(used
				for the corner)
PM(I,J)	V	radius	l	P.H. function at
				location (I,j)(used
			Ļ	for the corner)
AIII	μ	radius	real	lach angle
K(1,J)		i m	real 2-D   array	radius (or ordinate)     at (I i)
TETA(I.I)	Α	radius	real 2-11	flow direction at
1010(190)		Laurus	array	(T i)

# A.4 LIST OF MAIN SYMBOLS USED IN 'AXSYM' (CONTINUED)

				······································
Parameter	Physical News	Undto		
	Physical Name	Units	Type	Description
ALFAL		radians	lear	ning characteristics
ALFAR		radians	real	angle of a right run-
				ning characteristics
DENSF(I,J)		$k_{\sigma}/m^3$	real 2-D	gas density at point
		8	array	IJ
AMCOR(I,J)			real 2-D	llach number at mesh
			array	points in region (1)
				(region 1 is bounded
				by the two tail
				characteristics
TETAC(I,J)		radians	real 2-D	flow direction at
			array	mesh points (region
			L	1)
PMC(I,J)		radians	real 2-D	P.M. function at mesh
			array	points (region 1)
XC(I,J)		п	real 2-D	X coordinate at mesh
			array	points (region 1)
RC(I,J)		n	real 2-D	radius (ordinate) at
			array	mesh points (region
				1)
AMIL		radians	real	Mach angle far left
			ł	running character-
				istics
AIIR		radians	real	Mach angle far right
				running character-
DUCT				istics
DKSI	αξ	m	real	distance between mesh
D11/11 4				points
DETA	an	m	real	distance between mesh
DELNIT				
AMC		radians	real	P.M. differential
AIIG		radians	1	itemating sales
				iterative calcula-
DDEC			+	
TEMP			1	temperature
DN				pumber density
FP FP				mean free path
AKN				Knudsen number
SOUND	<u>.                                    </u>		<u> </u>	speed of sound
VEL			<u>+</u>	absolute local
				velocity
DDENS			<u> </u>	density difference
			i	between two points a-
				long a steamline
COLF				collision frequency
μ	<u></u>		<del> </del>	herealtdarm namenatan

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E

# A.4 LIST OF MAIN SYMBOLS USED IN 'AXSYM' (CONTINUED)

Press and the

A.5 AXSYM PROGRAM USER'S GUIDE

1. Input data:

2.

ambient pressure	PANB
Mach number (Exit plane)	AMO
Temperature (Exit plane)	то
Pressure (Exit plane)	РО
Half width of nozzle	X1
Radius of nozzle ring	K1
Specific heat ratio of jet gas	GALIA
average molecular diameter (jet)	DIAM
average molecular weight	Gì1
Options for flow geometry	
two dimensional flow	KD=2
ring jet	KD=3
default condition	KD=3

3. Resolution of mesh points

to change the resolution of the mesh points

- a change N1 and N2 as necessary
- b change 'DIMENSIONS' according to new values of  $\rm \ N_1$  and  $\rm \ N2$
- c define distribution of Mach lines in the Prandtl-Meyer fan as required (program lines 126-131)
- 4. Execution commands:

After copying program into USER'S FILE:

# WATFIV AXSYM \* (XTYPE

The program will run on user's terminal under WATFIV. A soft copy of program listing and output listing will be stored in user's disk named AXSY11 LISTING.

5. Hard Copy

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PRINT AXSYM LISTING.

6. Program Outputs.

All necessary outputs are automatically listed by the program. Figure (20) and Figure (21) show the resulting mesh of characteristics calculated for an altitude of 200 km for MO=4 and MO=2 respectively.

In these figures we also show some isotherms and the limit where the breakdown parameter equals 0.05. These lines are plotted (manually) using interpolation procedures. Data along the breakdown line is input data for the molecular flow.

# APPENDIX B SIMUL PROGRAM

# **B.1** DATA ORGANIZATION

Because of the large number of molecules, cells, regions and sectors in the simulation and the large number of data related to each molecule, each cell and region to be stored, special precautions should be taken in order not to overflow the available computer memory.

The following data organization was used in SIMUL. Figure 22 shows the geometry of one sector.


N N



cell volume =  $v(I) = R(I) * DDALFA \times DR \times RSI * DFI.$ 

$$\frac{\mathbf{v}(\mathbf{I})}{\mathbf{v}(1)} = \frac{\mathbf{R}(\mathbf{I}) \cdot \mathbf{RSI}(\mathbf{I})}{\mathbf{R}(1) \cdot \mathbf{RSI}}$$

v(1) is the volume of smallest cell in a region.

1. Tables of Molecules and Their Parameters

P1(L,N1M) -	Light	molecules	of	the	jet
-------------	-------	-----------	----	-----	-----

P2(L,N2M) - Heavy molecules of the jet

P3(L,N3M) - Ambient gas molecules (not used in the present program)

N1M, N2M, N3M - maximum number of molecules in simulation. Number of active molecules may be smaller or equal to (N<I>11).

L=1,2,3 - cartesian components of velocity  $v_x$ ,  $v_y$ ,  $v_z$  [m/s]

L=4 - radial coordinate [meters]

if r=-99 the particular molecule is inactive

L=5 - angular coordinate [radians].

This table is generated each time the simulation is initiated for a region. That means, the same group of molecules (as stored in the computer memory) is used to simulate the flow in all regions in the computation domain.

C(M,I,j) Tal	ble of Cells (in a Region)-Real Data
I = 1,10 ·	- radial index of the cell in a region
j = 1,10 ·	- angular index of the cell in a region
M = 19	- radial coordinate of cell center
M = 20	- angular coordinate of cell center
M = 1,9	- time parameter for collisions of different species in a
	cell
M = 10-18	- maximum relative velocity expected for collisions of
	different species in a cell

2.

3. IP(N1A+N2A+N3A) Table of the addresses of the active molecules arranged in order of their species and in the order of their cells IC(N,I,j) - table of cells (in a region) integer data I = 1,10 - radial index j = 1,10 - angular index N = 1 - number of molecules (spec 1) N = 2 - number of molecules (spec 2) N = 3 - number of molecules (spec 3) N = 4 - (starting address - 1) of molecules as ordered in (IP).

4.	Reg(N,kR,kS)	) ]	Data table for a specific region (real)
	kR = 1,10 ·	-	index of a region in a sector
	kS = 1,20 -	-	index of the sector
	N = 1 -	-	Dfl = differential angle (axisymmetric)
			DFl is a weighting factor
	N = 2 -	-	DN1 = number density (species 1)
	N = 3 -	-	DN2 = number density (species l)
	N = 4 -	-	VOL 1 = actual volume of smallest cell in kR
	N = 5 -	-	AREAL INPUT area of smallest cell in kR

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# 5. Region Geometry and Input Flux

(spec 1), (spec 2)

6.

## Input Flux From High Pressure Starting Line

FWP1(N,I,j) FWP2(N,I,j) \*\*\*\* species positive (input molecules) west flux I = 1,10 - number of the cell along the starting line in a region (j) j = 1,10 - number of the region along the starting line N = 1 - molecular flow for a given DF1 N = 2- mean molecular velocity Vx mean molecular velocity Vy N = 3 -N = 4 - mean input gas temperature 7. Output Flux FNN1(4,NAD,kR) FSN1(4,NAD,kR) FNN2(4,NAD,kR) FSN2(4,NAD,kR) \*\* 11 negative (output) negative (output) north south kR - number of region in the sector NAD - angular location The first index include the same parameters as (FWP1) FEN1(4,NRD) FWN1(4,NRD) FWN2(4,NRD) FEN2(4,NRD) †† \*\* negative negative east west

NRD + radial location

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FEN1, FEN2, FWN1, FWN2 are necessary for iterations within one sector.

8. Sampling of Output Flux from a Sector

After averaging they are transferred to FOE1, FOE2, FOW1, FOW2. FOW1(4,kC,kR,kS) output flow to the west FOW2(4,kC,kR,kS) FOE1(4,kC,kR,kS) output flow to the east FOE2(4,kC,kR,kS) kC - radial location (cell) of flow in a region kR - index of a region in a sector kS - index of the sector The first index (4 parameters) include the same parameters as FEP1( ).

# **B.2 MOLECULAR SIMULATION FOR A GIVEN REGION**

After we define the geometry of the whole sector resulting from the region geometry and cell geometry, we may start with the molecular simulation. This includes:

- initial setting of molecules in cells
- molecules are moved according to the time increment DTH
- new molecules are generated according to input (or output) flows
- collisions calculations

- integration of flow parameters for average parameters calculations
- repetition of the whole procedure as long as necessary to obtain reasonable statistical averaging
- calculate averages and flow weighting.

These routines are the core of the program and must be repeated for all regions in a sector and (or all sectors in the domain where the collisions are significant).

In the following sections we bring a detailed description of this part of the program.

- 1. Initial Setting of Molecules in Cells
  - a. The initial number of available molecules in a simulation is larger than the number of active molecules (Pl(data, number of molecules), P2(data, number of molecules) are the vectors used for species 1 and 2)
  - b. an inactive molecule is defined as

[P1(4,N) or P2(4,N)] = -99

c. calculation of number of molecules to be set in each cell

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d. calculation of cell coordinates

- e. deactivation of all available molecules in simulation
- f. definition of molecules coordinates

P1(4,N), P2(4,M) are polar radiuses

Pl(5,N), P2(5,M) are angular coordinate in radians

All molecules in a cell are set at random locations within the cell.

g. definition of molecular velocities

Pl(1,N), P2(1,M) velocity in X direction

P1(2,N), P2(2,M) velocity in Y direction

Pl(3,N), P2(3,M) velocity in Z direction

Thermal velocities are random function of temperatures and are added to the mean velocity as defined at initial boundary  $ALFA_0$  of the region.

As the thermal velocity has a Boltzmann distribution the thermal velocity setting is based on rejection-acceptance methods (for more details see Bird [4] Appendix D).

h. reset collision timers and relative velocity

i. reset general time counter: Time = 0

### 3. The Simulation

a. Move all molecules according to their velocity  $({\tt V}_{\tt X}, {\tt V}_{\tt y})$  and find their new coordinates

Note - A routine designed to calculate the collisions with the wall was included in the program; if the region (or sector) is bounded by the solid wall, the collision is calculated - resulting new velocities and directions and counted for wall flux calculations. If the program is stopped at an angle where the flow becomes collisionless, this routine becomes irrelevant and other type of calculations should be designed.

b. Output flow counting: all molecules that leave the region are counted and stored in specific vectors which are used as inputs to other regions. The output vectors are (X represent 1 or 2 for the two species in the program (FSNX)) FSNX(1,j,kR) → "south" boundary FNNX(1,j,kR) → "north" boundary FENX(1,I) → "east" boundary FENX(1,I) → "east" boundary FMNX(1,I) → "west" boundary I represents the radial location index of the cell j represents the angular location index kR is the index of the region within a sector Note - all molecules that move to

(j=NAD+1)(I=NRD+1) are placed in FENX(1,NRD) (j= -1)(X=NRD+1) are placed in FWNX(1,NRD) (j=NAD+1)(I= -1) are placed in FSNX(1,1,kR) (j= -1)(I= -1) are placed in FWNX(1,1,kR)

This was done only for simplification reasons.

c. Generation of new molecules due to input flows. Through the four sides E,N,W,S, of a region, molecules are allowed to enter the region according with the flows coming from the neighbouring regions:

for "W" side of the region in sector 1

FWPX(P, I, kR)

for other sectors

for "E" side of any region

for "N" side of any region

for "S" side of the region

FOWX(P,I,kR,kS+1)

FOEX(P,I,kR,kS-1)

FSNX(P,j,kR+1)

FNNX(P,j,kR-1)

The first parameter of all these arrays represent:

P = 1 - number flux (real number)

 $P = 2 - velocity component - (V_x)$ 

 $P = 3 - velocity component - (V_v)$ 

P = 4 - gas temperature

Note 1 - because every region has a different size of angle DFI, all fluxes have to be adjusted accordingly.

Note 2 - input fluxes are calculated, adjusted and stored as real numbers. The number of input molecules are by definition integers. In order not to "loose" molecules, the number of input molecules is increased by 1 on a random basis. (The average of many runs will result in the accurate average input flow.)

New molecules are set at random locations on the boundary of the specific cells and at random time within DTM. Then each molecule is allowed to enter the region according to its initial coordinate and velocity. At the end of the time interval the new location and velocity is stored in molecule array Pl or P2. If DTM is chosen to be too large and cell size is small (total region size too small) some molecules may cross the region and will not be counted in the simulation of the specific region. In order not to "loose" molecules:

- (a) DTM should be decreased
- (b) count these molecules as output fluxes from the specific region. (This is recommended only if there is no other choice.)

Note - Because the arrays of input flows store only averaged data for the molecules, the thermal velocity of each new molecule is calculated according to the Boltzmann distribution as a function of the averaged temperature.

d. Rearrangement of molecules in cells. Before collisions are calculated all simulated molecules which have been let to move and generated have to be rearranged and recounted for each cell.

(I,j)
k = 1 - is the number of molecules of species 1
k = 2 - is the number of molecules of species 2
k = 3 - is the number of molecules of species 3 (not used)
k = 4 - is the (address-1) of the first molecule in the cell
related to the vector IP(M)

The array IC(k,I,j) contains integer data for each cell

Vector IP(M) contains the list of the simulated molecules arranged in the order of species in cells and cells respectively. The following is a graphic description of IP(M)



Figure 23. Vector IP(M)

B.3 SIMUL Program Flowchart

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A simplified flowchart for the Monte Carlo simulation of the molecular flow is shown in Figure 24. The program is designed to solve the ring axisymmetric jet flow, however, minor changes may be done to enable a different geometry.





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**B.4** SIMUL Program Listing PROGRAM SIMUL SIM00010 THIS PROGRAM SIMUL THIS PROGRAM IS DESIGNED TO CALCULATE THE MOLECULAR FLOW OUTSIDE THE SIM00020 CONTINUUM REGION FLOW OF A HIGHLY UNDEREXPANDED AXISYMMETRIC RING JET.SIM00030 RESULTS FOR THE CONTINUUM FLOW MAY BE OBTAINED FROM 'AXSYM' PROGRAM SIM00040 WHICH GIVES THE 'METHOD OF CHARACTERISTICS' ISENTROPIC SOLUTION. SIM00050 THE BOUNDARY BETWEEN THE CONTINUUM AND MOLECULAR FLOW IS DEFINED BY THE BREAKDOWN PARAMETER 'P' AS PROPOSED BY G. A. BIRD. SIM00070 THE 'MOLECULAR DOMAIN' IS DIVIDED INTO POLAP DIVISIONS MAKING A SET THE MOLECULAR DOMAIN' IS DIVIDED INTO POLAR DIVISIONS MAKING A SET OF SECTORS. EACH SECTOR IS SUDIVIDED INTO 10 REGIONS NO APRIORY INFORMATION ABOUT THE GEOMETRY OF THE DIFFERENT SIM00080 SIM00090 SIM00100 REGIONS IS AVAILABLE, THEREFORE, MANUAL INTERVENTION MAY BE REQUIRED WHEN MOVING FROM ONE SECTOR TO THE OTHER. AN ACCEPTABLE GEOMETRY WILL RESULT A REASONABLE NUMBER OF SIMULATED MOLECULES. SIM00110 SIM00120 SIM00130 EACH REGION IS SUBDIVIDED INTO A NUMBER OF CELLS WITH A GEOMETRY DEFINED BY A POLAR MESH. A NUMBER OF MOLECULES IS SET IN EACH CELL PROPORTIONAL TO THE CELL VOLUME. THE BOUNDARY CONDITIONS FOR EACH REGION REQUIRE INPUT AND OUTPUT FLUX OF MOLECULES. NO APRIORY SIM00140 SIM00150 SIM00160 SIM00170 SIM00180 INFORMATION ON THE FLUX IS AVAILABLE. IT WILL BE CALCULATED IN AN ITERATIVE MODE SIM00190 IF THE BOUNDARY CONDITIONS FOR ALL CELLS ARE CONSTANT THE NUMBER Flux into each cell is proportional to cell wall area. To decrease the error when introducing molecules -(integer number)-SIM00200 SIM00210 SIM00220 DUE TO THE INPUT FLUX -(REAL NUMBER), AN ADDITIONAL MOLECULE IS GENERATED ON THE BASIS OF RANDOM NUMBERS SUCH THAT THE AVERAGE OF A LARGE NUMBER OF SAMPLINGS WILL EQUAL THE REAL INPUT FLUX. SIM00230 SIM00240 STM00250 \* SIM00260 THE MONTE CARLO SIMULATION THE JET GAS IS COMPOSED OF TWO SPECIES OF MOLECULES AMBIENT GAS IS REGARDED AS ONE SPECIES THE MOLECULAR MODEL IS - 'HARD SPHERE MOLECULE' SIM00270 SIM00280 SIM00290 SIM00300 NETWORK DEFINITION SIM00310 С THE MAXIMUM RADIUS (POLAR) OF THE DOMAIN IS ASSUMED TO BE RP=15 M. SIM00320 THE ANGLE OF THE BOUNDARY BETWEEN CONTINUUM AND MOLECULAR FLOW AND THE SOLID WALL IS SIM00330 000 SIM00340 ALFA (CALCULATED IN PROGRAM 'AXSYM') SIM00350 DEFINE A POLAR SECTOR WITH A RADIUS 'RP' AND AN ANGLE OF DALFA =5\*MFP\*NAD/RP CCCCCC SIM00360 SIM00370 THIS SECTOR IS SUBDIVIDED INTO A NUMBER OF RADIAL DIVISIONS SIM00380 MAKING 'N' REGIONS FOR SIMULATION CALCULATIONS FOR EACH 'DALFA'. Each region is devided into SIM00390 SIM00400 NAD -ANGULAR DIVISIONS (15) WITH AN ANGLE OF DDALFA=5\*MFP/RP SIM00410 -RADIAL DIVISIONS (10) MAKING NAD\*NRD CELLS NRD -RADIAL C C C C STM00420 SIM00430 THE SMALLEST CELL CONTAINS 'MIN' MOLECULES SIM00440 MIN = 15 TOTAL NUMBER OF ACTIVE MOLECULES IN A REGION IS LIMITED TO 6000 (3000 MOLECULES OF EACH SPECIES.) С STM00450 SIM00460 SIM00470 THE WIDTH OF A CELL DEFINED BY ANGLE 'DFI' MAY NOW BE EVALUATED. (MIN/NUMBER DENSITY = ACTUAL CELL VOLUME) C STM00480 SIM00490 \*\*\*\*\*\*\*\* STM00500 DEFINE PARAMETERS..... BLOCK 1SIM00510 COMMON IX SIM0052**0** SIM00530 DIMENSION P1(5,3000),P2(5,3000),IP(6000),C(20,10,15), \*IC(4,10,15),REG(5,10,20) SIM00540 С DIMENSION DFI(10), DN(10) SIM00550 DIMENSION R(10), A(10), VOL(10), M1(10), F1(10), F2(10) SIM00560 DIMENSION SS(2,10,10) SIM00570 DIMENSION FENI(4,10),FWN1(4,10),FNN1(4,15,10),FSN1(4,15,10) SIM00580 DIMENSION FEN2(4,10), FWN2(4,10), FNN2(4,15,10), FSN2(4,15,10) SIM00590 DIMENSION FWP1(4,10,10), FWP2(4,10,10) DIMENSION FOE1(4,10,10,20), FOW1(4,10,10,20) STMDDADD SIM00610 DIMENSION FOE2(4,10,10,20),FOW2(4,10,10,20) STM0.0620 DIMENSION NM(3), VRC(3), TOC(3,3), SPEC(3,5), NCOL(10,15) P1, P2, P3 CONTAIN INFORMATION ON UP TO M SIMULATED MOLECULES SIM00630 SIM00640 P1(1,N),P1(2,N),P1(3,N) ARE U,V,W VELOCITY COMPONENTS (CARTESIAN) STM00650 P1(4,N),P1(5,N) ARE R AND TETA COORDINATES (POLAR) SIM00660 SIM00670 IP(M) ARE THE M MOLECULES ARRANGED IN THE ORDER OF THEIR CELLS SIM00680 C(20, I, J) CONTAINS INFORMATION ON UP TO IXJ CELLS SIM00690 SIM00700 SIM00710 ALFA IS THE ANGLE WHERE THE BREAKDOWN PARAMETER EQUALS .05 SIM00720

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	PO = 101325.	SIM007
	$T_0 = 273.$	SIM008
	AVDG = 2.68699E+25	SIM008
	RG = 8314.	SIMOO8
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		51M008.
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	NIM = 15	STM009
	$N^{2}M = 15$	STM009
	NUMBER OF DIVISIONS IN A SIMULATED REGION	SIMOOS
	NAD = 15	SIMOOS
	NRDS=10	SIM009
	NRD=10	SIM009
	NRDI= 3	SIM010
	NIS =2	SIM010
	R1 IS THE RADIUS OF THE CYLINDER (WALL)	SIM010
	R(I) IS THE RADIAL COORDINATE OF CELL(I)	SIM010
	VOL(I) IS THE RATIO BETWEEN VOLUMES OF CELL(I) AND CELL(1)	SIM010
	A(I) IS THE RATIO BETWEEN INPUT FLOW AREAS OF CELL(I) AND CELL(I)	SIM010
	DR IS THE RADIAL SIZE OF A CELL (RADIAL INCREMENT)	SIM010
	INPUT_THE FOLLOWING AS 'DATA' OR 'READ' STATEMENTS ************************************	SIM010
	TETA = 1.2	SIMO10
	TETA IS THE FLOW DIRECTION (RADIANS) ON THE BREAKDOWN LINE AS FOUND	SIMOIO
	FROM THE AXSYM PROGRAM. VU IS THE FLOW VELOCITY (M/SEC)	SIMUII
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		STMOIL
	SET DATA FOR THE DIFFERENT SPECIES	SIMOII
	MOLECIII AR MASS	STMOIL
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	SPEC(2,1)=40./AV0G	SIM012
	SPEC(3,1)=29./AVOG	SIMOIZ
	MOLECULAR DIAMETER	SIM012
	SPEC(1,2)=2.19E-10	SIM012
	SPEC(2,2)=4.00E-10	SIM012
	SPEC(3,2)=	SIMOIZ
	SPEC(1,3)=	SIM012
	<u>SPEC(2,3)</u> = ADDITIONAL DATA IF REQUIRED	SIM012
	SPEC(3,3)=	SIM012
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	FOW1(KPAR, I, JR, JS) = 0.	SIMOLA

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DD 2001 J=1,10 FHP1(2,1,J)=V0X FHP2(2,1,J)=V0X FHP2(2,1,J)=V0Y FHP2(3,1,J)=V0Y FHP2(3,1,J)=V0Y FHP2(4,1,J)=TEMP SIM01630 Z001 FHP2(4,1,J)=TEMP SIM01640 Z001 FHP2(4,1,J)=TEMP SIM01650 Z005 CONTINUE C C C C C C C C C C C C C
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FMP1(3, f, J)=V0Y         SIM01620           FMP2(3, f, J)=V0Y         SIM01630           FMP2(3, f, J)=TEMP         SIM01640           2001 FMP2(4, f, J)=TEMP         SIM01660           C         SIM01670           C         SIM01670           C         SIM01670           C         SIM01670           C         SIM01700           C         RETURN TO 1000 FOR NEXT SECTOR           D00 KR=1         SIM01720           C         RETURN TO 1000 FOR NEXT SECTOR           D00 KR=1         SIM01720           D00 KR=1         SIM01760           D0 81 JR=1,NAD         SIM01770           D0 81 JR=1,NAD         SIM01770           D0 81 JR=1,10         SIM01770           D0 81 JR=1,10         SIM01780           FNN1(KPAR, I, JR)=0.         SIM01800           FNN1(KPAR, I, JR)=0.         SIM01800           C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFA SIM01800           G SUBTRACTED FROM PREVI
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DALFA=0. 1000 KR=1 C RESET SAMPLING OF FLOW VARIABLES (N AND S) SIM01760 D0 81 I=1,NAD SIM01760 D0 81 J=1,NAD SIM01780 D0 81 KPAR=1,4 FNN1(KPAR,I,JR)=0. FNN2(KPAR,I,JR)=0. SIM01820 81 FSN2(KPAR,I,JR)=0. C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFA SIM01820 81 FSN2(KPAR,I,JR)=0. C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFA SIM01820 81 FSN2(KPAR,I,JR)=0. C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFA SIM01820 ALFA=ALFA-DALFA DALFA=5.xFPMXFLOAT(NAD)/RP SIM01870 C DALFA IS THE ANGLE OF THE SECTOR IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2. SIM01880 IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2. SIM01890 IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2. SIM01900 DDALFA = DALFA/FLOAT(NAD) C DALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR ALFA=LAFA-DALFA/2. SIM01900 C DALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR SIM01900 C DALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR C MALFAJ=ALFA-DALFA/2. SIM01900 C DALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR C MALFAJ=ALFA-DALFA/2. SIM01900 C DEFINE REGION KR IN SECTOR. C RETURN TO 2000 FOR THE NEXT REGION KR 2000 CONTINUE C RESET SAMPLING OF FLOW VARIABLES PER REGION DO 82 I=1,NRD DO 02000 SIM
1000 KR=1SIM01750C RESET SAMPLING OF FLOW VARIABLES (N AND S)SIM01760D0 81 J=1,NADSIM01770D0 81 JR=1.10SIM01770D0 81 JRAT.1,GSIM01770D0 81 JRAR.1,GSIM01770FNN1(KPAR,I,JR)=0.SIM01790FNN2(KPAR,I,JR)=0.SIM01800FN1(KPAR,I,JR)=0.SIM0182081 FSN2(KPAR,I,JR)=0.SIM01820c ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFASIM01820c SUBTRACTED FROM PREVIOUS ALFA (PREVIOUS SECTOR) GIVES THE NEW ALFA.SIM01860DALFA = 5.*FFM*FL0AT(NAD)/RPSIM01870C DALFA IS THE ANGLE OF THE SECTORSIM01870C DALFA IS THE ANGLE OF THE SECTORSIM01870C DALFA IS THE ANGLE OF THE SECTORSIM01870C DALFA IS THE ANGLE OF THE SECTORSIM01900IF(DALFA.GT.ALFA/Z.)DALFA=ALFA/Z.SIM01900IF(DALFA.GT.ALFA/Z.)DALFA=ALFA/Z.SIM01910DDALFA = DALFA/FLOAT(NAD)SIM01910DDALFA = DALFA/FLOAT(NAD)SIM01910C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTORSIM01920C DFINE REGION KR IN SECTOR.SIM01960C RETURN TO 2000 FOR THE NEXT REGION KRSIM01970C RETURN TO 2000 FOR THE NEXT REGION KRSIM01900D0 82 I=1,NRDSIM02000D0 82 I=1,NRDSIM02000D0 82 KPAR=1,4SIM02010FEN2(KPAR,1)=0.SIM02010D0 82 KPAR=1,4SIM02010FEN2(KPAR,1)=0.SIM02000C RESET SAMPLING OF FLOW VARIABLES PER REGIONSIM02010D0 82 KPAR=1,4SIM0
C KISLI DAW LINDLESCK AND SYSIM01780D0 & 1 JR=1,NDSIM01770D0 & 1 JR=1,10SIM01770D0 & 1 KPAR=1,4SIM01770FNN1(KPAR,I,JR)=0.SIM01800FNN2(KPAR,I,JR)=0.SIM01820S1101760SIM01830C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFASIM01840C SUBTRACTED FROM PREVIOUS ALFA (PREVIDUS SECTOR) GIVES THE NEW ALFA.SIM01850ALFA=ALFA-DALFASIM01860SIM01870C DALFA IS THE ANGLE OF THE SECTORSIM01870IF(DALFA.GT.AFA/2.) DALFA=ALFA/2.SIM01880IF(DALFA.GT.(FPM*75/RP))DALFA=ALFA/2.SIM01880IF(DALFA.GT.(FPM*75/RP))DALFA=ALFA/2.SIM01900IF(ALFA-DALFA/2.0CSIM01910DALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTORSIM01930ALFA=ALFA-DALFA/2.SIM01940C RETURN TO 2000 FOR THE NEXT REGION KRSIM01990C RESET SAMPLING OF FLOW VARIABLES PER REGIONSIM01990D0 & 21 = 1,NRDSIM02010D0 & 22 L=1,NRDSIM02010D0 & 22 L=1,NRD <td< td=""></td<>
D0 81 JR=1,10         SIM01780           D0 81 KPAR=1,4         SIM01790           FNN1(KPAR,I,JR)=0.         SIM01800           FNN1(KPAR,I,JR)=0.         SIM01810           FSN2(KPAR,I,JR)=0.         SIM01820           S1 FSN2(KPAR,I,JR)=0.         SIM01830           C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFA         SIM01840           C SUBTRACTED FROM PREVIOUS ALFA (PREVIOUS SECTOR) GIVES THE NEW ALFA.         SIM01860           ALFA=ALFA-DALFA         SIM01870           C DALFA IS THE ANGLE OF THE SECTOR         SIM01880           IF(DALFA.GT.ALFA/2.) DALFA=ALFA/2.         SIM01880           IF(DALFA.GT.(FPM*75/RP))DALFA=ALFA/2.         SIM01900           IF(DALFA.GT.(AF/ELOFT (NAD))         SIM01920           DDALFA = DALFA/FLOAT(NAD)         SIM01920           C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR         SIM01930           ALFA=ALFA-DALFA/2.         SIM01940           C         SIM01950           C C         SIM01950           C RETURN TO 2000 FOR THE NEXT REGION KR         SIM01960           C O         SIM01960           C RETURN TO 2000 FOR THE NEXT REGION KR         SIM01990           C RESET SAMPLING OF FLOW VARIABLES PER REGION         SIM01990           C D0 82 KPAR=1,4
D0 81 KPAR:1,4 FNN1(KPAR,I,JR)=0. FNN2(KPAR,I,JR)=0. SIM01800 FSN1(KPAR,I,JR)=0. SIM01820 SIM01820 C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFA SIM01840 C SUBTRACTED FROM PREVIOUS ALFA (PREVIOUS SECTOR) GIVES THE NEW ALFA. SIM01850 ALFA=ALFA-DALFA DALFA = 5.×FPM*FLOAT(NAD)/RP C DALFA IS THE ANGLE OF THE SECTOR IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2. IF(DALFA.GT.(FPM*T5/RP))DALFA=ALFA SIM01890 DDALFA = DALFA/FLOAT(NAD) C DDALFA = CFM*TS/RP))DALFA=ALFA SIM01900 DDALFA = DALFA/FLOAT(NAD) C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR ALFAJ=ALFA-DALFA/2. SIM01930 C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR SIM01940 C DEFINE REGION KR IN SECTOR. C RESET SAMPLING OF FLOW VARIABLES PER REGION D0 82 I=1,NRD D0 82 I=1,NRD D0 82 KPAR=1,4 FEN2(KPAR,I)=0. FEN2(KPAR,I)=0. SIM02020 FEN2(KPAR,I)=0.
FNN2(KPAR, I, JR)=0. FSN1(KPAR, I, JR)=0. SIM01820 SIM01820 SIM01820 SIM01820 C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFA SIM01840 C SUBTRACTED FROM PREVIOUS ALFA (PREVIOUS SECTOR) GIVES THE NEW ALFA. SIM01850 ALFA=ALFA-DALFA DALFA = 5.*FPM*FLOAT(NAD)/RP C DALFA IS THE ANGLE OF THE SECTOR IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2. IF(DALFA.GT.(FPM*T5/RP))DALFA=ALFA IF(DALFA.GT.(FPM*T5/RP))DALFA=ALFA SIM01890 DDALFA = DALFA/FLOAT(NAD) C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR ALFAJ=ALFA-DALFA/2. C C C******************************
FSN1(KPAR, I, JR)=0.SIM0182081 FSN2(KPAR, I, JR)=0.SIM01830C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFASIM01830C SUBTRACTED FROM PREVIOUS ALFA (PREVIOUS SECTOR) GIVES THE NEW ALFA.SIM01860DALFA=ALFA-DALFASIM01860DALFA = 5.*FPM*FLOAT(NAD)/RPSIM01880C DALFA IS THE ANGLE OF THE SECTORSIM01880IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2.SIM01880IF(DALFA.GT.(FPM*75/RP))DALFA=ALFASIM01900DDALFA = DALFA/FLOAT(NAD)SIM01900DALFA = DALFA/FLOAT(NAD)SIM01900C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTORSIM01930ALFAJ=ALFA-DALFA/2.SIM01930C C***********************************
C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFA SIMO1830 C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFA SIMO1840 C SUBTRACTED FROM PREVIOUS ALFA (PREVIOUS SECTOR) GIVES THE NEW ALFA. SIMO1850 ALFA=ALFA-DALFA SIMO1860 DALFA = 5.*FPM*FLOAT(NAD)/RP SIMO1870 C DALFA IS THE ANGLE OF THE SECTOR SIMO1870 IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2. SIMO1890 IF(DALFA.GT.(FPM*75/RP))DALFA=ALFA SIMO1900 DDALFA = DALFA/FLOAT(NAD) C DDALFA = DALFA/FLOAT(NAD) C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR SIMO1930 ALFAJ=ALFA-DALFA/2. SIMO1920 C Z*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X
C SUBTRACTED FROM PREVIOUS ALFA (PREVIOUS SECTOR) GIVES THE NEW ALFA. SIMO1850 ALFA=ALFA-DALFA SIMO1860 DALFA = 5.*FPM*FLOAT(NAD)/RP SIMO1870 C DALFA IS THE ANGLE OF THE SECTOR SIMO1880 IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2. SIMO1890 IF(DALFA.GT.(FPM*75/RP))DALFA=ALFA SIMO1900 DDALFA = DALFA/FLOAT(NAD) SIMO1900 DDALFA = DALFA/FLOAT(NAD) SIMO1910 C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR SIMO1920 C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR SIMO1930 ALFAJ=ALFA-DALFA/2. SIMO1960 C DEFINE REGION KR IN SECTORBLOCK 5 SIMO1960 C DEFINE REGION KR IN SECTORBLOCK 5 SIMO1970 C RESET SAMPLING OF FLOW VARIABLES PER REGION SIMO2000 D0 82 I=1,NRD SIMO2000 D0 82 KPAR=1,4 SIMO2000 FEN1(KPAR,I)=0. SIMO2000
ALFA=ALFA-DALFASIM01860DALFA = 5.*FPM*FLOAT(NAD)/RPSIM01870C DALFA IS THE ANGLE OF THE SECTORSIM01880IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2.SIM01890IF(DALFA.GT.(FPM*75/RP))DALFA=ALFA/2.SIM01900DALFA = DALFA/FLOAT(NAD)SIM01910DALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTORSIM01920C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTORSIM01930ALFAJ=ALFA-DALFA/2.SIM01930C CSIM01950C X=XX=XX=XX=XX=XX=XX=XX=XX=XX=XX=XX=XX=X
C DALFA IS THE ANGLE OF THE SECTOR IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2. IF(DALFA.GT.(FPM*75/RP))DALFA=ALFA IF(DALFA.GT.(FPM*75/RP))DALFA=ALFA IF(ALFA.LE.0.)GO TO 2000 DDALFA = DALFA/FLOAT(NAD) C DDALFA = DALFA/FLOAT(NAD) C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR ALFAJ=ALFA-DALFA/2. C C C C C C C C C C C C C
IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2.       SIM01890         IF(DALFA.GT.(FPM*75/RP))DALFA=ALFA       SIM01900         IF(ALFA.LE.0.)GO TO 2000       SIM01910         DDALFA = DALFA/FLOAT(NAD)       SIM01920         C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR       SIM01930         ALFAJ=ALFA-DALFA/2.       SIM01940         C       SIM01950         C DEFINE REGION KR IN SECTOR.       SIM01960         C DEFINE REGION KR IN SECTOR.       SIM01970         C RETURN TO 2000 FOR THE NEXT REGION KR       SIM01980         2000 CONTINUE       SIM01990         C RESET SAMPLING OF FLOW VARIABLES PER REGION       SIM02000         D0 82 KPAR=1,4       SIM0200         FEN1(KPAR,I)=0.       SIM0200         FEN2(KPAR,I)=0.       SIM0200
IF(DALFA.GI.(FPM*75/KP))DALFA=ALFA IF(ALFA.LE.0.)GO TO 2000 DDALFA = DALFA/FLOAT(NAD) C DDALFA = DALFA/FLOAT(NAD) C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR ALFAJ=ALFA-DALFA/2. C C C C C C C C C C C C C
DDALFA = DALFA/FLOAT(NAD) DDALFA = DALFA/FLOAT(NAD) C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR ALFAJ=ALFA-DALFA/2. C C C C C C C C C C C C C
C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR SIM01930 ALFAJ=ALFA-DALFA/2. SIM01940 C SIM01940 C DEFINE REGION KR IN SECTOR
C       SIM01940         C       SIM01950         C×************************************
C************************************
C DEFINE REGION KR IN SECTORBLOCK 5 SIM01970 C RETURN TO 2000 FOR THE NEXT REGION KR SIM01980 2000 CONTINUE SIM01990 C RESET SAMPLING OF FLOW VARIABLES PER REGION SIM02000 DO 82 I=1,NRD SIM02010 DO 82 KPAR=1,4 SIM02020 FEN1(KPAR,I)=0. SIM02030 FEN2(KPAR,I)=0. SIM02040
2000 CONTINUE         SIM01990           C RESET SAMPLING OF FLOW VARIABLES PER REGION         SIM02000           D0 82 I=1,NRD         SIM02010           D0 82 KPAR=1,4         SIM02020           FEN1(KPAR,I)=0.         SIM02030           FEN2(KPAR,I)=0.         SIM02040
C RESET SAMPLING OF FLOW VARIABLES PER REGION SIM02000 D0 82 I=1,NRD SIM02010 D0 82 KPAR=1,4 SIM02020 FEN1(KPAR,I)=0. SIM02030 FEN2(KPAR,I)=0. SIM02040
D0 82 KPAR=1,4     SIM02020       FEN1(KPAR,I)=0.     SIM02030       FEN2(KPAR,I)=0.     SIM02040
FEN1(KPAR,I)=0. SIM02030 FEN2(KPAR,I)=0. SIM02060
FEN2(KPAR,I)=D. SIM02040
FWN1(KPAR, T)=0 STM02050
82 FWN2(KPAR,I)=0. SIM02050
MT=0 SIM02070
IF(KR.LT.2)NRD=NRD1 51M02080 STM02090
DO 100 I = 1,NRD SIM02100
C POLAR RADIUS MEASURED FROM THE NOZZLE LIP SIMO2110
IF(KR.EQ.2)R(I)=R(I)+FLOAT(NRDI)*DR SIM02120
IF(KR.GE.3)R(I)=R(I)+(FLOAT(NRD1+(KR-2)*NRD))*DR SIM02140
RSI=R(I)+R1/SIN(ALFAJ) SIMO2160

後後20月1月2月2日1月1日(19月2日)。 19月2日(19月2日) 19月2日(19月2日) 19月2日(19月2日) 19月2日(19月2日) 19月2日(19月2日) 19月2日(19月2日)

South States and the states of the states and the states of the

IF(I.EQ.1)RS1=RSI	SIM02170
A(I) = RSI/RS1	SIM02180
MI(I) = M(I)*K21/(K(I)*K21) MI(I) = M(I)*K21/(K(I)*K21)	SIM02200
MT = MT + M1(I)	SIM02210
C MI() IS THE INITIAL NUMBER OF MOLECULES IN EACH CELL	SIM02220
	SIM02230
REG(1,KR,KS)=FLOAT(MIN)/(DN1*R(1)*RS1*DR*DDALFA)	SIM02250
C DFI (REG(1,KR,KS)) IS THE SPHERICAL (AXISYMMETRIC) ANGLE	SIM02260
C WEIGHTING FACTOR. +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=	SIM02280
C (FNN1, FNN2, FSN1, FSN2, FEN1, FEN2, FWN1, FWN2) × DFI	SIM02290
C (FDE1,FDE2,FDW1,FDW2) X DF1 DA1 = PS1XDPXPEG(1,KP,KS)	SIMU2300 SIMU2310
C DA1 IS THE INPUT AREA OF CELL(1)	SIM02320
FN1 = VOXDA1XREG(2,KR,KS)XSIN(ALFA-TETA)	SIM02330
C TETA IS THE ANGLE BETWEEN FLOW DIRECTION AND THE WALL	SIM02340
$F1(I) = FN1 \times A(I)$	SIM02360
$F2(I) = FN2 \times A(I)$	SIM02370
99 FWP1(1,I,KR)=F1(I)	SIM02390
100 FWP2(1,I,KR)=F2(I)	SIM02400
C ACTUAL VOLUME AND INDUT APEA OF SMALLEST CELL IN REGION	SIM02410 STM02420
REG(4, KR, KS)=R(1)×DDALFA×DR×RS1×REG(1, KR, KS)	SIM02430
REG(5, KR, KS)=DA1	SIM02440
C INPUT NUMBER OF MOLECULES (INTEGER) WILL BE INTEGRATED TO MAKE AN	S1M02450
C AVERAGE OF FN1.	SIM02470
C F1(I) IS THE INPUT FLUX TO CELL(I)	SIM02480
102 RMIN=R(1)5×DR	SIM02500
RMAX=RMIN+DR*FLOAT(NRD)	SIM02510
IMAX=ALFA TMIN=AIFA-DAIFA	SIM02520 SIM02530
DO 9102 I = 1, NRD	SIM02540
WRITE (6,9101)R(I),A(I),VOL(I),M1(I),F1(I)	SIM02550
9102 CONTINUE	SIM02570
MTT= MT*NAD	SIM02580
103 FORMAT (' INITIAL NUMBER OF SIMULATED MOLECULES IS= '.15.' PER SPE	SIM02590
XCIES PER DDALFA, TOTAL NUMBER IS', I5)	SIM02610
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX	SIM02620
	SIM02640
	SIM02650
	SIM02670
C CALCULATE INITIAL NUMBER OF MOLECULES IN CELLSBLOCK 7	SIM02680
C SET INITIAL STATE OF GAS	SIMU2690
DO 150 I =1, NRD	SIM02710
DO 150 J= 1,NAD	SIM02720
Č SET SIMULATED MOLECULES IN THEIR CELLS	SIM02740
IC(1, I, J) = M1(I)	SIM02750
IC(2,1,J) = 0	SIM02770
	SIM02780
L SET CELL COURDINATES C(19.I.J) = R(I)	SIMU2790 SIM02800
$C(20, I, J) = ALFA-(FLOAT(J)5) \times DDALFA$	SIM02810
	SIM02820
C	SIM02840
C DEACTIVATE ALL MOLECULES	SIM02850
P1(4,N) = -99.	SIM02870
170 P2(4,N) = -99.	SIM02880

SIM02890 С SIM02900 SET INITIAL STATE OF THE GAS (LOCATION AND VELOCITY OF MOLECULES) SIM02910 С SIM02920 С NADR1 = 0SIM02930 NADR2 = 0SIM02940 SIM02950 DO 200 I = 1,NRD  $\overline{DO}$   $\overline{2OO}$   $\overline{J}$  = 1, NAD SIM02960 NM1 = IC(1, I, J)SIM02970 SIM02980 С DO 205 N = 1, NM1SIM02990 NADR1 = NADR1 + 1 SIM03000 CALL RANDU(PP) SIM03010 P1(4, NADR1) = C(19, I, J)+DR\*(PP-.5) SIM03020 CALL RANDU(P) SIM03030 P1(5, NADR1) = C(20, I, J) + DDALFA\*(P-.5)SIM03040 С SIM03050 DO 205 NV = 1,3 CALL RANDU(P) SIM03060 203 SIM03070  $V = -3.+6. \times P$ SIM03080  $B = EXP(-V \times V)$ SIM03090 CALL RANDU(P) SIM03100 IF(B.LT.P) GO TO 203 SIM03110 P1(NV,NADR1) = P\*SIN(B)\*VTER1 SIM03120 IF(NV.EQ.1)P1(NV,NADR1)=P1(NV,NADR1)+V0X SIM03130 IF(NV.EQ.2)P1(NV,NADR1)=P1(NV,NADR1)+V0Y SIM03140 **205 CONTINUE** SIM03150 С SIM03160 Ċ **REPEAT PROCEDURE FOR SPECIES 2** SIM03170 NM2 = IC(2, I, J) SIM03180 DO 210 N = 1, NM2 SIM03190 NADR2 = NADR2+1SIM03200 CALL RANDU(P) SIM03210  $P2(4, NADR2) = C(19, I, J) + DR \times (P-.5)$ SIM03220 CALL RANDU(P) SIM03230 P2(5, NADR2) = C(20, I, J) + DDALFA\*(P-.5)SIM03240 С SIM03250 DO 210 NV = 1,3SIM03260 207 CALL RANDU(P) SIM03270  $V = -3.+6. \times P$ SIM03280  $B = EXP(-V \times V)$ SIM03290 CALL RANDU(P) SIM03300 IF(B.LT.P) GO TO 207 SIM03310 P2(NV,NADR2) = P\*SIN(B)\*VTER2 SIM03320 IF(NV.EQ.1)P2(NV,NADR2)=P2(NV,NADR2)+V0X SIM03330 IF(NV.EQ.2)P2(NV,NADR2)=P2(NV,NADR2)+V0Y SIM03340 SIM03350 210 CONTINUE С SIM03360 С WHEN NECESSARY, REPEAT PROCEDURE FOR SPECIES 3. SIM03370 200 CONTINUE SIM03380 C SIM03390 SIM03410 DEFINE HERE ALL COLLISION PARAMETERS TO BE INCLUDED IN SIMULATION С С BLOCK 9 SIM03420 С RESET COLLISION TIMERS SIM03430 DO 19 I=1,NRD DO 19 J=1,NAD DO 19 L=1,3 SIM03440 SIM03450 SIM03460 DO 19M=1,3 SIM03470 KT=3\*(L-1)+M+9 SIM03480 C(KT,I,J)=0SIM03490 C SET EXPECTED MAXIMUM RELATIVE VELOCITY IN COLLISIONS SIM03500  $KV = 3 \times (L - 1) + M$ SIM03510 EM1=SPEC(L,1) SIM03520 EM2=SPEC(M,1) SIM03530 EMR=EM1×EM2/(EM1+EM2) SIM03540 С SIM03550 IF(KS.EQ.1)G0 T0 17 SIM03560 TEM=FOE1(4,I,KR,KS) SIM03570 GO TO 18 SIM03580 17 TEM=FWP1(4,I,KR) SIM03590 С SIM03600

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18 RV=2./SQRT(PI*2.*BOLTZ*TEM/EMR) 19 C(KV,I,J)=2.*RV	SIM03610 SIM03620 SIM03630
C MAXIMUM RELATIVE VELOCITY WILL BE RESET IF FASTER ENCOUNTERS OCCUR	SIM03640
	SIM03650 KSIM03660
TIME=0.	SIM03670
C LOOP OVER TIME INTERVALSBLOCK 10 DO 6000 JDTM = 1,NIS C	SIM03680 SIM03690 SIM03700
C	SIM03710
IIML=IIML+DIM Cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx	SIMUS/20 KSIM03730
C	SIM03740
C MOVE ALL MOLECULESBLUCK 12 C MOVE MOLECULES OF SPECIES 1 C	SIMU3750 SIM03760 SIM03770
DO 310 II = 1, NMOLI	SIM03780
IF (P1(4,I1).EQ99.) GO TO 310	SIM03800
VX = P1(1, I1)	SIM03810
VT = P1(2,11) RX = P1(4.11)	SIM03820 SIM03830
T = P1(5, I1)	SIM03840
	SIM03850 *STM03860
C FIND NEW COORDINATESBLOCK 14	SIM03870
XX=RX*COS(T)+VX*DTM	SIM03880
	SIM03900
T=ATAN(YY/XX)	SIM03910
C FOR LAST SECTOR FIND COLLISIONS WITH THE WALL AND SAMPLE THEM	SIM03920 SIM03930
C	SIM03940
IF(ALFA.GT.DALFA)GO TO 301 IE(T.GT.D.)GO TO 301	SIM03950
DTR=DTM×T/(T-TOLD)	SIM03970
C DTR IS THE TIME REMAINING AFTER A MOLECULE STRIKES THE WALL	SIM03980
RW=RX+(RNEW-RX)*DTR/DTM	SIM04000
IF(RW.LT.RMIN)RW=RMIN+DTR*.001	SIM04010
IF(RW.GT.RMAX)RW=RMAX~DTR¥.001 LOC=RW/DR+1	SIM04020 SIM04030
C	SIM04040
C COUNT COLLISIONS WITH THE WALL(MUST BE WAIGHTED =*DFI)	SIM04050
C 55(1,LUC,JSAMF)=55(1,LUC,JSAMF)+1	SIM04080
C SET VELOCITY AND LOCATION AFTER A MOLECULE STRIKES THE WALL	SIM04080
302 CALL RANDU(P) R=VWM1¥SORT(-ALOG(P))	S1M04090 S1M04100
CALL RANDU(P)	SIM04110
BB=2.XPIXP P1(1 NADPI)=BXCOS(BB)	SIM04120
VX=B×COS(BB)	SIM04140
P1(2,NADR1)=B*SIN(BB)	SIM04150
CALL RANDU(P)	SIM04160
P1(3,NADR1)=VWM1×SQRT(-ALOG(P))	SIM04180
XX=KX*CUS(T)+VX*U1K YY=RX*SIN(T)+VY*DTR	SIMU4190 SIM04200
RNEW=SQRT(XX**2+YY**2)	SIM04210
I=AIAN(YY/XX) C	51M04220 51Mn4230
Č*************************************	KSIM04240
C DEACTIVATE ALL MOLECULES THAT MOVED OUT	SIM04250
, JUL IFERNEMILIIRHAA ANDIRNEMIUIRHIN ANDIILIIHAA ANDIILUI HINJUU () ¥303	SIM04200
RI=(RNEW-RMIN)/DR+.999999	SIM04280
1K=K1 TI=(TMAX-T)/DDA1FA+,999999	51M04290 STM04300
IT=TI	SIM04310
C	SIM04320

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	IF(IT.LE.0)G0 T0_304	SIM04330
	IF(IT.GT.NAD)GO TO 305 TE(IR GT NRD)GO TO 306	SIM04340 SIM04350
C	COUNT S DIRECTION, SAMPLE	SIM04360
•	FSN1(1,IT,KR)=FSN1(1,IT,KR)+1.	SIM04370
Ċ	COUNT W DIRECTION, SAMPLE	SIM04380
_	304 IF(IR.LE.0)IR=1	SIM04400
	IF(IR.GT.NKD)IR=NKD FWN1(1.TR)=FWN1(1.TR)+1.	SIM04410 SIM04420
	GO TO 309	SIM04430
C	COUNT E DIRECTION, SAMPLE	SIM04440
	IF(IR.GT.NRD)IR=NRD	SIM04450
	FEN1(1, IR)=FEN1(1, IR)+1.	SIM04470
C	GUTU SUY COUNT N DIRECTION, SAMPLE	S1MU4480 STM04490
-	306 FNN1(1,IT,KR)=FNN1(1,IT,KR)+1.	SIM04500
ç	SET NEW VALUES IN THE MOLECULE TABLE	SIM04510
C	309 RNEW=-99.	SIM04520
	303 P1(4,I1)=RNEW	SIM04540
	310 CONTINUE	SIM04550 SIM04560
C		SIM04570
C.	REPEAT PROCEDURE FOR SPECIES 2 MOLECULES BLOCKS 12 TO18	SIM04580 STM04590
C	DO 320 I2=1,NMOL2	SIM04600
С	SKIP INACTIVE MOLECULES	SIM04610
	VX = P2(1, 12)	SIM04620
	VY = P2(2, I2)	SIM04640
	RX = P2(4, I2) T = P2(5, I2)	SIM04650 SIM04660
	TOLD=T	SIM04670
С		SIM04680
	YY=RX*SIN(T)+VY*DTM	SIM04870
	RNEW=SQRT(XX**2+YY**2)	SIM04710
С	COLLISIONS WITH THE WALL	SIM04720 SIM04730
ē.		SIM04740
	IF(ALFA.GT.DALFA)GO TO 311 IF(T GT 0 )GO TO 311	SIM04750 SIM04760
	DTR=DTM*T/(T-TOLD)	SIM04770
С	DTR IS THE TIME REMAINING AFTER A MOLECULE STRIKES THE WALL	SIM04780
	RW=RX+(RNEW-RX)*DTR/DTM	SIM04790 SIM04800
	IF(RW.LT.RMIN)RW=RW+DTR¥.001	SIM04810
	IF(RW.GT.RMAX)RW=RW~DTR*.001 LOC=RW/DR+1	SIMU4820 STM04830
С	COUNT COLLISIONS WITH THE WALL (MUST BE WEIGHTED =*DFI)	SIM04840
~	SS(2,LOC,JSAMP)=SS(2,LOC,JSAMP)+1	SIM04850
č	FIND THE NEW COORDINATES OF THE MOLECULE	SIM04880
	312 CALL RANDU(P)	SIM04880
	B=VWM2*SQRT(~ALUG(P)) CALL RANDU(P)	SIM04890 SIM04900
	BB=2. *PI*P	SIM04910
	P2(1,NADR2)=B*COS(BB) VX=B*COS(BR)	SIM04920 SIM04930
	P2(2,NADR2)=B*SIN(BB)	SIM04940
	VY=B×SIN(BB) CALL PANDU(P)	SIM04950
	XX=RX*COS(T)+VX*DTR	SIM04970
	YY=RXXSIN(T)+VYXDTR	SIM04980
	KNEM-SWRI(XXXXXZTIIXXZ) T=ATAN(YY/XX)	SIM05000
Ç		SIM05010
С	DEACLIVATE MULECULES THAT MOVED OUT.COUNT FOR OUTPUT FLUX EVALUATION. 311 IF(RNEW.LT.RMAX.AND.RNEW.GT.RMIN AND T.LT TMAX AND T GT TMINIGO T	SIM05020 0SIM05030
	¥313	SIM05040

RI = (RNEW-RMIN)/DR+.999999	SIM05050
IK = KI TT = (TMAY-T)/DDA! FA+ 000000	S1MU5U6U STM05070
II = II	SIM05080
IF (IT.LE.0)GO TO 314	SIM05090
IF (IT.GT.NAD)GO TO 315	SIM05100
IF(IR.GT.NRD)GO TO 316	SIM05110
FSN2(1, TT, KR) = FSN2(1, TT, KR) + 1.	STM05120
GO TO 319	SIM05140
C COUNT W DIRECTION, SAMPLE	SIM05150
314 IF(IR.LE.O)IR=1	SIM05160
IF(IK.GI.NKU)IK=NKU EUN2(1 TP)=EUN2(1 TP)+1	51M05170 SIM05180
GO TO 319	SIM05190
C COUNT E DIRECTION, SAMPLE	SIM05200
315 IF(IR.LE.0)IR=1	SIM05210
IF(IR.GT.NRD)IR=NRD	SIM05220
renz(1,1R) = renz(1,1R) + 1.	SIM05230
C COUNT N DIRECTION. SAMPLE	SIM05250
316 FNN2(1,IT,KR)=FNN2(1,IT,KR)+1.	SIM05260
C	SIM05270
$_{319}$ RNEW = -99.	SIM05280
	SIM05290
P2(4,12) = T	STM05310
320 CONTINUE	SIM05320
c ····································	SIM05330
Cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx	XSIM05340
C NOW NEW MOLECULES WILL BE INTRODUCED	SIM05350
C TUTAL JET FLUX INTO THE REGION WAS DETERMINED BY FI(I) MUL./SEC.	51M05360 STM05370
C NUMBER OF MOLECULES TO BE ACTIVATED PER DTM IS F(I)*DTM PER CELL.	SIM05380
c	SIM05390
Cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx	SIM05400
DO 390 I=1,NRD	SIM05410
L INPUT 'W' MULEUULES TECKS EN 1)GN TN 322	51M05420 STM05630
ANEW1 = FOE1(1.I.KR.KS-1)	SIM05440
ANEW2=F0E2(1,I,KR,KS-1)	SIM05450
GO TO 323	SIM05460
322 ANEWI=FWPI(1,I,KR)*DTM	SIM05470
ANEW2=FWF2(1,1,1,KK)*UIM 323 NEW1=ANEW1	SIMU548U SIMU5480
NEW2=ANEW2	SIM05500
REM1=ANEW1-NEW1	SIM05510
CALL RANDU(P)	SIM05520
IF(REMI.GT.P)NEWI=NEWI+1	SIM05530
KEMZ-ANEWZ-NEWZ	51M05550
IF(REM2.GT.P)NEW2=NEW2+1	SIM05560
C ACTIVATE NEW INPUT MOLECULES	SIM05570
C TIME, LOCATION AND VELOCITY COMP. OF NEW MOLS. ARE RANDOM FUNCTIONS	SIM05580
C SPECIES 1	SIM05590
C IF(NEWI.LI.I)00 TO 341	SIMU56UU
DO 340 I1=1,NEW1	SIM05620
CALL RANDU(P)	SIM05630
ATIME=P*DTM	SIM05640
LALL KANUU(M) PSTART=/FLOAT(T_1)+P)*DP+PMTN	SIMU5650
VFLX=FWP1(2.T.KR)	SIM05670
VELY=FWP1(3,I,KR)	SIM05680
TEM=FWP1(4,I,KR)	SIM05690
C THERMAL VELOCITY	SIM05700
VIEKIFOWKI(Z.*BULIZ*IEM/SPEC(I,I)) C TEMPERATURE IS TRANSEERRED THRONGH ENDING I VON	51MU5710 STM05720
XX=RSTART*COS(ALFA)+VFLY*ATIMF	STM05720
YY=RSTART*SIN(ALFA)+VELY*ATIME	SIM05740
RX=SQRT(XX**2+YY**2)	SIM05750
T=ATAN(YY/XX)	SIM05760

IF(RX.LT.RMIN.OR.RX.GT.RMAX)GO TO 340 SIM05770 IF(T.LT.TMIN.OR.T.GT.TMAX)GO TO 340 SIM05780 C FOR MORE ACCURATE CALCULATION SET THESE MOLECULES IN OUTPUT FLOWS SIM05790 SIM05800 C DEFINE THE VELOCITY COMPONENTS SIM05810 CALL RANDU(P) SIM05820 SIM05830 B=VTER1×SQRT(-ALOG(P)) CALL RANDU(P) SIM05840 BB=2.XPIXP SIM05850 VELX=VELX+B×COS(BB) SIM05860 VELY=VELY+B×SIN(BB) SIM05870 CALL RANDU(P) SIM05880 SIM05890 VELZ=VTER1×SQRT(-ALOG(P)) C DEFINE THE NEW MOLECULE TO BE ACTIVATED DO 325 IACT=1,NMOL1 IF(P1(4,IACT).EQ.-99.)GO TO 326 SIM05900 SIM05910 SIM05920 325 CONTINUE SIM05930 SIM05940 SIM05950 C C IF THERE IS NO ROOM FOR ADDITIONAL MOLECULE PRINT 'ALARM' IF(IACT.GE.NMOL1)GO TO 3004 SIM05960 SIM05970 SIM05980 326 P1(4, IACT)=RX P1(5, IACT)=T P1(1, IACT)=VELX SIM05990 P1(2, IACT)=VELY P1(3, IACT)=VELZ SIM06000 SIM06010 340 CONTINUE SIM06020 SIM06030 REPEAT PROCEDURE FOR SPECIES 2 341 IF(NEW2.LT.1)G0 TO 351 SIM06040 SIM06050 DO 350 I2=1,NEW2 CALL RANDU(P) ATIME=P\*DTM SIM06060 SIM06070 SIM06080 SIM06090 CALL RANDU(P) RSTART=RMIN+(FLOAT(I-1)+P)\*DR SIM06100 VELX=FWP2(2,I,KR) VELY=FWP2(3,I,KR) TEM=FWP2(4,I,KR) SIM06110 SIM06120 SIM06130 C THERMAL VELOCITY SIM06140 VTER2=SQRT(2.\*BOLTZ\*TEM/SPEC(2,1)) SIM06150 XX=RSTART\*COS(ALFA)+VELX\*ATIME SIM06160 YY=RSTART\*SIN(ALFA)+VELY\*ATIME SIM06170 RX=SQRT(XX\*\*2+YY\*\*2) T=ATAN(YY/XX) SIM06180 SIM06190 IF(RX.LT.RMIN.OR.RX.GT.RMAX)GO TO 350 IF(T.LT.TMIN.OR.T.GT.TMAX)GO TO 350 FOR MORE ACCURATE RESULTS SET THESE MOLECULES IN OUTPUT FLOWS SIM06200 SIM06210 SIM06220 SIM06230 DEFINE VELOCITY COMPONENTS CALL RANDU(P) SIM06240 SIM06250 B=VTER2×SQRT(-ALOG(P)) SIM06260 CALL RANDU(P) BB=2.\*PI\*P VELX=VELX+B\*COS(BB) VELY=VELY+B\*SIN(BB) SIM06270 SIM06280 SIM06290 SIM06300 CALL RANDU(P) SIM06310 VELZ=VTER2\*SQRT(-ALOG(P)) C FIND A NEW MOLECULE TO BE ACTIVATED D0 345 IACT=1,NMOL2 IF (P2(4,IACT).Eq.-99.)GO TO 346 SIM06320 SIM06330 SIM06340 SIM06350 345 CONTINUE SIM06360 C IF THERE IS NO PLACE THEN PRINT ALARM IF(IACT.EQ.NMOL2)GO TO 3004 SIM06370 SIM06380 346 P2(4, IACT)=RX P2(5, IACT)=T SIM06390 SIM06400 P2(1, IACT) = VELX SIM06410 P2(2, IACT)=VELY P2(3, IACT)=VELZ SIM06420 SIM06430 **350 CONTINUE** SIM06440 SIM06450 č **REPEAT PROCEDURE FOR SPEC-3** SIM06460 .....SIM06470 INPUT E MOLECULES SIM06480

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351 IF (TMIN.LE.0.)GO TO 390 C č ANEW1=FOW1(1,I,KR,KS+1) С Č NEW1 = ANEW1 REM=ANEW1-NEW1 CALL RANDU(P) IF(P.LT.REM)NEW1=NEW1+1 C ANEW2=FOW2(1,I,KR,KS+1) NEW2=ANEW2 REM=ANEW2-NEW2 CALL RANDU(P) IF(P.LT.REM)NEW2=NEW2+1 C C IF(NEW1.LE.0)G0 T0 370 С DO 362 I1=1,NEW1 CALL RANDU(P) T=TMIN+DDALFAXP CALL RANDU(P) RNEW=RMIN+(FLOAT(I-1)+P)×DR CALL RANDU(P) TEM=FOW1(4,I,KR,KS+1) VTER1=SQRT(2.\*BOLTZ\*TEM/SPEC(1,1)) B=VTER1×SQRT(-ALOG(P)) CALL RANDU(P) BB=2.\*PI\*P VELX=FOW1(2,I,KR,KS+1)+B\*COS(BB) VELY=FOW1(3, I, KR, KS+1)+B×SIN(BB) CALL RANDU(P) VELZ=VTER1×SQRT(-ALOG(P)) C FIND A NEW MOLECULE TO BE ACTIVATED DO 364 IACT=1,NMOL1 IF(P1(4,IACT).EQ.-99.)GO TO 366 **364 CONTINUE** C IF THERE IS NO ROOM FOR ADDITIONA' MOLECULE THEN PRINT 'ALARM' IF(IACT.EQ.NMOL1)GO TO 3004 366 P1(4, IACT) = RNEW P1(5, IACT)=T P1(1, IACT)=VELX P1(2, IACT)=VELY 362 P1(3, IACT)=VELZ **370 CONTINUE** С **REPEAT FOR SPECIES 2** IF(NEW2.LE.0)G0 TO 390 DO 382 I2=1,NEW2 CALL RANDU(P) T=TMIN+DDALFA×P CALL RANDU(P) RNEW=RMIN+(FLOAT(I-1)+P)\*DR CALL RANDU(P) TEM=FOW2(4,I,KR,KS+1) VTER2=SQRT(2.\*BOLTZ\*TEM/SPEC(2,1)) B=VTER2×SQRT(-ALOG(P)) CALL RANDU(P) BB=2.\*PI\*P VELX=FOW2(2, I, KR, KS+1)+B\*COS(BB) VELY=FOW2(3,I,KR,KS+1)+B\*COS(BB) CALL RANDU(P) VELZ=VTER2×SÓRT(-ALOG(P)) C FIND\_A NEW MOLECULE TO BE ACTIVATED DO 384 IACT=1, NMOL2 IF(P2(4, IACT). EQ. -99)GO TO 386 **384 CONTINUE** THERE IS NO ROOM FOR ADDITIONAL MOLECULE THEN PRINT ALARM IF(IACT.EQ.NMOL2) GO TO 3004 C IF 386 P2(4, IACT) = RNEW

soor as a recented market

SIM06490

SIM06500

SIM06510

SIM06520

SIM06530

SIM06540

SIM06550

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SIM06990 SIM07000

SIM07010

SIM07020

SIM07030

SIM07040 SIM07050 SIM07060

SIM07070

SIM07080 SIM07090

SIM07100

SIM07110 SIM07120

SIM07130 SIM07140

SIM07150

SIM07160

SIM07170

SIM07180 SIM07190

SIM07200

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	P2(5,IACT)=T P2(1,IACT)=VELX	SIM07210 SIM07220
382	P2(2,IACT)=VELY P2(3,IACT)=VELZ	SIM07230 SIM07240
		SIM07250
KEP	LAT FUR SPEC-S	SIM07260 SIM07270
390	CONTINUE	SIM07280
İNP	JT 'S' MOLECULES	SIM07290
	DO 460 J=1,NAD	SIM07310
	ANEW1=FNN1(1,J,KR-1)	SIM07320
	IF(ANEW1.LE00001)G0 TO 420	SIM07340
	REMI=ANEWI -NEWI	SIM07360
	CALL RANDU(P)	SIM07370
	DO 402 II=1,NEWI=NEWI+1	SIM07390
	CALL RANDU(P)	SIM07400
	CALL RANDU(P)	SIM07410 SIM07420
	RNEW=RMIN+P×DR	SIM07430
	CALL KANDU(P) TEM=FNN1(4.J.KR-1)	SIM07440 SIM07450
	VTER1=SQRT(2.*BOLTZ*TEM/SPEC(1,1))	SIM07460
	B=VIEKI#SQKI(-ALUG(P)) CALL RANDU(P)	51M07470 SIM07480
	BB=2.×PI×P	SIM07490
	VELX=FNN1(2,J,KR-1)+B*COS(BB) VELY=FNN1(3,J.KR-1)+B*SIN(BB)	SIM07500 SIM07510
	CALL RANDU(P)	SIM07520
FTN	VELZ=VTER1×SQRT(-ALOG(P)) D A NEW MOLECULE TO BE ACTIVATED	SIM07530 SIM07540
1 11	DO 404 IACT=1,NMOL1	SIM07550
606	IF(P1(4,IACT).EQ99.)GO TO 406 Continue	SIM07560 SIM07570
404	IF(IACT.EQ.NMOL1)GO TO 3004	SIM07580
406	P1(4,IACT)=RNEW P1(5,IACT)=T	SIM07590
	PI(1, IACT)=VELX	SIM07610
602	P1(2, IACT)=VELY P1(3, IACT)=VEL7	SIM07620
420	CONTINUE	SIM07640
REP	EAT FOR SPECIES 2 ANEW2=ENN2(1 LKP-1)	SIM07650
	IF(ANEW2.LT00001)G0 TO 440	SIM07670
		SIM07680
	CALL RANDU(P)	SIM07700
	IF(P.LT.REM)NEW2=NEW2+1	SIM07710
	CALL RANDU(P)	SIM07730
	T=TMIN+DDALFA×(P+FLOAT(J-1))	SIM07740
	RNEW=RMIN+P×DR	SIM07760
	CALL RANDU(P)	SIM07770
	VTER2=SQRT(2.*BOLTZ*TEM/SPEC(2,1))	SIM07790
	B=VTER2×SQRT(-ALOG(P))	SIM07800
	BB=2. XPIXP	SIM07820
	VELX=FNN2(2,J,KR-1)+B*COS(BB) VELY=ENN2(3, LKP-1)+B*SIN(BB)	SIM07830
	CALL RANDU(P)	SIM07850
ETAN	VELZ=VTER2*SQRT(-ALOG(P))	SIM07860
F1N.	DO 424 IACT=1,NMOL2	SIMU/8/0 SIM07880
6.94	IF(P2(4, IACT).EQ99)G0 T0 426	SIM07890
424	IF(IACT.EQ.NMOL2)GO TO 3004	SIM07900 SIM07910
426	P2(4, IACT)=RNEW	SIM07920
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	D9/ 5. TACT)=T	STM07930	7
	P2(1.IACT)=VELX	SIM07940	1
	P2(2, IACT)=VELY	SIM07950	Ţ
422	P2(3, IACT)=VELZ	SIM07960	1
. 440	CONTINUE	SIM079/0 CTM07080	1
PEP	EAT END CDEC-Z	.51MU/700 CTM07990	ļ
и Кърт 1.	LAI FUR JECTJ	STM08000	,
INP	UT 'N' MOLECULES	.SIM08010	ī
SPE	C-1	SIM08020	!
-	ANEW1=FSN1(1, J, KR+1)	SIMO8030	
	IF(ANEW1.LE00001)GO TO 450	SIMD8040	1
		SIMUBUJU CTMABALA	ť
	CVII BARDICD) KEMEANEMI-NEMI	S1000000	i
	TE (P   T.REM)NEW1=NEW1+1	STM08080	•
	DO 442 I1=1.NEW1	SIM08090	ŕ
	CALL RANDU(P)	SIM08100	
	T=TMIN +DDALFA×(P+FLOAT(J-1))	SIM08110	,
	CALL RANDU(P)	SIMUSIZU	-
		CIMU8130 SIMU8130	
	UALL KANDU(F) TEM=FGN1(6.1.KD+1)	STM08150	-
	VTFR1=SORT(2.*BOLTZ*TEM/SPEC(1.1))	STM08160	
	B=VTER1×SQRT(-ALOG(P))	SIM08170	ļ
	CALL RANDU(P)	SIM08180	1
	BB=2.XPIXP	SIM08190	•
	VELX=FSN1(2, J, KR+1)+B×COS(BB)	SIMOSZUU	
	VELY=FSNI(3, J, KR+1)+B*SIN(BB)	51MU8210 67M08220	
	CALL KANDU(P) VELZ=VTED1×SODT(_ALOG(P))	SIMUSZEU SIMUSZEU	
FIN	D A NEW MOI FOULE TO BE ACTIVATED	STM08240	•
/ • •••	DO 444 IACT=1, NMOL1	SIM08250	ľ
	IF(P1(4,IACT).EQ99.)GD TO 446	SIM08260	ļ
444	CONTINUE	SIM08270	
	IF(IACT.EQ.NMOL1)GO TO 3004	SIM0828U	
440	PI(4, IACT)=RNEW	51MU8270 CTM02300	
	P1(5,1AC/)=/ p1(1,1ACT)=VFLY	S100500	
	P1(2.IACT)=VELY	SIM08320	
442	P1(3, IACT)=VELZ	SIM08330	
450	CONTINUE	SIM08340	•
	······································	SIMO8350	
j lmr	UT N MULECULES SPEC-Z	51706360 CTMN8370	
	TECANEW2 I F. 00001 )GO TO 460	STM08380	
	NEW2=ANEW2	SIM08390	
	REM=ANEW2-NEW2	SIM08400	
	CALL RANDU(P)	SIM08410	
	IF(P.LT.REM)NEW2=NEW2+1	SIMO8420	
	DU 452 12=1,NEWZ	SIMU8430 CTM02660	
	T=TMTN+DDAIFA=(P+FLOAT(.(-1))	STM08450	
	CALL RANDU(P)	SIM08460	
	RNEW=RMAX-P×DR	SIM08470	
	CALL RANDU(P)	SIM08480	
	TEM=FSN2(4, J, KR+1)	SIM08490	
	VTER2=SQRT(2.XBOLTZXTEM/SPEC(Z,I))	SIMUSSUU	
	B=VICK2*SUKI("ALUG("))	S100510 STM08520	
	RR=2XPIXP	STM08530	
	VELX=FSN2(2,J,KR+1)+B*COS(BB)	SIM08540	
	VELY=FSN2(3,J,KR+1)+B*SIN(BB)	SIM08550	
	CALL RANDU(P)	SIM08560	
	VELZ=VTERZ=SQRT(-ALOG(P))	SIMO8570	
~ =TN	D A NEW MULECULE ID BE ACIIVAIED D0 464 TACT-1 AMOLO	SIMUOJOU Cimogegn	
C FIN	של 1754 באנו=ב,מחטוג זבוססוג זארדו גם בסטונה דה גגג	S100570	
C FIN		9711000000	
C FIN 454		STM08610	
C FIN 454	CONTINUE IF(IACT.EQ.NMOL2)GO TO 3004	SIM08610 SIM08620	
C FIN 454 456	CONTINUE IF(IACT.EQ.NMOL2)GO TO 3004 P2(4,IACT)=RNEW	SIM08610 SIM08620 SIM08630	

•	
P2(1, IACT)=VELX	SIM08650
	SIM08660
	51M08680
	SIMU8000
	STM08760
	*****SIM08710
Cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx	XXXXXSIM08720
C REARRANGE MOLECULES IN THEIR CELLS	SIM08730
C INITIALIZATION	SIM08740
5000 CONTINUE	SIM08750
Cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx	SIM08760 -
KIP=NMOL1+NMOL2+NMOL3	SIM08770
DO 1001 KADD=1,KIP	S1M08780
IUUI IF(KADD)=U	-21M08800
	SIMUSSUU .
	STM08820
	SIM08830
C NIA.NZA.NJA ARE THE NUMBER OF ACTIVE MOLECULES (COUNTED NEXT)	SIM08840
	SIM08850
DO 1100 I=1,NRD	SIM08860
DO 1100 J=1,NAD	SIM08870 ·
	SIM08880
DO 1005 K=1,4	5IM08890
_1005 IC(K,I,J)=0	SIM08900
C SET SPECIES 1	S1M08910
	SIM0920
	STM08950
N3C=0	STM08950
NTC=0	SIM08960
DO 1020 K1=1,NMOL1	SIM08970
ĪF(PÌ(4,KÌ).EQ99.)GO TO 1020	SIM08980
RLOC=ABS(C(19,I,J)-P1(4,K1))	SIMO8990
TLOC=ABS(C(20, I, J)-P1(5, K1))	SIM09000
IF(RLOC.GT.DR*.5)G0 T0 1020	SIM09010 ,
IF(ILUC:GI.DDALFA#.5)G0_I0_1020	SIMUYUZU
	SIMU9USU (
	STM09040 *
	SIMONAN
IF(NTC.E9.1)IC(4.I.J)=KADD	SIM09070
IC(1, I, J) = IC(1, I, J) + 1	SIM09080
KADD=KADD+1	SIM09090
IP(KADD)=K1	SIM09100 ·
1020 CONTINUE	SIM09110
U SEI SPEU-Z MULECULES	SIM09120
DU 1040 KZ=1,NMULZ 15/02/6 K2) 50 -00 100 TO 1060	51M09150
IF(F2(4,K2).EV79.JGU IU IU4U PIOC-ABS(7/10 T I)_P2(6 K2))	SIMU9140 *
TLOC=ABS(C(20.1.J)-P2(5.K2))	SIMOPISO
	STM09170
IF(TLOC.GT.DDALFAX.5)GO TO 1040	STM09180
Ç	SIM09190
N2A=N2A+1	SIM09200
NTC=NTC+1	SIM09210
IF(NTC.EQ.1)IC(4,I,J)=KADD	SIM09220
IC(2, I, J) = IC(2, I, J) + 1	SIM09230
KAUU=KAUU+1 TP/FADD)=F2	51MU924U
INGO CONTRILE	31MUY23U Stm09240
	STM09200
WRITE(6,1021)N1A,N2A	SIMD9280
1021 FORMAT( ' NUMBER OF ACTIVE MOLECULES SPEC1= ', 15. ' SPEC2='.I	5/) SIM09290
	SIM09300
Ĵ	SIM09310 . ;
C##XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX	*****SIM09320 /
C CALCULATE COLLISIONSBLOC	K SIM09330
C EXIERNAL LOOPS ARE OVER CELLS I, J	51M09340
└┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍┍	RRR 51M09550
	2140A20A

DO 999 I=1,NRD SIM09370 DO 999 J=1,NAD 999 NCOL(I,J)=0 SIM09380 SIM09390 SIM09400 DO 900 I=1,NRD DO 900 J=1,NAD SIM09410 SIM09420 C SIM09430 SIM09440 NM(1)=IC(1,I,J) NM(2)=IC(2,I,J) NM(3)=IC(3,I,J) SIM09450 SIM09460 SIM09470 NTOT=NM(1)+NM(2)+NM(3) DO 900 L=1,3 DO 900 M=1,3 SIM09480 SIM09490 C NUMBER OF SPECIES IN THE PROGRAM IS 2 (3) SIM09500 SIM09510 KV=(L-1)×3+M KT=KV+9 SIM09520 C KV, KT ARE THE ADDRESSES OF RELATIVE VELOCITY AND COLLISION TIMERS SIM09530 920 IF(C(KT,I,J).GE.TIME) GO TO 900 C C(KT,I,J)IS THE INTEGRATED TIME FOR L-M COLLISION SIM09540 SIM09550 KSEL=0 SIM09560 KREJ=0 SIM09570 IF(NM(L).GT.1.AND.NM(M).GT.1)GO TO 912 C NO COLLISIONS ARE CALCULATED IF THERE ARE NO MOLECULES SIM09580 SIM09590 911 C(KT, I, J)=C(KT, I, J)+DTM G0 T0 900 SIM09600 SIM09610 C SELECT NOW THE MOLECULES FOR COLLISION SIM09620 912 IF (KSEL.GE.100)GO TO 911 CALL RANDU(P) SIM09630 SIM09640 MOL1=P\*NM(L)+.999999 SIM09650 SIM09660 SIM09670 IF(MOL1.EQ.0)MOL1=1 C SIM09680 CALL RANDU(P) SIM09690 MOL2=P×NM(M)+.999999 IF(MOL2.EQ.0)MOL2=1 SIM09700 **SIM09710** C SIM09720 KSEL=KSEL+1 SIM09730 CHECK IF THE SAME MOLECULE HAS BEEN SELECTED TWICE IF(L.EQ.M.AND.MOL1.EQ.MOL2)GO TO 912 SIM09740 SIM09750 SIM09760 C FIND THE ACTUAL ADDRESSES OF THE SELECTED MOLECULES SIM09770 IF(L.EQ.1)K1=0 IF(L.EQ.2)K1=NM(1) SIM09780 SIM09790 IF(L.EQ.3)K1=NM(1)+NM(2) SIM09800 IF(M.EQ.1)K2=0 IF(M.EQ.2)K2=NM(1) IF(M.EQ.3)K2=NM(1)+NM(2) SIM09810 SIM09820 SIM09830 KADI=MOLI+KI+IC(4,I,J) KAD2=MOL2+K2+IC(4,I,J) C KAD1,KAD2 ARE THE LOCATION OF SELECTED MOLECULES IN IP( SIM09840 SIM09850 SIM09860 MAD1=IP(KAD1) SIM09870 MAD2=IP(KAD2) SIM09880 C MAD1, MAD2 ARE THE ACTUAL ADDRESSES OF THE SELECTED MOLECULES (THE SIM09890 C INDICATION OF WHAT SPECIES THEY ARE HAS BEEN DEFINED HERE) SIM09900 DO 930 N=1,3 SIM09910 IF(L.EQ.1)VN1=P1(N,MAD1) IF(L.EQ.2)VN1=P2(N,MAD1) IF(L.EQ.3)VN1=P2(N,MAD1) IF(L.EQ.3)VN1=P3(N,MAD1) SIM09920 SIM09930 С SIM09940 С SIM09950 IF(M.EQ.1)VN2=P1(N,MAD2) IF(M.EQ.2)VN2=P2(N,MAD2) SIM09960 SIM09970 IF(M.EQ.3)VN2=P3(N,MAD2) SIM09980 С SIM09990 930 VRC(N)=VN1-VN2 SIM10000 C VRC(3) CURTAIN THE THREE RELATIVE VELOCITY COMPONENTS SIM10010 VR=SQRT(VRC(1)\*VRC(1)+VRC(2)\*VRC(2)+VRC(3)\*VRC(3)) SIM10020 VR IS THE RELATIVE SPEED IN A SPECIFIC COLLISION IF(C(KV,I,J).LT.VR)C(KV,I,J)=VR SIM10030 SIM10040 LAST STATEMENT RESETS THE MAXIMUM RELATIVE VELOCITY FOR FURTHER SIM10050 CALCULATIONS SIM10060 SIM10070 IF(KREJ.GT.100)G0 TO 911 SIM10080

The second and the second second second second second second second second second second second second second s

С		SIM10090
	CALL RANDU(P)	SIM10100
	KREJ=KREJ+1	SIM10120
	IF(AVR.LT.P)GO TO 912	SIM10130
Č	LAST STATEMENT REJECTS THE CALCULATED COLLISION	SIM10140
0	NOW & SPECIES I -M COLLISION HAS REEN SELECTED	SIM10150
č	NON A DIEDIED E N ODEELDION NAD DEEN DEELDIED	SIM10170
C	CALCULATE NOW THE PROBABILITY THAT SUCH A COLLISION WILL BE COUNTED	SIM10180
C	FOR THE L AND M SPECIES RESPECTIVELY	SIM10190 SIM10200
		SIM10200
	CALL RANDU(P)	SIM10220
	ANM=FLOAT(NM(L))/FLOAT(NM(M))	SIM10230
	IF(ANM.LT.P)MP=0	SIM10240
	GO TO 955	SIM10260
Č		SIM10270
C	950 ANM=1 /ANM	SIM10280 SIM10290
	IF(ANM.LT.P)LP=0	SIM10300
ç		SIM10310
C	055 CVS-DTX/SDEC/1 2)+SDEC/M 2))XX2/6	SIM10320
	ALP=LP	SIM10340
	ALM=LM	SIM10350
C		SIM10360
c	VULUME=REG(4, KR, KS)*VUL(1)	STM10370
	DNL=FLOAT(NM(L))/VOLUME	SIM10390
~	DNM=FLOAT(NM(M))/VOLUME	SIM10400
5	USE EV.10.5 TDC(1.M)=A1P/(CXSXDNMXVRXNM(1))+A1M/(CXSXDN1XVRXNM(M))	STM10410
С		SIM10430
С	SET THIS VALUE INTO C(KT,I,J)	SIM10440
0	U(KI)1,J)=U(KI)1,J)T1UU(L)MJ	SIM10450
č	SAMPLE THIS COLLISION	SIM10470
~	NCOL(I,J)=NCOL(I,J)+1	SIM10480
ž	FIND RELATIVE MASSES	SIM10490
-	CALL RANDU(P)	SIM10510
	BB=12.XP	SIM10520
	VRC(1)=BBXVR	SIM10530
	CALL RANDU(P)	SIM10550
	BB=2.XPIXP	SIM10560
	VKC(Z)=AA*CUS(BD)*VK VRC(3)=AA*STN(RR)*VR	SIM105/0
С		SIM10590
C	FIND RELATIVE MASSES	SIM10600
	3M=3FEU(L,1)+3FEU(M,1) RML=SPEC(L,1)/SM	SIM10610
	RMM=SPEC(M, 1)/SM	SIM10630
С.		SIM10640
<u>ب</u>	**************************************	EXSIM10650
ć	THEIR NEW VELOCITIES (NEW VELOCITY COMPONENTS ARE ADDED TO THE	SIM10670
С	VELOCITY OF THE CENTER OF MASS VCCM)	SIM10680
	DU 960 N=1,5 TECH EQ I)VI=PICN MADI)	SIM10690
	IF(L.EQ.2)V1=P2(N,MAD1)	SIM10710
С	IF(L.EQ.3)V1=P3(N,MAD1)	SIM10720
	IF(M.EQ.I)VZ=PI(N,MADZ) TF(M.EQ.2)V2=P2(N.MADZ)	SIM10730
C	IF(M.EQ.3)V2=P3(N.MAD2)	SIM10740
č		SIM10760
	VCCM=RML×V1+RMM×V2	SIM10770
		SIM10/80
С		SIM10800

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						_
CHANGE IN VELOCI IF(LP.NE.1)G IF(L.EQ.1)P1 IF(L.EQ.2)P2	TY IS INPUTED 0 TO 961 ((N,MAD1)=VCCM1 2(N.MAD1)=VCCM1	ONLY IF	PROBABILITY	Y OF COLLISIO	IN.GT.1 SIM108 SIM108 SIM108 SIM108 SIM108	LO 20 30 40
IF(L.EQ.3)P3	(N,MAD1)=VCCM1	•			SIM108	50
961 IF(LM.NE.1)G	0 TO 960				SIM108	70
IF(M.EQ.1)P1 IF(M.EQ.2)P2	l(N,MAD2)=VCCM2 2(N,MAD2)=VCCM2				SIM1088 SIM1089	50 90
IF(M.EQ.3)P3	S(N,MAD2)=VCCM2				SIM1090 Stm1091	00
960 CONTINUE					SIM109	20
GU TO 920 900 CONTINUE					SIM1093 SIM1094	50 40
WRITE(6,4545	5)TOC(1,1),TOC( 451,5510 3)	1,2),TOC	(2,1),TOC(	2,2),TIME	SIM109	50 K n
		-			SIM109	70
NOW NEW TEMPERAT	URES MAY BE CA	LCULATED	IN EACH C	ELL	SIM109	50 90
AVERAGE VELOCITY	IN CELLS				SIM1101 STM1101	00
WRITE(6,4547		NOF	754001	754000	SIMIIO	ŽŎ
1 VAVY1	VAVX2	NZE VAVY2	NCOL '	1 EMPK2	VAVXI SIMIIU. SIMIIU	50 40
DO 1110 T=1.	NPD				SIM110	50
DO 1110 J=1,	NAD				SIMIIO	70
NIE=IC(1,1,J N2E=IC(2,I,J	))				SIMILO	50 90
KAD1=IC(4,1, KAD2=IC(6,1	, J)				SIMIII	00
IF(N1E.LT.1)	GO TO 1112				SIMIII	20
VX1=0.					SIM111 SIM111	30 40
VX2=0.					SIMIII	50
VY2=0.					SIMIII SIMIII	70
DO 1111 IM=1	.NIE				SIM111 SIM111	80 90
MAD1=KAD1+IM					SIM112	00
VX1=VX1+P1(1	, I,IAD)				SIMII2 SIMI12	20
111 VY1=VY1+P1(2 112 IF(N2F.LF.0)	2,IAD) 160 TO 1110		•		SIM112	30 4 n
					SIM112	50
DU 1115 IM=1 MAD2=MAD1+IN	1, NZE 1				SIM1120 SIM1127	50 70
IAD=IP(MAD2) VY2=VY2+P2(1	) 				SIM1128	30
115 VY2=VY2+P2(2	2,1AD)				SIM113	ŐŐ
THE AVERAGE VELC	CITIES IN THE	CELL WIL	L RESULT-		SIM1131 SIM1132	50 1 0
VAVX1=VX1/N1 VAVY1=VY1/N1	E				SIM113	30 4 n
VAVX2=VX2/N2	Ē				SIM113	50
IF(I.NE.1)G0	TO 1116				SIM1136 SIM1137	50 70
FSN1 (2.1. KP)	)=VAVX1+FSN1(7.	1.KB)			SIM1138 STM1130	30 30
FSN1(3, J, KR)	=VAVY1+FSN1(3,	J,KR)			SIM1140	ŐŐ
FSN2(3, J, KR)	=VAVX2+F5N2(2, )=VAVY2+F5N2(3,	J,KR)			SIM1141 SIM1142	20
116 IFCT NE NEDI	GO TO 1117				SIM1143 STM1144	30 40
FNN1(2,J,KR)	=VAVX1+FNN1(2,	J,KR)			SIM114	50
FNN1(3,J,KR) FNN2(2,J,KR)	)=VAVT1+FNN1(3, )=VAVX2+FNN2(2,	J,KR) J,KR)			SIM1146 SIM1147	50 70
FNN2(3, J, KR)	=VAVY2+FNN2(3,	J,KR)			SIM1148	30
1117 IF(J.NE.1)60	TO 1118				SIM1150	00
FEN1(2,I)=VA FEN1(3,I)=VA	VX1+FEN1(2,I) VY1+FEN1(3,I)				SIM1151 SIM1152	10 20
		0.2				

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FEN2(2,1)=VAVX2+FEN2(2,1) SIM11530 FEN2(3,I)=VAVY2+FEN2(3,I) SIM11540 C SIM11550 1118 IF(J.NE.NAD)GO TO 1119 SIM11560 FWN1(2,I)=VAVX1+FWN1(2,I)
FWN1(3,I)=VAVY1+FWN1(3,I) SIM11570 SIM11580 FWN2(2,I)=VAVX2+FWN2(2,I) FWN2(3,I)=VAVY2+FWN2(3,I) SIM11590 SIM11600 1119 CONTINUE SIM11610 SIM11620 Č THERMAL VELOCITIES AND TEMPERATURES SIM11630 ENRGI=0. SIM11640 ENRG2=0. SIM11650 IF(NIE.LT.1)GO TO1131 DO 1130 IM=1,NIE MAD1=KAD1+IM SIM11660 SIM11670 SIM11680 IAD=IP(MAD1) SIM11690 CX1=P1(1,IAD)-VAVX1 SIM11700 CY1=P1(2,IAD)-VAVY1 CZ1=P1(3,IAD) 1130 ENRG1=ENRG1+CX1\*CX1+CY1\*CY1+CZ1\*CZ1 SIM11710 SIM11720 SIM11730 1131 IF(N2E.LT.1)GO TO 1150 SIM11740 DO 1140 IM=1,N2E MAD2=KAD2+IM SIM11750 SIM11760 IAD=IP(MAD2) SIM11770 SIM11780 CX2=P2(1,IAD)-VAVX2 CY2=P2(2,IAD)-VAVY2 SIM11790 CZ2=P2(3, IAD) SIM11800 C SIM11810 С SIM11820 1140 ENRG2=ENRG2+CX2\*CX2+CY2\*CY2+CZ2\*CZ2 SIM11830 SIM11840 C 1150 TEMPR1=(ENRG1/N1E)\*SPEC(1,1)/(3.\*BOLTZ) SIM11850 TEMPR2=(ENRG2/N2E)\*SPEC(2,1)/(3.\*BOLTZ) SIM11860 С SIM11870 IF(1.NE.1)G0 T0 1151 FSN1(4,J,KR)=TEMPR1+FSN1(4,J,KR) SIM11880 SIM11890 FSN2(4, J, KR)=TEMPR2+FSN2(4, J, KR) SIM11900 С SIM11910 SIM11920 1151 IF(I.NE.NRD)G0 T0 1152 FNN1(4, J, KR)=TEMPR1+FNN1(4, J, KR) SIM11930 FNN2(4, J, KR) = TEMPR2+FNN2(4, J, KR) SIM11940 SIM11950 С 1152 IF(J.NE.1)GO TO 1153 FWN1(4,I)=TEMPR1+FWN1(4,I) SIM11960 SIM11970 FWN2(4,I) = TEMPR2 + FWN2(4,I)SIM11980 SIM11990 1153 IF(J.NE.NAD)GO TO 1154 FEN1(4,I)=TEMPR1+FEN1(4,I) SIM12000 SIM12010 FEN2(4, I) = TEMPR2+FEN2(4, I) renz(4,I 1154 CONTINUE C SIM12020 SIM12030 SIM12040 WRITE(6,4548)I, J,N1E,N2E, TEMPR1, TEMPR2, VAVX1, VAVY1, VAVX2, VAVY2, NCOSIM12050 1L(I,J)SIM12060 4548 FORMAT(\* \*,415,6F12.3,17) SIM12070 С SIM12080 1110 CONTINUE SIM12090 С SIM12100 6000 CONTINUE SIM12110 C CALCULATE AVERAGED PARAMETERS, WEIGHTED BY DFI SIM12120 DO 6010 I=1,NRD SIM12130 DO 6010 KPAR=1,4 SIM12140 FOW1(KPAR, I, KR, KS)=FWN1(KPAR, I)/(NIS) SIM12150 FOW2(KPAR, I, KR, KS)=FWN2(KPAR, I)/(NIS)
FOE1(KPAR, I, KR, KS)=FEN1(KPAR, I)/(NIS) SIM12160 SIM12170 6010 FOE2(KPAR, I, KR, KS)=FEN2(KPAR, I)/(NIS) SIM12180 C SIM12190 DO 6020 J=1,NAD DO 6020 KPAR=1,4 SIM12200 SIM12210 FSN1(KPAR, J, KR)=FSN1(KPAR, J, KR)/NIS SIM12220 FSN2(KPAR, J, KR)=FSN2(KPAR, J, KR)/NIS SIM12230 FNN1(KPAR, J, KR)=FNN1(KPAR, J, KR)/NIS SIM12240

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6020 FNN2(KPAR, J, KR)=FNN2(KPAR, J, KR)/NIS
                                                                          SIM12250
                                                                          SIM12260
 TO PREPARE FLOWS FOR THE NEXT REGION OR SECTOR, DIVIDE F()N() BY LOCALSIMI2270
C
 DFI AND MULTIPLY BY NEXT DFI WHEN STARTING NEW REGION
                                                                          SIM12280
Ĉ
                                                                          SIM12290
С
 CALCULATE HERE THE MEAN FREE PATH AND STORE INTO REG(,,)
                                                                          SIM12300
                                                                          SIM12310
 STOP PROGRAM IF FLOW BECOMES COLLISIONLESS OR NUMBER DENSITY IS EQUAL SIM12320
TO THE AMBIENT NUMBER DENSITY. STORE FOEL, FOE2 IN A SEPARATE FILE TO SIM12330
C
Ĉ
 BE USED IN A DIFFERENT PROGRAM.
Č
                                                                           SIM12340
                                                                          SIM12350
Č
 PRINT AVERAGED RESULTS
                                                                          SIM12360
 WRITE(6,6029)
6029 FORMAT(' ',////)
                                                                          SIM12370
                                                                          SIM12380
 WRITE(6,6030)NIS,KR SIM12390
6030 FORMAT(' AVERAGED OUTPUT FLOWS AFTER',15,' TIME INCREMENTS IN REGISIM12400
                                                                           SIM12390
     10N',15)
WRITE(6,6031)
                                                                           SIM12410
                                                                           SIM12420
 6031 FORMAT('0
                   T
                        FEN1(1,I)
                                      FEN2(1,I)
                                                    FWN1(1,I)
                                                                FWN2(1,I) *SIM12430
     1)
                                                                           SIM12440
      DO 6033 I=1,NRD
                                                                           SIM12450
 WRITE(6,6032)I, FEN1(1,I), FEN2(1,I), FWN1(1,I), FWN2(1,I)
6032 FORMAT(''', I5,4F13.3)
                                                                          SIM12460
                                                                           SIM12470
 6033 CONTINUE
                                                                           SIM12480
                                                                          SIM12490
 WRITE (6,6034)
6034 FORMAT(*0 J
                                                                       FSNSIM12500
                         FNN1(1, J, KR)
                                        FNN2(1, J, KR)
                                                        FSN1(1, J, KR)
     12(1, J, KR) *)
D0 6036 J=1, NAD
                                                                           SIM12510
                                                                           SIM12520
SIM12520
WRITE(6,6037)J,FNN1(1,J,KR),FNN2(1,J,KR),FSN1(1,J,KR),FSN2(1,J,KR)SIM12530
6037 FORMAT(' ',I5,4F15.5)
 6036 CONTINUE
                                                                           SIM12550
C
                                                                           SIM12560
SIM12570
                                                                           SIM12580
С
 START A NEW REGION
                                                                           SIM12590
      IF(KR.EQ.10) GO TO 7000
KR=KR+1
С
                                                                           SIM12600
Ĉ
                                                                          SIM12610
      GO TO 2000
                                                                           SIM12620
                                                                           SIM12630
SIM12640
                                                                           SIM12650
С
 7000 CONTINUE
                                                                           SIM12660
                                                                           ŠĪM12670
                                                                           SIM12680
SIM12690
                                                                           SIM12700
 FIND IF FLOW BECAME COLLISIONLESS IN THE WHOLE SECTOR
                                                                           SIM12710
 IF POSITIVE, STORE FOEL, FOE2 IN A SEPARATE FILE AND STOP PROGRAM
C
                                                                          SIM12720
                                                                           SIM12730
С
 PREPARE DATA FOR THE NEXT SECTOR
                                                                           SIM12740
Č
      KR=1
                                                                           SIM12750
      STOP PROGRAM IF KS WAS BOUNDED BY THE WALL
                                                                           SIM12760
      KS=KS+1
С
                                                                           SIM12770
č
      GO TO 1000
                                                                           SIM12780
                                                                           SIM12790
SIM12800
С
                                                                          SIM12810
Č
 IF THERE IS BACK FLOW (FWN1, FWN2) NONZERO CALCULATE NEXT ITERATION
                                                                           SIM12820
      ITER=ITER+1
С
                                                                           SIM12830
Ċ
      KS=KR=1
                                                                          SIM12840
Č
      GO TO 3000
                                                                          ŠĪM12850
                                                                           SIM12860
SIM12870
                                                                          SIM12880
С
 WRITE(6,6099)
6099 FORMAT('1 DATA FOR TEN MOLECULES SPEC.2')
                                                                           SIM12890
                                                                          SIM12900
SIM12910
      DO 3003 I=1,10
 WRITE(6,3002) P2(1,1),P2(2,1),P2(3,1),P2(4,1),P2(5,1)
3002 FORMAT(' ',4F10.3,E18.10)
                                                                           SIM12920
                                                                          SIM12930
 3003 CONTINUE
                                                                          SIM12940
      GO TO 3009
                                                                          SIM12950
 3004 WRITE(6,3005)
                                                                          SIM12960
```

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	•
FORMAT(' NO PLACE FOR ADDITIONAL MOLECULES')	SIM12970
Continue	SIM12980
Stop	SIM12990
END	SIM13000 SIM13010 SIM13020
SUBROUTINE RANDU(P)	SIM13030
Common IX	SIM13040
IV = IXX65539	SIM13050
IF (IY) 5,6,6	SIM13060
IY = IY+2147483647+1	SIM13070
P = IY	SIM13080
$P = P \times .4656613E - 9$	SIM13090
IX = IY	SIM13100
Return	SIM13110
End	SIM13120
	FORMAT(' NO PLACE FOR ADDITIONAL MOLECULES') CONTINUE STOP END SUBROUTINE RANDU(P) COMMON IX IY = IXx65539 IF (IY) 5,6,6 IY = IY+2147483647+1 P = IY P = PX.4656613E-9 IX = IY RETURN END

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B.5 Program SIMUL - User's Guide

Preparation: Run AXSYII program. From its output data evaluate:

ALFA - The averaged angle for the continuum breakdown

 $(P \sim 0.05)$ 

TETA - Flow direction along the breakdown limit.

Flow parameters along this line - Pressure, temperature, velocity, mean free path.

Input Data:

Radius of nozzle ring	RI
Radial size of a cell	DR
Maximum radius in simulation	RP
Angle of breakdown limit	ALFA
Flow direction along (ALFA)	TETA
Averaged flow velocity along (ALFA)	Vo
Molecular weight of each species	<pre>Spec(1,1)</pre>
Molecular diameter of each species	Spec (1,2)
Mean free path along (ALFA)	FPM
Averaged Temperature (ALFA)	TEMP
Time increment	DTH
Number of time increments	NIS

#### Options

a. Geometry

The program is designed to run for axisymmetric ring flow. For a two dimensional planar flow the molecular motion, collisions and flow calculation remain unchanged. The flow cross section remain
unchanged. Instead of the angle DFI the two dimensional flow requires the definition of the width of each region (or cell). To keep the number of molecules within reasonable computational limits this size has to decrease in the same manner as DFI.

The part of the program which has to be changed for this purpose is lines 230 to 250.

b. Wall flux calculations:

The program may run for the whole molecular region resulting the flux towards the wall (this part needs additional debugging). However in order to make it more efficient we may stop the program at a sector where the flow becomes collisionless. The remaining part of the flow may be regarded either as collisionless or if we define a much larger size of cells we may calculate the molecular collisions on this basis.

This part need additional analysis and programming.

**Execution** Commands

Without additional changes the program runs under WATFIV compiler using the following command:

## WATFI AXSYM \* (XTYPE)

Further developments will be required to run the program for each sector separately and the output intermediate results on the mass storage.

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#### B.6 The Influence of the Ambient Gas

The temperature, pressure and density of the ambient gas are shown in Table 1. Because its temperature is much higher than in the jet gas, the thermal velocity of ambient gas molecules is much higher than jet molecules. the following contribution may be expected due to the ambient gas:

- a. Collisions between the "hot" ambient molecules with the "cold" jet molecules may cause an increase in the dissipation in the outer layer of the jet and increase in the flux towards the walls.
- b. For higher ambient pressures, those collisions become rare because of the low number density therefore, the influence of the collisions may decrease.

The only way to evaluate the influence of these two controversial factors. is by an additional simulation program to be designed for this region. The following are the main factors to be included in this program:

Boundary Conditions:

- a. The jet side: FOE1 and FOE2 obtained from the last simulated sector (SIHUL) supply the number flux, flow velocity componetns and temperatures. These parameters are given for all points along the radius R(I) at constant distances DR. In the low density domain the resolution DR is much too large compared with the expected mean free path. A different mesh has to be designed for this purpose. It is possible that one cell may be sufficient.
- b. Far Field Condition: The boundary conditions where the gas may be regarded "undisturbed" by the jet are as follows

- Jet gas molecules are allowed to go out the simulation region (these molecules will be regarded as "lost" molecules).
- Ambient gas is allowed to enter the simulated region according with their thermal velocity and number density.
- c. Solid Wall Bondaries. The solid wall may be assumed to have a constant temperature  $T_{w}$ . Incident molecules of either species are reflected back from the wall. Different models of collisions with the wall may be employed.

- Elastic collisions 'specular reglection' (this calculation has been included in SIMUL program)
- Collisions with ideal heat transfer (diffuse reflections)
- Other models depending on the materials and surface parameters.

The collision with the wall was included as an internal routine in the program SIMUL. If the general molecular simulation contains the program proposed here the collision with the wall will be omitted from SIMUL and become the core of the additional collisionless program. Figure 25 shows the low density (collisionless) region and its boundaries.



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#### SUMMARY OF REPORT

Algorithms for the continuum regime and for the region where molecular collisions are significant have been developed.

Program AXSYM contains the calculation of planar jet flow and axisymmetric ring jet flow. This program supplies data for the limits where the continuum approach become invalid and molecular approach should be employed.

Program SINUL contains the molecular simulation for the axisymmetric ring flow. This program may run for the whole molecular region to result in the calculation of flux towards the solid wall. For a more efficient simulation it is proposed to design an additional program for the collisionless region where ambient gas may be included.

For the two dimensional flow, program SINUL may be used after changing the definition of the cell geometry.

To run the whole program it may be required to make separate runs for each sector and store results on the mass storage.

## LIST OF REFERENCES

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