CONTRACTOR REPORT

GAS DYNAMICS OF LASER EXHAUST EXTERNAL TO SPACECRAFT

Shaul Abramovich

November 1985

Approved for public release; distribution unlimited.

Prepared for:
Defense Advanced Research Projects Agency
Arlington, VA 22209
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.

Reproduction of all or part of this report is authorized.

This report was prepared by:

DR. SHAUL ABRAMOVICH
Contracted Research Associate

Reviewed by:

ALLEN E. FUHS
Distinguished Professor
Department of Aeronautics

M. F. PLATZER
Chairman
Department of Aeronautics

Released by:

JOHN N. DYER
Dean of Science and Engineering
**Title:** Gas Dynamics of Laser Exhaust External to Spacecraft

**Author(s):** Shaul Abramovich

**Performing Organization Name and Address:** Naval Postgraduate School, Monterey, California 93943

**Contract or Grant Number(s):** N62271-3140-5157

**Program Element, Project, Task Area & Work Unit Numbers:** DARPA ORDER-4573 ELEMENT: 62301E

**Security Class. (of this report):** UNCLASSIFIED

**Distribution Statement (of this Report):** Approved for public release; distribution unlimited.

**Supplementary Notes:**

**Key Words:**
- Spacecraft Laser Exhaust
- Method of Characteristics
- Direct Simulation - Monte Carlo
- Molecular Simulation - Monte Carlo
- Ring Jet
- Underexpanded Flow
- Hard Sphere Molecules

**Abstract:** Some procedures have been developed to analyze the flowfield of highly underexpanded axisymmetric ring jets operated at high altitudes. The Method of Characteristics (MOC) was used to compute the Prandtl-Meyer expansion fan and 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 compression part downstream, when the ambient pressure goes below certain limits.
Abstract (continued)

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 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.
ACKNOWLEDGMENT

The author wishes to acknowledge the valuable help and cooperation that Professor Allen E. Fuhs has given him throughout this work.
# TABLE OF CONTENTS

I. **INTRODUCTION** .................................................. 1

II. **THE CONTINUUM REGIME** ..................................... 5
   A. **THE TWO DIMENSIONAL ISENTROPIC UNDEREXPANDED JET** ..................... 5
   B. **THE TWO-DIMENSIONAL PLANAR JET** .................................. 7
   C. **THE HODOGRAPH PLANE FOR A TWO DIMENSIONAL JET** ...................... 8
   D. **THE SHAPES OF TWO DIMENSIONAL JETS** ................................ 11
      1. **SIMPLE UNDEREXPANDED JETS** ........................................ 11
      2. **CRITICAL UNDEREXPANDED JETS** ..................................... 11
      3. **HIGHLY UNDEREXPANDED JETS** ....................................... 13
      4. **EXPANSION INTO COMPLETE VACUUM - Pamb = 0** .......................... 17
   E. **THE METHOD OF CHARACTERISTICS, COMPUTATION OF PLANAR AND
      AXISYMMETRIC TWO DIMENSIONAL FLOWS** ................................ 21

III. **THE BREAKDOWN OF CONTINUUM THEORY** ...................... 24
   A. **GENERAL CRITERIA** ............................................. 24
   B. **THE EMPIRICAL CRITERION** ...................................... 26

IV. **THE MOLECULAR FLOW IN AN AXISYMMETRIC KING JET** .......... 28
   A. **GENERAL CONSIDERATIONS** ........................................ 28
      1. **THE DIRECT SIMULATION MONTE CARLO METHOD** .......................... 30
   B. **THE GEOMETRY OF THE SIMULATED DOMAIN, SECTORS, REGIONS AND
      CELLS** .............................................................. 32
   C. **INITIAL NUMBER OF MOLECULES IN CELLS** ................................ 34
   D. **DEFINITION OF INPUT AND OUTPUT FLOWS FOR A REGION** .................. 36
   E. **COLLISIONLESS FLOW** ........................................... 38
   F. **TWO DIMENSIONAL PLANAR FLOW VS. AXISYMMETRIC FLOW** ................ 38

**APPENDIX A: THE AXSYM PROGRAM** ................................... 39

iv
A.1 DIFFERENT REGIONS IN THE JET .............................................. 39
A.2 PROGRAM FLOWCHART .......................................................... 40
A.3 PROGRAM AXSYM LISTING ....................................................... 47
A.4 LIST OF SYMBOLS IN AXSYM PROGRAM .................................... 56
A.5 AXSYM PROGRAM - USER'S GUIDE ........................................... 59
APPENDIX B: SIMUL PROGRAM ...................................................... 61
  B.1 DATA ORGANIZATION .......................................................... 61
  B.2 MOLECULAR SIMULATION FOR A GIVEN REGION ...................... 70
  B.3 SIMUL PROGRAM FLOWCHART ................................................ 76
  B.4 PROGRAM LISTING ............................................................. 78
  B.5 SIMUL PROGRAM - USER'S GUIDE ......................................... 97
  B.6 THE INFLUENCE OF THE AMBIENT GAS .................................. 99
SUMMARY OF REPORT ................................................................. 102
LIST OF REFERENCES ................................................................. 103
INITIAL DISTRIBUTION LIST ..................................................... 106
# LIST OF FIGURES

1. THE SPACECRAFT LASER ................................................. 2
2. THE HODOGRAPH PLANE .................................................. 9
3. FLOW AT EXIT OF A SIMPLE UNDEREXPANDED JET ....................... 12
4. THE HODOGRAPH PLANE FOR A CRITICAL UNDEREXPANDED JET ........ 14
5. DEPENDENCE OF CRITICAL VALUES OF $P_{amb}/P_0$ ON THE MACH NUMBER AT THE EXIT PLANE ($N_0$) FOR DIFFERENT VALUES OF SPECIFIC HEAT RATIO ($\gamma$) .................................................... 15
6. THE HODOGRAPH PLANE FOR A HIGHLY UNDEREXPANDED JET ........... 16
7. HODOGRAPH PLANE SHOWING THE POINTS ON THE MESH OF CHARACTERISTICS (RELATED TO PHYSICAL PLANE FIGURE 8) ......................... 19
8. SCHEMATIC SHAPE OF A HIGHLY UNDEREXPANDED JET ................. 20
9. THE CALCULATION OF $\nu$ AND $\theta$ FOR POINT (3) IS BASED ON DATA FOR POINTS 1 AND 2 ..................................................... 21
10. CALCULATION OF $\nu$ AND $\theta$ FOR AXISYMMETRIC FLOW ........... 22
11. LIMITS FOR CONTINUUM APPROACH ..................................... 25
12. REGIONS IN A KING JET .................................................. 29
13. CROSS SECTION OF THE MOLECULAR SIMULATION DOMAIN, DEFINITION OF SECTORS, REGIONS, CELLS AND COORDINATES ....................... 33
14. VARIATION OF THE ANGLE $\omega$ ........................................ 35
15. DEFINITION OF INPUT AND OUTPUT FLOWS OF SPECIES 1 TO A REGION (KR) IN A SECTOR (KS) .................................................. 37
16. THE THREE REGIONS IN AN UNDEREXPANDED JET ....................... 39
17. INDEXING OF MESH POINTS IN THE AXSYM PROGRAM .................. 41
18. AXSYM PROGRAM FLOWCHART ........................................... 42
19. ITERATIVE PROCEDURE FOR MACH NUMBER CALCULATION ............ 44
20. THE MESH OF CHARACTERISTICS IN REGION 2 AND REGION 3 ‐ AXISYMMETRIC KING JET. $N_0=4$ ALTITUDE=200km ........................................ 45
21. THE MESH OF CHARACTERISTICS IN REGION 2 AND REGION 3 - AXISYMMETRIC RING JET. $M_0=2$ ALTITUDE=200km .................. 46

22. DEFINITION OF SECTOR GEOMETRY AND CELL VOLUME .................. 62

23. VECTOR $\mathbf{P}(\mathbf{n})$ ........................................ 75

24. SIMUL PROGRAM FLOWCHART ........................................ 77

25. THE LOW DENSITY REGION IN THE JET .................................. 101

LIST OF TABLES

1. ATMOSPHERIC DATA ........................................ 6

2. CALCULATION OF CHARACTERISTICS ON PHYSICAL PLANE ................. 18
ABSTRACT

Some procedures have been developed to analyze the flowfield of highly underexpanded axisymmetric ring jets operated at high altitudes. The Method of Characteristics (MOC) 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 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 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.
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.
Figure 1. The Spacecraft Laser.

\( M_0 \) - Mach number at the exit surface \( \sim 4 \) 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 Mach 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 $10^6$ 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.

In the following chapters we bring the detailed description of the computer programs which solve the different parts of the flowfield.
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 parameters of a jet emerging from a gas dynamics spacecraft laser are:

a. The Mach number at the exit surface $M_o = 4$. The static pressure at the exit plane $P_o = 136$ 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 $\text{DF, HF, He}$ and other species. In the programs we limit the composition 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 compressible flow is isentropic

$$T_T = T(1 + \frac{r-1}{2} M^2)$$  \hspace{1cm} (1)

$$P_T = P(1 + \frac{r-1}{2} M^2) \frac{T}{T_1}$$  \hspace{1cm} (2)

$$\rho_T = \rho(1 - \frac{r-1}{2} M^2) \frac{1}{T_1}$$  \hspace{1cm} (3)
TABLE 1

ATMOSPHERIC DATA
(Abstracted from U.S. Standard Atmosphere 1976)

<table>
<thead>
<tr>
<th>Altitude (km)</th>
<th>Pressure (m bar)</th>
<th>Number density (m$^{-3}$)</th>
<th>Particle speed (m/sec)</th>
<th>Collision frequency (sec$^{-1}$)</th>
<th>Mean free path (m)</th>
<th>Molecular weight (kg/kmol)</th>
<th>Density (kg/m$^3$)</th>
<th>Temperature (°k)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>3.2011 -4</td>
<td>1.189 +19</td>
<td>381.4</td>
<td>2.68 +3</td>
<td>1.42 -1</td>
<td>28.4</td>
<td>5.604 -7</td>
<td>195.08</td>
</tr>
<tr>
<td>200</td>
<td>8.4736 -7</td>
<td>7.182 +15</td>
<td>921.6</td>
<td>3.9</td>
<td>2.4 +2</td>
<td>21.3</td>
<td>2.541 -10</td>
<td>854.56</td>
</tr>
<tr>
<td>300</td>
<td>8.7704 -8</td>
<td>6.509 +14</td>
<td>1079.7</td>
<td>4.2 -1</td>
<td>2.6 +3</td>
<td>17.73</td>
<td>1.916 -11</td>
<td>976.01</td>
</tr>
<tr>
<td>400</td>
<td>1.4518 -8</td>
<td>1.056 +14</td>
<td>1148.5</td>
<td>7.2 -2</td>
<td>1.6 +4</td>
<td>15.98</td>
<td>2.803 -12</td>
<td>995.83</td>
</tr>
<tr>
<td>500</td>
<td>3.0236 -9</td>
<td>2.192 +13</td>
<td>1215.0</td>
<td>1.6 -2</td>
<td>7.7 +4</td>
<td>14.33</td>
<td>5.215 -13</td>
<td>999.24</td>
</tr>
<tr>
<td>600</td>
<td>8.2130 -10</td>
<td>5.950 +12</td>
<td>1356.4</td>
<td>4.8 -3</td>
<td>2.8 +5</td>
<td>11.51</td>
<td>1.137 -13</td>
<td>999.85</td>
</tr>
<tr>
<td>700</td>
<td>3.1908 -10</td>
<td>2.311 +12</td>
<td>1627.0</td>
<td>2.2 -3</td>
<td>7.3 +5</td>
<td>8.00</td>
<td>3.070 -14</td>
<td>999.97</td>
</tr>
<tr>
<td>800</td>
<td>1.7036 -10</td>
<td>1.234 +12</td>
<td>1954.3</td>
<td>1.4 -3</td>
<td>1.4 +6</td>
<td>5.54</td>
<td>1.136 -14</td>
<td>999.99</td>
</tr>
<tr>
<td>900</td>
<td>1.0873 -10</td>
<td>7.876 +11</td>
<td>2192.6</td>
<td>1.0 -3</td>
<td>2.1 +6</td>
<td>4.40</td>
<td>5.759 -15</td>
<td>1000.00</td>
</tr>
<tr>
<td>1000</td>
<td>7.5138 -11</td>
<td>5.442 +11</td>
<td>2318.1</td>
<td>7.5 -4</td>
<td>3.1 +6</td>
<td>3.94</td>
<td>3.561 -15</td>
<td>1000.00</td>
</tr>
</tbody>
</table>
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

$$\mu = \arcsin \left( \frac{1}{M} \right)$$

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 ($M$) as

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

$$\nu(M) = \frac{\gamma + 1}{\gamma - 1} \arctg \frac{\gamma - 1}{\gamma + 1} (M^2 - 1) - \arctg (M^2 - 1)$$  \hspace{1cm} (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 $\nu$ 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
The initial turning angles for $M_0 > 1$

$\theta_1^-, \theta_1^+ -$ maximum turning angles for a highly under-expanded jet

$\theta_{\max} -$ maximum turning angle for the specific gas.

Figure 2. The Hodograph Plane.

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 $P_{amb2} \ll P_0$, 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 families 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 $M_0 > 1$, an initial turn of the flow $\theta_0$ is made within the nozzle. An additional 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 $M_0 = 1$ 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 $H_0$ or $P/P_{\infty} = 0$. This means that there is a core within the jet where the pressure approaches zero and Mach approaches infinity. This core is theoretically bounded at its upstream side by expansion waves and downstream by compression waves.
Jet boundary (freestream), $P = P_{amb}$

---

Streamline:

1. Uniform axial flow ($P = P_0$)
2. Uniform flow parallel to $L_2$ ($P = P_{amb}$)
3. Uniform axial flow (lowest pressure $P_{\text{min}}$)
4. Uniform flow parallel to $L_4$ ($P = P_{amb}$)
5. Uniform axial flow ($P = P_0$)

---

Figure 3. Flow at exit of a simple underexpanded jet.

(a) Physical Plane

(b) Hodograph Plane
Using the theoretical expressions for isentropic ideal flow one may derive the values of $\frac{P_{\text{amb}}}{P_T}$ or $\frac{P_{\text{amb}}}{P_0}$ as function of $M_o$ which causes a jet to be critical underexpanded.

Figure 5 shows results of $\frac{P_{\text{amb}}}{P_0}$ as functions of $M_o$ for gases with different specific heat ratio.

3. Highly Underexpanded Jets

When $P_{\text{amb}}$ 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 $\theta_{\text{lim}}$ (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".
Figure 4. The Hodograph Plane for a Critical Underexpanded Jet.

(1-2-3-4-1), (\gamma=1.4)
Figure 5. Dependence of critical values of $P_{amb}/P_0$ 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

\( \gamma = 1.4 \)

- \( \theta_{\text{max}} \) - maximum turning angle
- \( \theta \) - total turning angle in the specific jet \( \theta > \theta_{\text{max}}/2 \)
- \( \theta_{\text{lim}} \) - limiting angle of compression region.
Figure (7) shows the hodograph plane for an air jet (γ=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 - \(P_{amb}=0\)

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 \(P=0\) without being reflected by the jet boundaries.
<table>
<thead>
<tr>
<th>State</th>
<th>$\theta_\alpha^+$</th>
<th>$\theta_\alpha^-$</th>
<th>$\theta$</th>
<th>$\nu$(M)</th>
<th>$\mu$</th>
<th>$\theta+\mu$</th>
<th>$\theta-\mu$</th>
<th>$P/P_E$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>90°</td>
<td>-90°</td>
<td>0.5283</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>10</td>
<td>10</td>
<td>10</td>
<td>1.435</td>
<td>44.15</td>
<td>54.15</td>
<td>-34.15</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>1.775</td>
<td>34.3</td>
<td>54.3</td>
<td>-14.3</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>40</td>
<td>30</td>
<td>30</td>
<td>2.135</td>
<td>27.93</td>
<td>57.93</td>
<td>-2.07</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>60</td>
<td>40</td>
<td>40</td>
<td>2.54</td>
<td>23.18</td>
<td>63.18</td>
<td>16.82</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>80</td>
<td>50</td>
<td>50</td>
<td>3.013</td>
<td>19.38</td>
<td>69.38</td>
<td>30.62</td>
</tr>
<tr>
<td>7</td>
<td>0</td>
<td>100</td>
<td>60</td>
<td>60</td>
<td>3.595</td>
<td>16.15</td>
<td>76.15</td>
<td>43.85</td>
</tr>
<tr>
<td>8</td>
<td>0</td>
<td>120</td>
<td>67.7</td>
<td>67.7</td>
<td>4.145</td>
<td>13.96</td>
<td>88.7</td>
<td>53.74</td>
</tr>
<tr>
<td>9</td>
<td>20</td>
<td>135.4</td>
<td>20</td>
<td>20</td>
<td>1.775</td>
<td>34.3</td>
<td>34.3</td>
<td>-34.3</td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>20</td>
<td>10</td>
<td>30</td>
<td>2.135</td>
<td>27.93</td>
<td>37.93</td>
<td>-17.93</td>
</tr>
<tr>
<td>11</td>
<td>20</td>
<td>40</td>
<td>20</td>
<td>40</td>
<td>2.54</td>
<td>23.18</td>
<td>43.18</td>
<td>-3.18</td>
</tr>
<tr>
<td>12</td>
<td>20</td>
<td>60</td>
<td>30</td>
<td>50</td>
<td>3.013</td>
<td>19.38</td>
<td>49.38</td>
<td>10.62</td>
</tr>
<tr>
<td>13</td>
<td>20</td>
<td>80</td>
<td>40</td>
<td>60</td>
<td>3.595</td>
<td>16.15</td>
<td>56.15</td>
<td>23.85</td>
</tr>
<tr>
<td>14</td>
<td>20</td>
<td>100</td>
<td>50</td>
<td>70</td>
<td>4.339</td>
<td>13.315</td>
<td>63.32</td>
<td>36.69</td>
</tr>
<tr>
<td>15</td>
<td>20</td>
<td>120</td>
<td>57.7</td>
<td>77.7</td>
<td>5.085</td>
<td>11.34</td>
<td>69.04</td>
<td>46.4</td>
</tr>
<tr>
<td>16</td>
<td>40</td>
<td>135.4</td>
<td>0</td>
<td>40</td>
<td>2.54</td>
<td>23.18</td>
<td>23.18</td>
<td>-23.18</td>
</tr>
<tr>
<td>17</td>
<td>40</td>
<td>40</td>
<td>10</td>
<td>50</td>
<td>3.013</td>
<td>19.38</td>
<td>29.38</td>
<td>-9.38</td>
</tr>
<tr>
<td>18</td>
<td>40</td>
<td>60</td>
<td>20</td>
<td>60</td>
<td>3.595</td>
<td>16.15</td>
<td>36.15</td>
<td>3.85</td>
</tr>
<tr>
<td>19</td>
<td>40</td>
<td>80</td>
<td>30</td>
<td>70</td>
<td>4.339</td>
<td>13.315</td>
<td>43.32</td>
<td>16.69</td>
</tr>
<tr>
<td>20</td>
<td>40</td>
<td>120</td>
<td>40</td>
<td>80</td>
<td>5.347</td>
<td>10.777</td>
<td>50.78</td>
<td>29.23</td>
</tr>
<tr>
<td>21</td>
<td>40</td>
<td>135.4</td>
<td>47.7</td>
<td>87.7</td>
<td>6.433</td>
<td>8.943</td>
<td>56.64</td>
<td>38.76</td>
</tr>
<tr>
<td>22</td>
<td>60</td>
<td>60</td>
<td>0</td>
<td>60</td>
<td>3.595</td>
<td>16.15</td>
<td>16.15</td>
<td>-16.15</td>
</tr>
<tr>
<td>23</td>
<td>60</td>
<td>80</td>
<td>10</td>
<td>70</td>
<td>4.339</td>
<td>13.315</td>
<td>23.32</td>
<td>-3.32</td>
</tr>
<tr>
<td>24</td>
<td>60</td>
<td>100</td>
<td>20</td>
<td>80</td>
<td>5.347</td>
<td>10.777</td>
<td>30.78</td>
<td>9.22</td>
</tr>
<tr>
<td>25</td>
<td>60</td>
<td>120</td>
<td>30</td>
<td>90</td>
<td>6.8190</td>
<td>8.433</td>
<td>38.43</td>
<td>21.57</td>
</tr>
<tr>
<td>26</td>
<td>60</td>
<td>135.4</td>
<td>37.7</td>
<td>97.7</td>
<td>9.2105</td>
<td>6.2330</td>
<td>43.93</td>
<td>31.5</td>
</tr>
<tr>
<td>27</td>
<td>80</td>
<td>80</td>
<td>0</td>
<td>80</td>
<td>5.347</td>
<td>10.777</td>
<td>10.777</td>
<td>-10.77</td>
</tr>
<tr>
<td>28</td>
<td>80</td>
<td>100</td>
<td>10</td>
<td>90</td>
<td>6.8190</td>
<td>8.433</td>
<td>18.433</td>
<td>1.57</td>
</tr>
<tr>
<td>29</td>
<td>80</td>
<td>120</td>
<td>20</td>
<td>100</td>
<td>9.2105</td>
<td>6.233</td>
<td>26.23</td>
<td>13.8</td>
</tr>
<tr>
<td>30</td>
<td>80</td>
<td>135.4</td>
<td>27.7</td>
<td>107.7</td>
<td>12.45</td>
<td>4.61</td>
<td>32.3</td>
<td>23.1</td>
</tr>
<tr>
<td>31</td>
<td>100</td>
<td>100</td>
<td>0</td>
<td>100</td>
<td>9.2105</td>
<td>6.233</td>
<td>+6.233</td>
<td>-6.233</td>
</tr>
<tr>
<td>32</td>
<td>100</td>
<td>120</td>
<td>10</td>
<td>110</td>
<td>13.874</td>
<td>4.1331</td>
<td>14.13</td>
<td>5.9</td>
</tr>
<tr>
<td>33</td>
<td>100</td>
<td>135.4</td>
<td>17.7</td>
<td>117.7</td>
<td>21.4</td>
<td>2.678</td>
<td>20.37</td>
<td>15.0</td>
</tr>
<tr>
<td>34</td>
<td>120</td>
<td>120</td>
<td>0</td>
<td>120</td>
<td>27.335</td>
<td>2.097</td>
<td>2.097</td>
<td>-2.097</td>
</tr>
<tr>
<td>35</td>
<td>120</td>
<td>135.4</td>
<td>7.7</td>
<td>127.7</td>
<td>104</td>
<td>0.546</td>
<td>8.2</td>
<td>7.2</td>
</tr>
<tr>
<td>36</td>
<td></td>
<td></td>
<td>11°</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>51</td>
<td>20</td>
<td>115.4</td>
<td>47.7</td>
<td>67.7°</td>
<td>4.145</td>
<td>13.96</td>
<td>33.7</td>
<td>.5437</td>
</tr>
<tr>
<td>52</td>
<td>40</td>
<td>115.4</td>
<td>37.7</td>
<td>77.7</td>
<td>5.085</td>
<td>11.34</td>
<td>26.36</td>
<td></td>
</tr>
<tr>
<td>53</td>
<td>40</td>
<td>95.4</td>
<td>+27.7</td>
<td>67.7°</td>
<td>4.145</td>
<td>13.96</td>
<td>13.7</td>
<td>.5437</td>
</tr>
<tr>
<td>54</td>
<td>60</td>
<td>75.4</td>
<td>+7.7</td>
<td>67.7°</td>
<td>4.145</td>
<td>13.96</td>
<td>-6.26</td>
<td>.5437</td>
</tr>
<tr>
<td>55</td>
<td>60</td>
<td>95.4</td>
<td>17.7</td>
<td>77.7</td>
<td>5.085</td>
<td>11.34</td>
<td>6.4</td>
<td></td>
</tr>
<tr>
<td>56</td>
<td>60</td>
<td>115.4</td>
<td>27.7</td>
<td>87.7</td>
<td>6.433</td>
<td>8.943</td>
<td>18.8</td>
<td></td>
</tr>
</tbody>
</table>
Figure 7. Hodograph plane showing the points on the mesh of characteristics. (Related to physical plan Figure 8).
Figure 8. Schematic shape of a highly underexpanded jet.

(See Figure 7 - The Hodograph Plane)

The arrows indicate flow direction.
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))

\[
\begin{align*}
\nu_3 &= \frac{1}{2} (\nu_1 + \nu_2) + \frac{1}{2} (\theta_1 - \theta_2) \\
\theta_3 &= \frac{1}{2} (\nu_1 - \nu_2) + \frac{1}{2} (\theta_1 + \theta_2)
\end{align*}
\]

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 ($v$) and the flow direction ($\theta$) which are given by:

$$v_3 = \frac{1}{2} (v_1 + v_2) + \frac{1}{2} (\theta_1 - \theta_2) + \frac{1}{2} [\sin \theta_1 \frac{\sin \theta_1}{r_1} \Delta \xi_{13} + \sin \theta_2 \frac{\sin \theta_2}{r_2} \Delta \eta_{23}]$$

(9)

$$\theta_3 = \frac{1}{2} (v_1 - v_2) + \frac{1}{2} (\theta_1 + \theta_2) + \frac{1}{2} [\sin \theta_1 \frac{\sin \theta_1}{r_1} \Delta \xi_{13} - \sin \theta_2 \frac{\sin \theta_2}{r_2} \Delta \eta_{23}]$$

(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-Heyer 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 Reference [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 x 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

\[ P \equiv \frac{q}{\rho v} \left| \frac{d\rho}{dS} \right| = 0.05 \]  

where  
- \( q \) = stream velocity  
- \( \rho \) = density  
- \( v \) = molecular collision frequency  

\[ \left| \frac{d\rho}{dS} \right| = \text{absolute change in density while moving a distance} \]  

\[ dS \text{ along a streamline} \]

Introducing the breakdown parameter \( P \) into the program, gives the definition 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$^3$. 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
Figure 12. Regions in a ring jet.
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 Monte 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. The size of a cell must be such that the change in flow properties across each cell is small. The time is advanced in discrete steps ∈t, such that ∈t is small compared with the mean collision time per molecule. If there is a flow going through the domain, ∈t should be small compared with the mean time required for the mean flow to cross the cells.* Both cell size ((DR),(DDLFA) - radial size and angular size as they appear in the program) and ∈t 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

*If ∈t 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 ∈t 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 $N_L$ and $N_M$ molecules with collision cross section $\sigma_{LM}$, number densities $n_L$ and $n_M$ and relative velocity $C_r$, is given by

$$\Delta t_c = \frac{LP}{N_L} \frac{1}{\sigma_{LM} n_L C_r} + \frac{MP}{N_M} \frac{1}{\sigma_{LM} n_M C_r}$$ (12)

where $LP$ and $MP$ are the probabilities that the collision will be effective for the $L$ and $M$ 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:
To maintain the number of simulated molecules within computational limits, the 'width' of each region defined by DFI is such that:

\[
\text{MIN} = \text{number of molecules in smallest cell in a region} \\
\text{MIN} = \text{VOLUME (smallest cell)} \times \text{number density} \\
= f(R, \text{ALFA, DALFA}) \times \text{DFI} \times \text{number density for flux calculations} \\
\text{DFI is a weighting factor.}
\]
DFI*(constant) * (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 DFI 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.)
Figure 15. Definition of input and output flows of species 1 to a region (KR) in a sector (KS).

(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.
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.](image)

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 MOC 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 \((\text{TETA})\), 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 Mach angles, coordinates of mesh points and distances \( d_\zeta \) 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
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 Prandtl-Meyer angle. It is calculated by iterations with an initial guess or 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.
Figure 19. Iterative procedure for Mach number calculation.

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. $M_o = 4$. Altitude=200km.
Figure 21. The mesh characteristics in Region 2 and Region 3

Axisymmetric ring jet. $M_o = 2$. Altitude = 200 km.
A.3 PROGRAM 'AXSYM' LISTING

$JOB

PROGRAM AXSYM

C THIS PROGRAM CALCULATES THE ISENTROPIC EXPANSION OF A JET BY MEANS OF AXSYM.
C THE METHOD OF CHARACTERISTICS.
C
C FOR A TWO DIMENSIONAL JET 'KD' SHOULD BE SET EQUAL TO 2
C FOR AN AXISYMMETRIC RING JET 'KD' SHOULD BE SET EQUAL TO 3
C
C IMPLICIT REAL*(A-H,O-Z,$)
C
DIMENSION TETA(20,50),AM(20,50),R(20,50),X(20,50),PM(20,50)
DIMENSION AMCOR(20,20),TETAC(20,20),XC(20,20),RC(20,20),PMC(20,20)
DIMENSION DENSFC(20,50)
DIMENSION AMX(50,50),TETAX(50,50),XX(50,50),RX(50,50),PMX(50,50)
C
C TETA IS THE FLOW ANGLE (RADIANS) MEASURED FROM X AXIS.
C AM IS THE MACH NUMBER
C R IS THE RADIUS (NORMAL TO THE WALL)
C X IS THE AXIAL LOCATION (PARALLEL TO THE WALL)
C PM IS THE PRANDTL MEYER FUNCTION

C THE FOLLOWING IS DATA FOR THE SPECIFIC PROBLEM

PAMB = 8.4736E-5
KD = 3
C FOR TWO DIMENSIONAL FLOW KD=2 , FOR AXISYMMETRICAL FLOW KD=3

C CONSTANTS
PI = 3.141593
BOLTZ = 1.38032E-23
AVOG = 6.0225E+26
RG = 8314.3

C EXIT SURFACE
AM0 = 4.00
T0 = 300.0
P0 = 136.0
R1 = 2.5
X1 = 0.5

C GAS DATA
GAMA = 1.535
DIAM = 2.95E-10
GM = 17.0
RJ = RG/GM
CXS = PI*DIAM*DIAM
GMM = GM/AVOG

C MESH DEFINITION
N1=CHARACTERISTICS FROM THE EXIT PLANE
N2=CHARACTERISTICS FROM THE CORNERS
N1 = 20
N2 = 50

C CONSTANTS FOR THE ISENTROPIC EXPANSION
A1 = (GAMA-1.0)/GAMA
B1 = 1.0/A1
A2 = DSQRT((GAMA+1.0)/(GAMA-1.0))
B2 = 1.0/A2
A3 = (GAMA-1.0)/2.
C
C MACH*MACH*A3 + 1.
D = MACH*MACH -1.

C DEFINE STAGNATION PARAMETERS
C
C = (1.0+A3*AM0*AM0)
C PRESSURE
C DEFINE FREE STREAM PARAMETERS AT THE RIGHT CORNER
C
MACH NUMBER
FSM = DSQRT(((PSTG/PAMB)*NA1-1.)/A3)
C TEMPERATURE
FST = TSTG/(1.+A3*FSM)
C DENSITY
FSD = PAMB/(RJ*FST)
C MACH ANGLES FOR HEAD AND TAIL OF FAN
AMIT = DARSIN(1./AMO)
AMIH = DARSIN(1./FSM)
C PRANDTL MEYER FUNCTION FOR HEAD AND TAIL OF FAN
D1 = DSQRT(AMO*AMO-1.)
D2 = DSQRT(FSM*FSM-1.)
PMH = A2*DATAN(B2*D2)-DATAN(D1)
PMT = A2*DATAN(B2*D1)-DATAN(D1)
C EXTERNAL TURNING ANGLE (FREE STREAM ANGLE)=EXTA
EXTA = PMH - PMT
C PRANDTL MEYER FAN ANGLE PMFA
PMFA = EXTA - AMIH + AMIT
C
WRITE(6,1)PSTG,TSTG,DSTG,DIAM,GM
1 FORMAT('STAGNATION PRESSURE=',E12.5,' TEMPERATURE=',F10.5)
2 FORMAT('PRESSURE=',E12.5,' TEMPERATURE=',F10.5)
WRITE(6,2)PO,TO,DO
2 FORMAT('EXIT PLANE PRESSURE=',E12.5,' TEMPERATURE=',F10.5)
WRITE(6,3)PAMB,FST,FSD,FSM
3 FORMAT('FREE STREAM PRESSURE=',E12.5,' TEMPERATURE=',F10.5)
WRITE(6,4)'
4 FORMAT('PRANDTL MEYER FAN LINE MACH')
WRITE(6,5)DO
5 FORMAT('P.M. ANGLE TETA'/)
R(N) = R1
X(I,N) = X1
ALFAL = TETA(1,N)*AM0

C ALFAL IS THE ANGLE OF THE LEFT RUNNING CHARACTERISTICS

C PRESSURE, TEMPERATURE AND DENSITY VARIATION AT THE CORNER
C
C = AM(1,N)*AM(1,N)*AM0+1.
PRES = PSTG/(C*X*B1)
TEMP = TSTG/C
DENSF(1,N) = PRES/(RJ*TEMP)

C
WRITE(6,5) N,AM(1,N),PM(1,N),TETA(1,N)
5 FORMAT(' ',I15,3E20.5)

CONTINUE

C
WRITE(6,10) I,J,MACH,R,X,TETA
ITEMP,PRESS,VELOCITY,KNUDSEN,MFP,ND
10 FORMAT(O',',15E16.5)

C
THE EXIT PLANE IS DIVIDED INTO (N1-1) DIVISIONS (N1 POINTS)

DO 25 J = 1,N1
AMCOR(1,J) = AM0
D = DSQRT(AM0*AM0-1.)
PMC(1,J) = A2*DATAN(B2ND)-DATAN(D)
25 TETAC(1,J) = PI/2.

C
THE EXIT PLANE IS DIVIDED INTO (N1-1) DIVISIONS (N1 POINTS)

DO 30 J = 1,20
SOUND = DSQRT(GAMA*RJNTO)
VELO = AMCOR(1,J)*SOUND
DNO = PO/(BOLTZ*TO)
FPO = .707/(DNO*CXS)
DX = XI*2./FLOAT(NI)
AKNO = FPO/DX

C
XC(1,J) = X1*(1.-FLOAT(J-1)/FLOAT(NI-1)*2.)
CENTR = DABS(XC(1,J))
IF(CENTR.LT.0.001) XC(1,J) = 0.
RC(1,J) = RI

C
IF(J.GT.1) GO TO 29
C
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
C THE MESH DIMENSION.
C
SCALE = DX*DATAN(DARSIN(1./AM0))/2.
TIME1 = SCALE/VELO
TIME2 = 3./((.CXS*DNO)*DSQRT(BOLTZ/TO/(PI*GMM)))
P = TIME2/TIME1
DENSF(1,1) = P

CONTINUE

C
WRITE(6,11) J,AMCOR(1,J),R1,XC(1,J),TETAC(1,J),TO,PO,VELO,AKNO,FPO
11 FORMAT(' ',214.5F10.3,3E12.5,F9.4,2E12.3)

CONTINUE

C
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

WRITE (6,198)
198 FORMAT('1', ' CORE '/)
APM = 0.
BPM = 0.
CPM = 0.

DO 199 I = 2, N1
WRITE (6,10)
DO 199 J = 1, N1
IF (CI+J-1).GT.N1) GO TO 199
AMIL = DARSINC1./AMCORCI-1,J))
ALFAL = PI-(TETAC(I-1,J)+AMIL) AMIR = DARSINC1./AMCOR(I-1,J+1))
ALFAR = TETAC(I-1,J+1)-AMIR
XC(I,J) = (RC(I-1,J)-RC(I,J+1)+XCI-I,J)*DTAN(ALFAL)+XCI-I,J+1)*DTAN(ALFAR)
CENTR = DABS(XC(I,J))
IF (CENTR.LT.0.001) XC(I,J) = 0.
RC(I,J) = RC(I-1,J+1)+(XC(I,J)-XC(I-1,J+1))*DTAN(ALFAR)
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)

APM = PMC(I-1,J)+PMC(I-1,J+1)+TETAC(I-1,J+1)-TETAC(I-1,J)
IF (KD.EQ.2) GO TO 151
BPM = DSINC(AMIL)*DSIN(TETAC(I-1,J+1)))/RC(I-1,J+1)*DKSI
CPM = DSINC(AMIL)*DSIN(TETAC(I-1,J))/RC(I-1,J)*DETA
PMCI(I,J) = (APM+BPM+CPM)/2.0

AMG = AMCOR(I-1,J+1) KZ = 0
154 IF (KZ.GE.100) GO TO 160
KZ = KZ+1
C = AMG*AMG*A3+1.
D = DSQRT(AMG*AMG-1.) PMCAL = A2*DATAN(B2*D)-DATAN(D)
DELNI = PMCAL - PMCI(I,J)
DEL = DABS(DELNI)
IF (DEL.LT.0.000002) GO TO 160
IF (DELNI.LT.0.) GO TO 156
AMG = AMG*.999
GO TO 154
156 AMG = AMG*(1.-DELNI*C/D)
GO TO 154
160 AMCOR(I,J) = AMG

CALCULATE FLOW PARAMETERS IF (J.GT.1) GO TO 197
C = AMCOR(I,J)*AMCOR(I,J)*A3+1.
PRES = PSTG/(C*X@B1) TEMP = TSTG/C DN = PRES/(BOLTZ*TEMP) FP = .707/(DN*CXS) SCALE = DKSI * DSINC(ALFAL) AKN = FP/SCALE

50
SOUND = DSQRT(GAMA*RJ*TEMP)
VEL = SOUND*AMCOR(I,J)

BREAKDOWN PARAMETER AS DEFINED BY 'BIRD'.
DENSF(I,J) = PRES/(RJ*TEMP)
DDENS = DENSF(I-1,J) - DENSF(I,J)
COLF = 4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM))
P = VEL*DDENS/(SCALE*DENSF(I,J)*COLF)

197 CONTINUE

TIME1 = SCALE/VEL
TIME2 = 3./(4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM)))
P = TIME2/TIME1

WRITE(6,11)I,J,AMCOR(I,J),RC(I,J),XC(I,J),TETAC(I,J),TEMP,PRES,VEL

199 CONTINUE

MATCH CORE AND FAN POINTS
DO 200 I=1,N1
X(I,1) = XC(I,1)
R(I,1) = RC(I,1)
AM(I,1) = AMCOR(I,1)
PM(I,1) = PMCCI,1)
TETA(I,1) = TETAC(I,1)
GO TO 207
200 TETA(I,1) = TETAC(I,1)

CALCULATE FLOW PARAMETERS IN REGION 2 (SIMPLE PRANDTL MEYER FAN).
WRITE(6,298)

298 FORMAT ('1', ' REGION 2/')

C CHECK ANGLES AND CALCULATE COORDINATES
ANGLE1 = PI/2.-.000001
ANGLE2 = PI/2.+0.000001
IF (ALFAL.LE.ANGLE1.OR.ALFAL.GE.ANGLE2) GO TO 201
X(I,J) = X(I-1,J)
GO TO 207
201 IF (ALFAR.LE.ANGLE1.OR.ALFAR.GE.ANGLE2) GO TO 205
X(I,J) = X(I,J-1)
GO TO 207

205 X(I,J) = (RI-1,J)-R(I,J-1)+X(I,J-1)*DTAN(ALFAR)+X(I-1,J)*DTAN(ALFAXS0350)

1AL))/DTAN(ALFAL)+DTAN(ALFAR))

207 IF (ALFAL.LE.0.000001.OR.ALFAL.GE.0.000001) GO TO 209
R(I,J) = R(I-1,J)
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

211 R(I,J) = (X(I,J)-X(I,J-1))*DTAN(ALFAR)+R(I,J-1)
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)  
  C
  IF (R(I,J).GT.0.AND.X(I,J).GT.0.) GO TO 219
  Kfin = J-1
  WRITE(6,12)
  12 FORMAT(' FURTHER POINTS ON THE CHARACTERISTICS ARE DIVERGENT')
  219 CONTINUE
  C LOCATION OF THE NEW MESH POINT HAS BEEN FOUND
  C
  C CALCULATE NOW PRANDTL MEYER FUNCTION AND FLOW DIRECTION FOR NEW POINT
  APM = Pmci,J-1)Pm(I-1,J)-Tetaci-1,J)+Teta(I,J-1)
  IF (KD.EQ.2) GO TO 251
  BPM = DSINCAMIR)*DSINTETA(I,J-1)/R(I,J-1)*DKSI
  CPM = DSINCAMIL)*DSINTETA(I-1,J)/R(I-1,J)*DETA
  251 Pm(I,J) = .5*(APM+BPM+CPM)
  C
  C CALCULATE NOW MACH NUMBER FOR EACH POINT
  C
  INITIAL GUESS AM(I,J) = AM(I-1,J)
  AMG = AM(I-1,J)
  KZ = 0
  254 IF (AM.GT.200.) GO TO 257
  D = DSQRT(AM*AM-1.)
  GO TO 258
  257 D = AMG
  258 IF (KZ.GE.100) GO TO 260
  PMCAL = A2DATAN(B2*D)-DATAN(D)
  DELNI = PMCAL - PM(I,J)
  DEL = DABS(DELNI)
  IF (DEL.LT.0.000002) GO TO 257
  IF (DELNI.LT.0.)GO TO 256
  AMG = AMG*.999
  GO TO 254
  C
  256 IF (AM.GT.2000.)GO TO 2560
  KFIN = J-1
  GO TO 299
  C
  2560 D1 = (A3*AMG*AMG-1.)
  AMG = AMG*(1.-DELNI*D1/D)
  GO TO 254
  C
  260 AM(i,J) = AMG
  C CALCULATE NOW LOCAL TEMPERATURE,PRESSURE,VELOCITY,KNUDSEN NO.
  C = AMI,J)AAM(I,J)AAS+1
  Pres = PSTG/C**B1
  Temp = TSTG/C
  Dn = PRES/(BOLTZ*TEMP)
  DENSF(I,J) = PRES/(RJ*TEMP)
  DDENS = DENSF(I-1,J)-DENSF(I,J)
  SCALE = DSQRT((X(I,J)-X(I-1,J-1))**2+(R(I,J)-R(I-1,J-1))**2)
  C
  271 FP = .707/(DN*CXS)
  C
  AKN = FP/SCALE
  SOUND =DSQRT(GAMMA*RJ*TEMP)
  VEL = AM(I,J)*SOUND
  C
  COLF = 4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI**GMM))
  P = VEL*DDENS/(SCALE*DENSF(I,J)*COLF)
  C
  PRINT RESULTS FOR MESH POINTS
  KL = (-1)**I
  IF (KL.LT.0) GO TO 299
  WRITE(6,11)I,J,AM(I,J),R(I,J),X(I,J),TETA(I,J),TEMP,PRES,VEL,AKN
1FP,DN,P

299 CONTINUE
C
C MATCH 'REGION 2' AND 'REGION 3' POINTS
C
L = KFIN- 1
DO 300 J = 1,L
XX(1,J) = X(20,J)
RX(1,J) = R(20,J)
AMX(1,J) = AM(20,J)
PMX(1,J) = PM(20,J)
300 TETAX(1,J) = TETA(20,J)
C CACULATE FLOW PARAMETERS FOR REGION 3
C
WRITE (6,397)
397 FORMAT ('1',"REGION 3/")
DO 399 I = 2,L
DO 399 J = I,L
IF (J.GT.KFIN) GO TO 399-
IF (J.GT.I)GO TO 320
WRITE (6,10)
320 KZ = 0
C
AMIL = DARSIN(1./AMX(I-1,J))
ALFAL = PI-(TETAX(I-1,J)+AMIL)
IF (J.GT.I) GO TO 301
ALFAR = ALFAL
TETAX(I-1,J) = PI-TETAX(I-1,J)
XX(I,J) = 0.
RX(I,J) = RX(I-1,J)+XX(I-1,J)*DTAN(ALFAL)
RX(I,J-1) = RX(I-1,J)
XX(I,J-1) = -XX(I-1,J)
DKSI = (RX(I,J)-RX(I-1,J))/DSIN(ALFAL)
DETA = DKSI
PMX(I,J-1) = PMX(I-1,J)
GO TO 316
301 AMIR = DARSIN(1./AMX(I-1,J))
ALFAR = TETAX(I-1,J)-AMIR
C
IF (ALFAL.LE.ANGLE1.OR.ALFAL.GE.ANGLE2) GO TO 302
XX(I,J) = XX(I-1,J)
GO TO 307
302 IF(ALFAR.LE.ANGLE1.OR.ALFAR.GE.ANGLE2) GO TO 305
XX(I,J) = XX(I-1,J)
GO TO 307
305 XX(I,J) = (RX(I-1,J)-RX(I,J-1)+XX(I-1,J)-XX(I,J-1))**2+XX(I-1,J)**2)
1N(ALFAL))**2+DTAN(ALFAL)**2)
C
IF (ALFAL.LE.0.000001.OR.ALFAL.GE.0.000001) GO TO 309
RX(I,J) = RX(I-1,J)
GO TO 315
309 IF(ALFAR.LE.0.000001.OR.ALFAR.GE.0.000001) GO TO 311
RX(I,J) = RX(I,J-1)
GO TO 315
311 RX(I,J) = RX(I,J-1)+XX(I,J)-XX(I,J-1))**2+XX(I,J)**2)
316 CONTINUE
C
IF (RX(I,J).GE.0..AND.XX(I,J).GE.0.)GO TO 319
KFIN = J-1
WRITE (6,398)

53
398 FORMAT ('FURTHER POINTS ON THE CHARACTERISTICS ARE DIVERGENT')

C LOCATION OF THE NEW POINT HAS BEEN FOUND

C CALCULATE NORMAL P.M. ANGLE AND FLOW DIRECTION
319 APM = PMX(I-1,J-1)+PMX(I,J)+TETA(I,J-1)+TETA(I-1,J)
IF(KD.EQ.2) GO TO 351
BMP = DSIN(AMIR)*DSIN(TETA(I,J-1))/RX(I,J-1)*DKSI
CPI = DSIN(AMIR)*DSIN(TETA(I-1,J))/RX(I-1,J)*DETA

351 PMX(I,J) = .5*(APM+BMP+CPI)
APM = PMX(I-1,J-1)+PMX(I,J)+TETA(I-1,J)+TETA(I,J-1)
TETA(I,J) = .5*(APM+BMP+CPI)

C CALCULATE THE MACH NUMBER FOR EACH POINT

C INITIAL GUESS
AMX(I,J) = AMX(I-1,J)
AMG = AMX(I,J)
KZ = 0
KH = 0
KL = 0
KFIN = J-1
GO TO 399

354 IF (AMG.GT.2000.) GO TO 357
D = DSQRT(AMG*AMG-1.)
GO TO 358

357 D = AMG

358 IF (KZ.GE.50) GO TO 360
DELNI = PMCAL-PMX(I,J)
DEL = DABS(DELNI)
IF (DEL.LT.0.) GO TO 356
AMG = AMG.*.98
GO TO 354

356 IF (AMG.LT.5000.) GO TO 3560
KFIN = J-1
GO TO 399

3560 D1 = AMG*AMG+1.*C
DDELNI = DELNI
IF (AMG.GT.20.) DDELNI = DELNI*(.95**KZ)

C CALCULATE THE LOCAL TEMPERATURE, PRESSURE, VELOCITY, KNUDSEN
C = AMX(I,J)*AMX(I,J)*A3+1.
PRES = PST/(C**B1)
TEMP = TSTG/C
DN = PRES/(BOLTZ*TEMP)
DENSF(I,J) = PRES/(RJ*TEMP)
DDENS = DENSF(I-1,J)-DENSF(I,J)
SCALE = DSQRT((XX(I,J)-XX(I-1,J-1))**2+(RX(I,J)-RX(I-1,J-1))**2)
AKN = FP/SCALE
C
C ALFALL = -ALFALL+PI
AF = ALFALL-PI/2.
AF = DABS(AF)
IF (AF.LT.00001) GO TO 370
BF = 1./DSQRT(1.+DTAN(ALFALL)**2)
SCALE = BF*(RX(I,J-1)-DTAN(ALFALL)*(XX(I,J-1)-XX(I-1,J)-RX(I-1,J-1)))
C
SOUND = DSQRT(GAMA*RJ*TEMP)
VEL = AMX(I,J)*SOUND
C
C COLF = COLF/SCALE*DENSF(I,J)*COLF
P = PRES/(SCALE*DENSF(I,J)*COLF)

C
C PRINT RESULTS
WRITE(6, 11)I, J, AMX(I, J), RX(I, J), XX(I, J), TETAX(I, J), TEMP, PRES, VEL
1AKN, FP, DN, P
399 CONTINUE
STOP
END
$ENTRY
### A.4 LIST OF MAIN SYMBOLS USED IN 'AXSYM'.

<table>
<thead>
<tr>
<th>Parameter Name</th>
<th>Physical Name</th>
<th>Units</th>
<th>Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PAMB</td>
<td>ambient pressure</td>
<td>pascals</td>
<td>real</td>
<td>ambient atmosphere pressure</td>
</tr>
<tr>
<td>KD</td>
<td>K dimensions</td>
<td>-</td>
<td>integer</td>
<td>KD=2 for two dimensional jet</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>KD=3 for axisymmetric ring jet</td>
</tr>
<tr>
<td>PI</td>
<td>π</td>
<td>-</td>
<td>real</td>
<td>constant</td>
</tr>
<tr>
<td>BOLTZ</td>
<td>Boltzmann constant</td>
<td>Joule</td>
<td>real</td>
<td>1.38032 x 10^{-23} joules/degree</td>
</tr>
<tr>
<td>AVOG</td>
<td>Avogadro's constant</td>
<td>molecules mol</td>
<td>real</td>
<td>6.0225 x 10^{26} 1/kmol</td>
</tr>
<tr>
<td>RG</td>
<td>Universal gas constant</td>
<td>Joule mol.deg</td>
<td>real</td>
<td>8314.3</td>
</tr>
<tr>
<td>AMO</td>
<td>Mach No. (E.P)</td>
<td>-</td>
<td>real</td>
<td>Mach number at exit plane</td>
</tr>
<tr>
<td>TO</td>
<td>Temperature (E.P)</td>
<td>°k</td>
<td>real</td>
<td>Temperature at exit plane</td>
</tr>
<tr>
<td>PO</td>
<td>Pressure (E.P)</td>
<td>pascals</td>
<td>real</td>
<td>Pressure at exit plane</td>
</tr>
<tr>
<td>R1</td>
<td>Cylinder radius</td>
<td>m</td>
<td>real</td>
<td>Radius of the cylindrical vehicle</td>
</tr>
<tr>
<td>X1</td>
<td>0.5* nozzle width</td>
<td>m</td>
<td>real</td>
<td>Half width of nozzle</td>
</tr>
<tr>
<td>GAMA</td>
<td></td>
<td>-</td>
<td>real</td>
<td>averaged heat capacity ratio (jet)</td>
</tr>
<tr>
<td>DIAM</td>
<td>Molecule diameter</td>
<td>m</td>
<td>real</td>
<td>averaged molecular diameter (jet)</td>
</tr>
<tr>
<td>GM</td>
<td>Molecular mass</td>
<td>kg/kmol</td>
<td>real</td>
<td>averaged molecular weight (jet)</td>
</tr>
<tr>
<td>RJ</td>
<td>Gas constant</td>
<td>joules kj.deg</td>
<td>real</td>
<td>gas constant (jet)</td>
</tr>
<tr>
<td>CXS</td>
<td></td>
<td>m²</td>
<td>real</td>
<td>collision cross section (hard sphere)</td>
</tr>
<tr>
<td>GMM</td>
<td>mass of a molecule</td>
<td>kg</td>
<td>real</td>
<td>averaged mass of a molecule</td>
</tr>
<tr>
<td>N1</td>
<td></td>
<td>integer</td>
<td></td>
<td>number of divisions (characteristics from the exit plane)</td>
</tr>
<tr>
<td>N2</td>
<td></td>
<td>integer</td>
<td></td>
<td>number of characteristics in the Prandtl Meyer fan</td>
</tr>
<tr>
<td>A1</td>
<td></td>
<td>real</td>
<td></td>
<td>γ - 1</td>
</tr>
<tr>
<td>B1</td>
<td></td>
<td>real</td>
<td></td>
<td>γ</td>
</tr>
</tbody>
</table>

56
### A.4 LIST OF MAIN SYMBOLS USED IN 'AXSYM' (CONTINUED)

<table>
<thead>
<tr>
<th>Parameter Name</th>
<th>Physical Name</th>
<th>Units</th>
<th>Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A2</td>
<td>real</td>
<td>((y + 1)/(y - 1))</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B2</td>
<td>real</td>
<td>(1/A2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A3</td>
<td>real</td>
<td>(\gamma - 1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>real</td>
<td>(H^2 \gamma - 1 + 1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D, D1, D2</td>
<td>real</td>
<td>(H^2 - 1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PSTG</td>
<td>pascals</td>
<td>real</td>
<td>stagnation pressure</td>
<td></td>
</tr>
<tr>
<td>TSTG</td>
<td>°k</td>
<td>real</td>
<td>stagnation temperature</td>
<td></td>
</tr>
<tr>
<td>DSTG</td>
<td>kg/m³</td>
<td>real</td>
<td>stagnation density</td>
<td></td>
</tr>
<tr>
<td>FSH</td>
<td>real</td>
<td>free stream Mach number</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FST</td>
<td>°k</td>
<td>real</td>
<td>free stream temperature</td>
<td></td>
</tr>
<tr>
<td>FSD</td>
<td>kg/m³</td>
<td>real</td>
<td>free stream density</td>
<td></td>
</tr>
<tr>
<td>AMIT</td>
<td>(\nu_T)</td>
<td>radius</td>
<td>real</td>
<td>Mach angle (tail of P.H. fan)</td>
</tr>
<tr>
<td>ANIH</td>
<td>(\nu_H)</td>
<td>radius</td>
<td>real</td>
<td>Mach angle (head of P.H. fan)</td>
</tr>
<tr>
<td>PMT</td>
<td>(\nu_T)</td>
<td>radius</td>
<td>real</td>
<td>P.H. function (tail)</td>
</tr>
<tr>
<td>PINH</td>
<td>(\nu_H)</td>
<td>radius</td>
<td>real</td>
<td>P.H. function (head)</td>
</tr>
<tr>
<td>NAT, RAT2, E1</td>
<td>real</td>
<td>used to define a logarithmic division of the corner characteristics (50 lines in P.H. fan) (a linear division would have resulted in concentration of characteristics at high Mach numbers)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DELIH</td>
<td>real</td>
<td>difference of Mach numbers</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ANH(I,J)</td>
<td>(H)</td>
<td>real</td>
<td>2-D array</td>
<td>Mach number at location ((I,j)) (used for the corner)</td>
</tr>
<tr>
<td>PH(I,J)</td>
<td>(\nu)</td>
<td>radius</td>
<td>P.H. function at location ((I,j)) (used for the corner)</td>
<td></td>
</tr>
<tr>
<td>ANH</td>
<td>(\mu)</td>
<td>radius</td>
<td>real</td>
<td>Mach angle</td>
</tr>
<tr>
<td>R(I,J)</td>
<td>(m)</td>
<td>real</td>
<td>2-D array</td>
<td>radius (or ordinate) at ((I,j))</td>
</tr>
<tr>
<td>TETA(I,J)</td>
<td>(\theta)</td>
<td>radius</td>
<td>real</td>
<td>2-D array</td>
</tr>
</tbody>
</table>
### A.4 LIST OF MAIN SYMBOLS USED IN 'AXSYM' (CONTINUED)

<table>
<thead>
<tr>
<th>Parameter Name</th>
<th>Physical Name</th>
<th>Units</th>
<th>Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALFAL</td>
<td>radians real</td>
<td>angle of a left running characteristics</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ALFAR</td>
<td>radians real</td>
<td>angle of a right running characteristics</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DENSF(I,J)</td>
<td>kg/m³ real 2-D array</td>
<td>gas density at point L_I</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AMCOR(I,J)</td>
<td>real 2-D array</td>
<td>Mach number at mesh points in region (1) (region 1 is bounded by the two tail characteristics</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TETAC(I,J)</td>
<td>radians real 2-D array</td>
<td>flow direction at mesh points (region 1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PHC(I,J)</td>
<td>radians real 2-D array</td>
<td>P.M. function at mesh points (region 1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>XC(I,J)</td>
<td>m real 2-D array</td>
<td>X coordinate at mesh points (region 1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>RC(I,J)</td>
<td>m real 2-D array</td>
<td>radius (ordinate) at mesh points (region 1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AHIL</td>
<td>radians real</td>
<td>Mach angle for left running characteristics</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AHIR</td>
<td>radians real</td>
<td>Mach angle for right running characteristics</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DKSI</td>
<td>dξ m real</td>
<td>distance between mesh points</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DETA</td>
<td>dη m real</td>
<td>distance between mesh points</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DELNI</td>
<td>dv radians real</td>
<td>P.M. differential</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AMG</td>
<td>radians real</td>
<td>Mach number (used for iterative calculation)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PRES</td>
<td>pressure</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>TEMP</td>
<td>temperature</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DN</td>
<td>number density</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>FP</td>
<td>mean free path</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>AKH</td>
<td>Knudsen number</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOUND</td>
<td>speed of sound</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>VEL</td>
<td>absolute local velocity</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>UDENS</td>
<td>density difference between two points along a streamline</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>COLF</td>
<td>collision frequency</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P</td>
<td>breakdown parameter</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
A.5 AXSYM PROGRAM USER'S GUIDE

1. Input data:
   ambient pressure \( P_{AMB} \)
   Mach number (Exit plane) \( A_H \)
   Temperature (Exit plane) \( T_O \)
   Pressure (Exit plane) \( P_O \)
   Half width of nozzle \( X_1 \)
   Radius of nozzle ring \( R_1 \)
   Specific heat ratio of jet gas \( G_{AI} \)
   average molecular diameter (jet) \( D_{IA} \)
   average molecular weight \( G_{H} \)

2. 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 \( N_1 \) and \( N_2 \) as necessary
   b - change 'DIMENSIONS' according to new values of \( N_1 \) and \( N_2 \)
   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:
   \[
   \text{WATFIV AXSYM *(XTYPE)}
   \]
   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
   AXSYM LISTING.
5. Hard Copy

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 \( n_0 = 4 \) and \( n_0 = 2 \) 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.
Figure 22. Definition of sector geometry and cell volume.

Cell volume = \( v(I) = R(I) \times \Delta \alpha \times \Delta r \times RSI \times DF \).

\[
\frac{v(I)}{v(l)} = \frac{R(I)}{R(l)} \times RSI(I)
\]

\( v(I) \) 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<1M).

L=1,2,3 - cartesian components of velocity \( v_x, v_y, v_z \) [m/s]
L=4 - radial coordinate [meters]
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.
2. \( C(M,I,j) \) Table 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
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 1)
N = 4 - VOL 1 = actual volume of smallest cell in kR
N = 5 - AREAl INPUT area of smallest cell in kR
5. **Region Geometry and Input Flux**

- **R(10)** - polar radius of a cell in a region
- **A(10)** - input area of a cell
  input area of smallest cell
- **VOL(10)** - volume of a cell
  volume of smallest cell
- **M1(10)** - initial number of molecules in cells
  (equal number of molecules of either jet species)
- **F1(10), F2(10)** - input flux through high pressure starting line
  (spec 1), (spec 2)
6. **Input Flux From High Pressure Starting Line**

FWP1(N,I,j)

FWP2(N,I,j)

<table>
<thead>
<tr>
<th>species</th>
</tr>
</thead>
<tbody>
<tr>
<td>positive (input molecules)</td>
</tr>
</tbody>
</table>

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 DFI

N = 2 - mean molecular velocity Vx

N = 3 - mean molecular velocity Vy

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)

<table>
<thead>
<tr>
<th>species</th>
</tr>
</thead>
<tbody>
<tr>
<td>negative (output)</td>
</tr>
</tbody>
</table>

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)

FEN2(4,NRD)  FWN2(4,NRD)

<table>
<thead>
<tr>
<th>species</th>
</tr>
</thead>
<tbody>
<tr>
<td>negative</td>
</tr>
</tbody>
</table>

east west
NRD = radial location

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)** output flow to the east
- **FOE1(4,kC,kR,kS)**
- **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 ($P_1(data, number \ of \ molecules)$, $P_2(data, number \ of \ molecules)$ are the vectors used for species 1 and 2)

b. an inactive molecule is defined as

$$[P_1(4,N) \ or \ P_2(4,N)] = -99$$
c. calculation of number of molecules to be set in each cell

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
   \[ P1(5,N), P2(5,M) \] are angular coordinate in radians

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

  
g. definition of molecular velocities
   \[ P1(1,N), P2(1,M) \] velocity in X direction
   \[ P1(2,N), P2(2,M) \] velocity in Y direction
   \[ P1(3,N), P2(3,M) \] velocity in Z direction

   Thermal velocities are random function of temperatures and are added to the mean velocity as defined at initial boundary \( \alpha \) 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
1. reset general time counter: $\text{Time} = 0$

3. The Simulation

a. Move all molecules according to their velocity $(V_x, V_y)$ 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 $(FSNX))$

$$FSNX(1,j,kR) \rightarrow \text{"south" boundary}$$
$$FNNX(1,j,kR) \rightarrow \text{"north" boundary}$$
$$FENX(1,I) \rightarrow \text{"east" boundary}$$
$$FWNX(1,I) \rightarrow \text{"west" boundary}$$

$I$ 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

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

for "E" side of any region

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

for "N" side of any region

FSNX(P, j, kR+1)

for "S" side of the region

FNNX(P, j, kR-1)

The first parameter of all these arrays represent:
P = 1 - number flux (real number)
P = 2 - velocity component - (Vx)
P = 3 - velocity component - (Vy)
P = 4 - gas temperature

73
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 P1 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.
The array IC(k,i,j) contains integer data 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)

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).

![Graphic Description of IP(M)](image)

Figure 23. Vector IP(M)
B.3 SIMUL Program Flowchart

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.
Figure 24. SIMUL program flowchart.
B.4 SIMUL Program Listing

C PROGRAM SIMUL
C THIS PROGRAM IS DESIGNED TO CALCULATE THE MOLECULAR FLOW OUTSIDE THE
C CONTINUUM REGION FLOW OF A HIGHLY UNDEREXPANDED ASYMMETRIC RING JET.
C RESULTS FOR THE CONTINUUM FLOW MAY BE OBTAINED FROM 'AXSYM' PROGRAM
C WHICH GIVES THE CHARACTERISTICS OF ISENTROPIC SOLUTION.
C THE BOUNDARY BETWEEN THE CONTINUUM AND MOLECULAR FLOW IS DEFINED BY
C THE BREAKDOWN PARAMETER 'P' AS PROPOSED BY G. A. BIRD.
C THE 'MOLECULAR DOMAIN' IS DIVIDED INTO POLAR DIVISIONS MAKING A SET
C OF SECTORS. EACH SECTOR IS SUBDIVIDED INTO 10 REGIONS
C NO APRIORY INFORMATION ABOUT THE GEOMETRY OF THE DIFFERENT
C REGIONS IS AVAILABLE, THEREFORE, MANUAL INTERVENTION MAY BE
C REQUIRED WHEN MOVING FROM ONE SECTOR TO THE OTHER. AN ACCEPTABLE
C GEOMETRY WILL RESULT A REASONABLE NUMBER OF SIMULATED MOLECULES.
C EACH REGION IS SUBDIVIDED INTO A NUMBER OF CELLS WITH A GEOMETRY
C DEFINED BY A POLAR MESH. A NUMBER OF MOLECULES IS SET IN EACH CELL
C PROPORTIONAL TO THE CELL VOLUME. THE BOUNDARY CONDITIONS FOR EACH
C REGION REQUIRE INPUT AND OUTPUT FLOW OF MOLECULES. NO APRIORY
C INFORMATION ON THE FLUX IS AVAILABLE. IT WILL BE CALCULATED IN
C AN ITERATIVE MODE.
C IF THE BOUNDARY CONDITIONS FOR ALL CELLS ARE CONSTANT THE NUMBER
C OF MOLECULES IN EACH CELL IS PROPORTIONAL TO CELL WALL AREA.
C TO DECREASE THE ERROR WHEN INTRODUCING MOLECULES - (INTEGER NUMBER) -
C DUE TO THE INPUT FLUX - (REAL NUMBER), AN ADDITIONAL MOLECULE IS
C GENERATED ON THE BASIS OF RANDOM NUMBERS SUCH THAT THE AVERAGE OF A
C LARGE NUMBER OF SAMPLINGS WILL EQUAL THE REAL INPUT FLUX.
C******************************************************************************
C THE MONTE CARLO SIMULATION
C THE JET IS COMPOSED OF TWO SPECIES OF MOLECULES
C AMBIENT GAS IS REGARDED AS ONE SPECIES
C THE MOLECULAR MODEL IS - 'HARD SPHERE MOLECULE'
C NETWORK DEFINITION
C THE MAXIMUM RADIUS (POLAR) OF THE DOMAIN IS ASSUMED TO BE RP=15 M.
C THE ANGLE OF THE BOUNDARY BETWEEN CONTINUUM AND MOLECULAR FLOW
C AND THE SOLID WALL IS
C ALFA (CALCULATED IN PROGRAM 'AXSYM')
C DEFINE A POLAR SECTOR WITH A RADIUS 'RP' AND AN ANGLE OF
C ALFA = 5*RP/NAD/2/R
C THIS SECTOR IS SUBDIVIDED INTO A NUMBER OF RADIAL DIVISIONS
C MAKING 'N' REGIONS FOR SIMULATION CALCULATIONS FOR EACH 'DALFA'.
C EACH REGION IS DIVIDED INTO
C NAD-ANGULAR DIVISIONS (15) WITH AN ANGLE OF DDALFA=5*RP/NAD/R
C NRD - RADIAL DIVISIONS (10)
C MAKING NAD*NRD CELLS
C THE SMALLEST CELL CONTAINS 'MIN' MOLECULES
C N = 15
C TOTAL NUMBER OF ACTIVE MOLECULES IN A REGION IS LIMITED TO 6000
C (3000 MOLECULES OF EACH SPECIES.)
C THE WIDTH OF A CELL DEFINED BY ANGLE 'DFI' MAY NOW BE EVALUATED.
C (MIN/NUMBER DENSITY = ACTUAL CELL VOLUME)
C******************************************************************************
C THE COMMON PARAMETERS ARE
C******************************************************************************
C DIMENSION P1(5,3000),P2(5,3000),IP(6000),C(20,10,15),
* D(4,10,15),REG(5,10,20)
C DIMENSION DF1(10),DN(10)
C DIMENSION R(10),A(10),VOL(10),MI(10),F1(10),F2(10)
C DIMENSION SS(2,10,10)
C DIMENSION FEN(4,10),FNN1(4,10),FNN1(4,15,10),FSN1(4,15,10)
C DIMENSION FEN2(4,10),FNN2(4,10),FNN2(4,15,10),FSN2(4,15,10)
C DIMENSION FHP1(4,10,10),FHP2(4,10,10)
C DIMENSION FEN3(4,10,10,20),FNN1(4,10,20,20),
C FNN2(4,10,20,20),FNN3(4,10,20,20)
C DIMENSION NN0(3,5),VRC(3,5),TOC(3,5),SPEC(3,5),NCOL(10,15)
C P1,P2,P3 CONTAIN INFORMATION ON UP TO M SIMULATED MOLECULES
C P1(1,N),P1(2,N),P1(3,N) ARE U,V,W VELOCITY COMPONENTS (CARTESIAN)
C P1(4,N),P1(5,N) ARE R AND TETA COORDINATES (POLAR)
C IP(M) ARE THE M MOLECULES ARRANGED IN THE ORDER OF THEIR CELLS
C C(20,1,1) CONTAINS INFORMATION ON UP TO IJ) CELLS
C******************************************************************************
C ALFA IS THE ANGLE WHERE THE BREAKDOWN PARAMETER EQUALS .05
C FPM IS THE MEAN FREE PATH AT ALFA.

C ################################################################################################################### SIMO0730
C SET GENERAL CONSTANTS.................................................. BLOCK 2 SIMO0740
IX = 529814367
PI = 3.141593
BOLTZ = 1.380464E-23
PO = 101325.
TO = 273.
AVOG = 2.68699E+25
RG = 8314.

C################################################################################################################### SIMO0750
C SET PROGRAM CONSTANTS.................................................. BLOCK 3 SIMO0800
ISPEC=2
RI = 2.5
DR=.15
RP=15.

C NUMBER OF SIMULATED MOLECULES IN SMALLEST CELL (DIFFERENT SPECIES)
NMOL1=3000
NMOL2=3000
NMOL3=0
MIN = 15
NIM = 15
N2M = 15

C NUMBER OF DIVISIONS IN A SIMULATED REGION
NAD = 15
NRDS=10
NRD=10
NAD1 = 3
NIS =2
DR IS THE RADIUS OF THE CYLINDER (WALL)
C RI IS THE RADIAL COORDINATE OF CELL(I)
C VOL(I) IS THE RATIO BETWEEN VOLUMES OF CELL(I) AND CELL(1)
C AC(I) IS THE RATIO BETWEEN INPUT FLOW AREAS OF CELL(I) AND CELL(1)
C INPUT THE FOLLOWING AS 'DATA' OR 'READ' STATEMENTS **

TETA = 1.2
C TETA IS THE FLOW DIRECTION (RADIANS) ON THE BREAKDOWN LINE AS FOUND
C FROM THE AXSYM PROGRAM. VO IS THE FLOW VELOCITY (M/SEC)

V0 = 2100
VOX = V0*COS(TETA)
VOY = V0*Sin(TETA)
TWALL=300.
DN01=1.1E21
DN02=1.1E21
DTM=1.5E-6

C SET DATA FOR THE DIFFERENT SPECIES
C MOLECULAR MASS
SPEC(1,1)=4./AVOG
SPEC(2,1)=40./AVOG
SPEC(3,1)=29./AVOG
C MOLECULAR DIAMETER
SPEC(1,2)=2.19E-10
SPEC(2,2)=4.00E-10
SPEC(3,2)=
C SPEC(1,3)=
C SPEC(2,3)=
C SPEC(3,3)= ADDITIONAL DATA IF REQUIRED

C THERMAL VELOCITIES AT WALL TEMPERATURE
VM11=SQR(2.*BOLTZ*TWALL/SPEC(1,1))
VM12=SQR(2.*BOLTZ*TWALL/SPEC(2,1))

C INITIATION..RESET ALL SAMPLING VARIABLES
DO 80 I=1,NRD
DO 80 JR=1,10
DO 80 JS=1,20
DO 80 KPAR=1,4
FOEI(KPAR,I,JR,JS)=0.
FOE2(KPAR,I,JR,JS)=0.
FOW1(KPAR,I,JR,JS)=0.
FOW2(KPAR,I,JR,JS)=0.
80 CONTINUE
C SET INPUT PARAMETERS ........................................... BLOCK 3
ITER=1

C RETURN TO 3000 FOR ADDITIONAL ITERATIONS
3000 KS=1
ALFA=1.3
FPM=.001
TEMP=40.
VTER1=SQR(2.*BOLTZ*TEMP/SPEC(1,1))
VTER2=SQR(2.*BOLTZ*TEMP/SPEC(2,1))
IF (ITER.GT.1)GO TO 2005
DO 2001 I=1,10
REG(2,I,1)=DNO1
REG(3,I,1)=DNO2
DO 2001 J=1,10
FWP1(2,I,J)=VOX
FWP2(2,I,J)=VOX
FWP1(3,I,J)=VOY
FWP2(3,I,J)=VOY
FWP1(4,I,J)=TEMP
FWP2(4,I,J)=TEMP
2005 CONTINUE

C DEFINE SECTOR GEOMETRY ........................................ BLOCK 4
C KR IS THE INDEX FOR A REGION IN ONE SECTOR
C RETURN TO 1000 FOR NEXT SECTOR
DALFA=0.
1000 KR=1
C RESET SAMPLING OF FLOW VARIABLES (N AND S)
DO 81 I=1,NAD
DO 81 JR=1,10
DO 81 KPAR=1,4
FNN1(KPAR,I,JR)=0.
FNN2(KPAR,I,JR)=0.
FSN1(KPAR,I,JR)=0.
FSN2(KPAR,I,JR)=0.
81 CONTINUE
C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFA SUBTRACTED FROM PREVIOUS ALFA (PREVIOUS SECTOR) GIVES THE NEW ALFA.
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*75/RP))DALFA=ALFA
IF(ALFA.LE.0.)GO TO 2000
DALFA = DALFA/FLOAT(NAD)
C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR
ALFAJ=ALFA-DALFA/2.
C
C DEFINE REGION KR IN SECTOR .................................... BLOCK 5
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 82 KPAR=1,4
FEN1(KPAR,I)=0.
FEN2(KPAR,I)=0.
82 CONTINUE
MT=0
NRD=NRDS
IF(KR.LT.2)NRD=NRD1
DO 100 I = 1,NRD
R(i) =(FLOAT(I)-.5)*DR
IF(KR.EQ.3)R(i)=R(i)+FLOAT(NRDI)*DR
100 CONTINUE
C POLAR RADIUS MEASURED FROM THE NOZZLE LIP
R(I) =(FLOAT(I)-.5)*DR
IF(KR.EQ.2)R(I)=R(I)+FLOAT(NRDI)*DR
C RSI IS THE RADIUS MEASURED FROM THE AXIS OF SYMMETRY
RSI=R(I)+R1/SIN(ALFAJ)
IF(I.EQ.1)RS1=RSI
A(I) = RSI/RSI
VOL(I) = R(I)*RSI/(R(I)*RS1)
M1(I) = MIN(VOL(I)
MT = MT+M1(I)

C M1() IS THE INITIAL NUMBER OF MOLECULES IN EACH CELL
DN1=REG(2,KR,KS)
DN2=REG(3,KR,KS)

C DFI (REG(1,KR,KS)) IS THE SPHERICAL (AXISYMMETRIC) ANGLE
C THIS ANGLE HAS DIFFERENT VALUES FOR EACH KR, THEREFORE IT IS A
C WEIGHTING FACTOR.

C (FNN1,FNN2,FSN1,FSN2,FEN1,FEN2,FWN1,FWN2) * DFI
C (FOE1,FOE2,FOW1,FOW2) * DFI

C DA1 IS THE INPUT AREA OF CELL(I)
FN1 = VO*DA1*REG(2,KR,KS)*SIN(ALFA-TETA)
FN2 = VO*DA1*REG(3,KR,KS)*SIN(ALFA-TETA)

C TETA IS THE ANGLE BETWEEN FLOW DIRECTION AND THE WALL
F1(I) = FN1*A(I)
F2(I) = FN2*A(I)

C F1(I) IS THE INPUT FLUX TO CELL(I)
C FOLLOWING ARE THE REGION BOUNDARIES

C DEFINE ACTUAL VOLUME AND INPUT AREA OF SMALLEST CELL IN REGION
REG(4,KR,KS)=R(1)*DDALFADR*RSINREG(1,KR,KS)
REG(5,KR,KS)=DA1

C FN1 IS THE NUMBER FLUX TO THE SMALLEST CELL (REAL NUMBER) PER SECOND.
C INPUT NUMBER OF MOLECULES (INTEGER) WILL BE INTEGRATED TO MAKE AN
C AVERAGE OF FN1.
C F1(I) IS THE INPUT FLUX TO CELL(I)
C FOLLOWING ARE THE REGION BOUNDARIES

DO 9102 I = 1, NRD
WRITE (6,9101)R(I),A(I),VOL(I),M1(I),F1(I)
9101 FORMAT(' ',3F13.5,I10,E15.5)
9102 CONTINUE

WRITE(6, 103)MT
103 FORMAT(I

C INITIAL NUMBER OF SIMULATED MOLECULES IS 'IS' PER SPES
X CIES PER DDALFA, TOTAL NUMBER IS 'IS'

C DEFINE INPUT FLOWS TO KR W,E,N,S ................................................................... BLOCK 6
C
C SET INITIAL STATE OF GAS.............................................................................. " &

C DO 150 I =1,NRD
DO 150 J = 1,NAD

C SET SIMULATED MOLECULES IN THEIR CELLS
IC(1,I,J) = M1(I)
IC(2,I,J) = M1(I)
IC(3,I,J) = 0

C SET CELL COORDINATES
C(19,I,J) = R(I)
C(20,I,J) = ALFA-(FLOAT(J)-.5)*DDALFA

150 CONTINUE

C DEACTIVATE ALL MOLECULES
DO 170 N = 1,NMOL
P1(N) = -99.
P2(N) = -99.
C******************************************************************************
C SET INITIAL STATE OF THE GAS (LOCATION AND VELOCITY OF MOLECULES)
C******************************************************************************

NADR1 = 0
NADR2 = 0
DO 200 I = 1, NRD
DO 200 J = 1, NAD
NM1 = IC(1, I, J)

DO 205 N = 1, NM1
NADR1 = NADR1 + 1
CALL RANDU(P)
PI(4, NADR1) = C(19, I, J) + DX*(P - .5)
CALL RANDU(P)
PI(5, NADR1) = C(20, I, J) + DDALFA*(P - .5)

DO 205 NV = 1, 3
203 CALL RANDU(P)
V = -.3 + 6 * RP
B = EXP(-V*V)
CALL RANDU(P)
IF(B.LT.P) GO TO 203
PI(NV, NADR1) = PI(NV, NADR1) + VOX
IF(NV.EQ.2) PI(NV, NADR1) = PI(NV, NADR1) + VOY

C******************************************************************************
C REPEAT PROCEDURE FOR SPECIES 2
C******************************************************************************

NM2 = IC(2, I, J)
DO 210 N = 1, NM2
NADR2 = NADR2 + 1
CALL RANDU(P)
P2(4, NADR2) = C(19, I, J) + DX*(P - .5)
CALL RANDU(P)
P2(5, NADR2) = C(20, I, J) + DDALFA*(P - .5)

DO 210 NV = 1, 3
207 CALL RANDU(P)
V = -.3 + 6 * RP
B = EXP(-V*V)
CALL RANDU(P)
IF(B.LT.P) GO TO 207
P2(NV, NADR2) = P*SIM01090
IF(NV.EQ.1) P2(NV, NADR2) = P2(NV, NADR2) + VOX
IF(NV.EQ.2) P2(NV, NADR2) = P2(NV, NADR2) + VOY

210 CONTINUE

C******************************************************************************
C WHEN NECESSARY, REPEAT PROCEDURE FOR SPECIES 3.
C******************************************************************************

200 CONTINUE

C******************************************************************************
C DEFINE HERE ALL COLLISION PARAMETERS TO BE INCLUDED IN SIMULATION
C******************************************************************************

C BLOCK 9
C RESET COLLISION TIMERS

DO 19 I = 1, NRD
DO 19 J = 1, NAD
DO 19 L = 1, 3
KT = 3*(L-1) + M + 9
C(KT, I, J) = 0

C SET EXPECTED MAXIMUM RELATIVE VELOCITY IN COLLISIONS

KV = 3*(L-1) + M
EM1 = SPEC(L, 1)
EM2 = SPEC(M, 1)
EMR = EM1*EM2/(EM1 + EM2)

IF(KS.EQ.I) GO TO 17
TEM = F0EI(4, I, KR, KS)
GO TO 18
17 TEM = FHP1(4, I, KR)

82
RV=2./SQRTCPIN2.XBOLTZXTE/EMR)

C MAXIMUM RELATIVE VELOCITY WILL BE RESET IF FASTER ENCOUNTERS OCCUR
C TIME=0.
C LOOP OVER TIME INTERVALS.......................... BLOCK 10
DO 6000 JDTM = 1, NIS
C
C TIME=TIME+DTM
C MOVE ALL MOLECULES .................. BLOCK 12
C MOVE MOLECULES OF SPECIES 1
C
DO 310 I = 1, NMOL1
C SKIP INACTIVE MOLECULES .................. BLOCK 13
IF (Pl(4,I1).EQ.-99.) GO TO 310
VX = P1(1,I1)
VY = P1(2,I1)
RX = P1(4,I1)
T = P1(5,I1)
TOLD=T
C FIND NEW COORDINATES .................. BLOCK 14
XX=RX*COS(T)+VX*DTM
YY=RX*SIN(T)+VY*DTM
RNEW=SQRT(XX**2+YY**2)
T=ATAN(YY/XX)
C FOR LAST SECTOR FIND COLLISIONS WITH THE WALL AND SAMPLE THEM
C
C ........................... BLOCK 15,16
C IF(ALFA.GT.DALFA)GO TO 301
IF(T.GT.0.)GO TO 301
C DTR IS THE TIME REMAINING AFTER A MOLECULE STRIKES THE WALL
C IF(DTR.LT.1E-10)DTR=1E-10
RW=RX+(RNEW-RX)*DTR/DTM
IF(RW.LT.RMIN)RW=RMIN+DTR*.001
IF(RW.GT.RMAX)RW=RMAX-DTR*.001
LOC=RW/DR+.999999
C COUNT COLLISIONS WITH THE WALL(MUST BE WAIGHTED =**DFI)
SS(1,LOC,JSAMP)=SS(1,LOC,JSAMP)+1
C SET VELOCITY AND LOCATION AFTER A MOLECULE STRIKES THE WALL
CALL RANDU(P)
B=VWM1*SQRT(-ALOG(P))
B=VWM1*SQRT(-ALOG(P))
CALL RANDU(P)
BB=2.*PI*P
CALL RANDU(P)
P1(1,NADR1)=B*COS(BB)
VX=B*COS(BB)
P1(2,NADR1)=B*SIN(BB)
VY=B*SIN(BB)
CALL RANDU(P)
P1(3,NADR1)=VWM1*SQRT(-ALOG(P))
XX=RX*COS(T)+VX*DDT
YY=RX*SIN(T)+VY*DDT
RNEW=SQRT(XX**2+YY**2)
T=ATAN(YY/XX)
C DEACTIVATE ALL MOLECULES THAT MOVED OUT .................. BLOCK 17
301 IF(RNEW.LT.RMAX.AND.RNEW.GT.RMIN.AND.T.LT.TMAX.AND.T,.GTTMIN)GO TO 303

303 RI=(RNEW-RMIN)/DR+.999999
IR=RI
TI=(TMAX-T)/DDALFA+.999999
IT=IT
IF(IT.LE.0)GO TO 304
IF(IT.GT.NAD)GO TO 305
IF(IR.GT.NRD)GO TO 306

C COUNT S DIRECTION, SAMPLE
FSNL(1,IT,KR)=FSNL(1,IT,KR)+1.
GO TO 309

C COUNT W DIRECTION, SAMPLE
IF(IR.LE.0)IR=1
IF(IR.GT.NRD)IR=NRD
FSNW(1,IR)=FSNW(1,IR)+1.
GO TO 309

C COUNT E DIRECTION, SAMPLE
IF(IR.LE.0)IR=1
IF(IR.GT.NRD)IR=NRD
FSNE(1,IR)=FSNE(1,IR)+1.
GO TO 309

C COUNT N DIRECTION, SAMPLE
FNIN(1,IT,KR)=FNIN(1,IT,KR)+1.
C SET NEW VALUES IN THE MOLECULE TABLE

C 309 RNEW=-99.
303 P1(4,11)=RNEW
P1(5,11)=T
310 CONTINUE

C REPEAT PROCEDURE FOR SPECIES 2 MOLECULES BLOCKS 12 TO 18
DO 320 12=1,NMOL2

C SKIP INACTIVE MOLECULES
IF(P2(4,12).EQ.-99.)GO TO 320
VX = P2(1,12)
VY = P2(2,12)
RX = P2(4,12)
T = P2(5,12)

TOLD=T

XX=RX*COS(T)+VX*DTM
YY=RX*SIN(T)+VY*DTM
RNEW=SQRT(XX**2+YY**2)
T=ATAN(YY/XX)

C COLLISIONS WITH THE WALL
IF(ALFA.GT.DALFA)GO TO 311
IF(T.GT.0.)GO TO 311

T=DTM*(T-TOLD)

C DTR IS THE TIME REMAINING AFTER A MOLECULE STRIKES THE WALL
IF(DTR.LT.1E-10)DTR=1E-10
RH=RX+(RNEW-RX)*DTR/DTM
IF(RH.LT.RMIN)RH=RH+DTR*.001
IF(RH.GT.RMAX)RH=RH-DTR*.001
LOC=RH/DR+1

C COUNT COLLISIONS WITH THE WALL (MUST BE WEIGHTED =FDI)
SS(2,LOC,JSAMP)=SS(2,LOC,JSAMP)+1

C FIND THE NEW COORDINATES OF THE MOLECULE
312 CALL RANDU(P)
B=1.2*M2*SQR(-ALOG(P))
CALL RANDU(P)
BB=2.*PI*P
PZ(1,NADR2)=B*COS(BB)
VX=B*COS(BB)
PZ(2,NADR2)=B*SIN(BB)
VY=B*SIN(BB)

CALL RANDU(P)
XX=RX*COS(T)+VX*DTR
YY=RX*SIN(T)+VY*DTR
RNEW=SQRT(XX**2+YY**2)
T=ATAN(YY/XX)

C DEACTIVATE MOLECULES THAT MOVED OUT.COUNT FOR OUTPUT FLUX EVALUATION.
IF(RNEW.LT.RMAX.AND.RNEW.GT.RMIN.AND.T.LT.TMAX.AND.T.GT.TMIN)GO TO 303

84
RI = (RNEW-RMIN)/DR+.999999
IR = RI
TI = (TMAX-T)/DDALFA+.999999
IT = TI
IF (IT.LE.0) GO TO 314
IF (IT.GT.NAD) GO TO 315
IF (IR.GT.NRD) GO TO 316

C COUNT S DIRECTION, SAMPLE ........................................ 18
FSN2(1,IT,KR)=FSN2(1,IT,KR)+1.

C COUNT H DIRECTION, SAMPLE .......................................... 19
P2(4, IZ) = RNEW
P2(5, IZ) = T
320 CONTINUE

C
319 RNEW = -99.

C
313 P2(4, IZ) = RNEW
P2(5, IZ) = T
320 CONTINUE

C
FSN2(1,IT,KR)=FSN2(1,IT,KR)+1.

C
FWN2(1,IR)=FWN2(1,IR)+1.

C
FEN2(1,IR)=FEN2(1,IR)+1.

C
FNN2(1,IR,KR)=FNN2(1,IR,KR)+1.

C
RNEW = -99.

C

C
FSN2(1,IT,KR)=FSN2(1,IT,KR)+1.

C
FWN2(1,IR)=FWN2(1,IR)+1.

C
FEN2(1,IR)=FEN2(1,IR)+1.

C
FNN2(1,IR,KR)=FNN2(1,IR,KR)+1.

C

C

C
FSN2(1,IT,KR)=FSN2(1,IT,KR)+1.

C
FWN2(1,IR)=FWN2(1,IR)+1.

C
FEN2(1,IR)=FEN2(1,IR)+1.

C
FNN2(1,IR,KR)=FNN2(1,IR,KR)+1.

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C
IF(RX.LT.RMIN.OR.RX.GT.RMAX)GO TO 340
IF(T.LT.TMIN.OR.T.GT.TMAX)GO TO 340
C FOR MORE ACCURATE CALCULATION SET THESE MOLECULES IN OUTPUT FLOWS
C
C DEFINE THE VELOCITY COMPONENTS
CALL RANU(P)
B=VTER1*SQRT(-ALOG(P))
CALL RANU(P)
BB2=2.*PI*P
VELX=VELX+B*COS(BB)
VELY=VELY+B*SIN(BB)
CALL RANU(P)
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
325 CONTINUE
C IF THERE IS NO ROOM FOR ADDITIONAL MOLECULE PRINT 'ALARM'
IF(CIACT.GE.NMOL1)GO TO 3004
326 P1(4,IACT)=RX
P1(5,IACT)=T
P1(1,IACT)=VELX
P1(2,IACT)=VELY
P1(3,IACT)=VELZ
340 CONTINUE
C
C REPEAT PROCEDURE FOR SPECIES 2
341 IF(NEW2.LT.1)GO TO 351
DO 350 I=1,NEW2
CALL RANU(P)
ATIME=P**DTM
CALL RANU(P)
RSTART=RMIN+(FLOAT(I-i)+P)*DR
VELX=FWP2(2,I,KR)
VELY=FNP2(3,I,KR)
TEM=FWP2(4,I,KR)
C THERMAL VELOCITY
VTER2=SQRT(2.*BOLTZ*TEM/SPEC(2,1))
XX=RSTART*COS(ALFA)+VELX*ATIME
YY=RSTART*SIN(ALFA)+VELY*ATIME
RX=SQRT(XX**2+YY**2)
T=ATAN(YY/XX)
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
C
C DEFINE VELOCITY COMPONENTS
CALL RANU(P)
B=VTER2*SQRT(-ALOG(P))
CALL RANU(P)
BB2=2.*PI*P
VELX=VELX+B*COS(BB)
VELY=VELY+B*SIN(BB)
CALL RANU(P)
VELZ=VTER2*SQRT(-ALOG(P))
C FIND A NEW MOLECULE TO BE ACTIVATED
DO 345 IACT=1,NMOL2
IF(P2(4,IACT).EQ.-99.)GO TO 346
345 CONTINUE
C IF THERE IS NO PLACE THEN PRINT ALARM
IF(CIACT.EQ.NMOL2)GO TO 3004
346 P2(4,IACT)=RX
P2(5,IACT)=T
P2(1,IACT)=VELX
P2(2,IACT)=VELY
P2(3,IACT)=VELZ
350 CONTINUE
C
C REPEAT PROCEDURE FOR SPEC-3
C
C INPUT E MOLECULES
IF (TMIN.LE.0.) GO TO 390

ANEW1 = FMIN1(I, I, KR, KS+1)

REM = ANEW1 - NEW1
CALL RANDU(P)
IF (P.LT.REM) NEW1 = NEW1+1

ANEW2 = FMIN2(I, I, KR, KS+1)
NEW2 = ANEW2
REM = ANEW2 - NEW2
CALL RANDU(P)
IF (P.LT.REM) NEW2 = NEW2+1

IF (NEW1.LE.0.) GO TO 370

DO 362 II=1, NEW1
CALL RANDU(P)
T = TMIN + DDALFA*P
CALL RANDU(P)
RNEW = RMIN + (FLOAT(I-1)+P)*DR
CALL RANDU(P)
TEM = FMIN1(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 = FMIN2(2, I, KR, KS+1)+B*COS(BB)
VELY = FMIN2(3, I, KR, KS+1)+B*SIN(BB)
CALL RANDU(P)
VELZ = VTER2*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
362 P1(5, IACT) = T
P1(1, IACT) = VELX
P1(2, IACT) = VELY
P1(3, IACT) = VELZ
370 CONTINUE

C REPEAT FOR SPECIES 2
IF (NEW2.LE.0.) GO 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 = FMIN2(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 = FMIN2(2, I, KR, KS+1)+B*COS(BB)
VELY = FMIN2(3, I, KR, KS+1)+B*SIN(BB)
CALL RANDU(P)
VELZ = VTER2*SQRT(-ALOG(P))

C FIND A NEW MOLECULE TO BE ACTIVATED
DO 384 IACT=1, NMOL2
IF(P2(4, IACT).EQ.-99.) GO TO 386
382 P2(5, IACT) = T
P2(1, IACT) = VELX
P2(2, IACT) = VELY
P2(3, IACT) = VELZ
390 CONTINUE

C IF THERE IS NO ROOM FOR ADDITIONAL MOLECULE THEN PRINT 'ALARM'
IF(IACT.EQ.NMOL1) GO TO 3004

C IF THERE IS NO ROOM FOR ADDITIONAL MOLECULE THEN PRINT 'ALARM'
IF(IACT.EQ.NMOL2) GO TO 3004
P2(5, IACT) = T
P2(1, IACT) = VELX
P2(2, IACT) = VELY
P2(3, IACT) = VELZ

C REPEAT FOR SPEC-3

C 390 CONTINUE

C INPUT 'S' MOLECULES
DO 460 J = 1, NAD
  IF(KR.LT.2) GO TO 460
  ANEW1 = FNN1(1, J, KR-1)
  IF(ANEW1.LT.00001) GO TO 420
  NEW1 = ANEW1
  REM = ANEW1 - NEW1
  CALL RANDU(P)
  IF(P.LT.REM) NEW1 = NEW1 + 1
  DO 402 I1 = 1, NEW1
    CALL RANDU(P)
    T = TMIN + DDALFA*(P + FLOAT(J-1))
    CALL RANDU(P)
    RN1 = RM1*P
    CALL RANDU(P)
    TEM = FNN1(4, J, KR-1)
    VTER1 = SQRT(2.*BOLTZ*TEM/SPEC(1,1))
    B = VTER1*SQRT(-ALOG(P))
    CALL RANDU(P)
    BB = 2.*PI*P
    VELX = FNN1(2, J, KR-1) + B*COS(BB)
    VELY = FNN1(3, J, KR-1) + B*SIN(BB)
    CALL RANDU(P)
    VELZ = VTER1*SQRT(-ALOG(P))
  C FIND A NEW MOLECULE TO BE ACTIVATED
  DO 404 IACT = 1, NMOL1
    IF(P(4, IACT).EQ.-99) GO TO 406
    IF(IACT.EQ.NMOL1) GO TO 3004
    PI(4, IACT) = RNEW
    P1(5, IACT) = T
    P1(1, IACT) = VELX
    P1(2, IACT) = VELY
    P1(3, IACT) = VELZ
  C REPEAT FOR SPECIES 2
    ANEW2 = FNN2(1, J, KR-1)
    IF(ANEW2.LT.00001) GO TO 440
    NEW2 = ANEW2
    RM2 = ANEW2 - NEW2
    CALL RANDU(P)
    IF(P.LT.REM) NEW2 = NEW2 + 1
    DO 422 I2 = 1, NEW2
      CALL RANDU(P)
      T = TMIN + DDALFA*(P + FLOAT(J-1))
      CALL RANDU(P)
      RNEW = RM2*P
      CALL RANDU(P)
      TEM = FNN2(4, J, KR-1)
      VTER2 = SQRT(2.*BOLTZ*TEM/SPEC(2,1))
      B = VTER2*SQRT(-ALOG(P))
      CALL RANDU(P)
      BB = 2.*PI*P
      VELX = FNN2(2, J, KR-1) + B*COS(BB)
      VELY = FNN2(3, J, KR-1) + B*SIN(BB)
      CALL RANDU(P)
      VELZ = VTER2*SQRT(-ALOG(P))
  C FIND A NEW MOLECULE TO BE ACTIVATED
  DO 426 IACT = 1, NMOL2
    IF(P2(4, IACT).EQ.-99) GO TO 426
    IF(IACT.EQ.NMOL2) GO TO 3004
    P2(3, IACT) = RNEW
P2(5, IACT) = T
P2(1, IACT) = VELX
P2(2, IACT) = VELY
422 P2(3, IACT) = VELZ
440 CONTINUE

C REPEAT FOR SPEC-3
C
C INPUT 'N' MOLECULES
C
C SPEC-1
ANEW1 = FSN1(1, J, KR+1)
IF(ANEW1 .LE. 0.0001) GO TO 450
NEM1 = ANEW1
REM = ANEW1 - NEW1
CALL RANDU(P)
IF (P .LT. REM) NEW1 = NEW1 + 1
DO 442 II = 1, NEW1
CALL RANDU(P)
T = TMIN + DDALFA*(P + FLOAT(J-1))
CALL RANDU(P)
RNEM = RMAX - PXDR
CALL RANDU(P)
TEM = FSN1(4, J, KR+1)
VTER1 = SQRT(2. * BOLTZ * TEM / SPEC1(J, 1))
B = VTER1 * SQRT(-ALOG(P))
CALL RANDU(P)
BB = 2. * PI * P
VELX = FSN1(2, J, KR+1) + BB * COS(BB)
VELY = FSN1(3, J, KR+1) + BB * SIN(BB)
CALL RANDU(P)
VELZ = VTER1 * SQRT(-ALOG(P))
C
C FIND A NEW MOLECULE TO BE ACTIVATED
DO 444 IACT = 1, NMOL1
IF(P1(4, IACT).EQ.-99) GO TO 446
444 CONTINUE
IF(IAct.EQ.NMOL1) GO TO 3004
446 P1(4, IACT) = RNEM
P1(5, IACT) = T
P1(1, IACT) = VELX
P1(2, IACT) = VELY
P1(3, IACT) = VELZ
450 CONTINUE

C
C INPUT 'N' MOLECULES SPEC-2
ANEW2 = FSN2(1, J, KR+1)
IF(ANEW2 .LE. 0.0001) GO TO 460
NEM2 = ANEW2
REM = ANEW2 - NEW2
CALL RANDU(P)
IF(P .LT. REM) NEW2 = NEW2 + 1
DO 452 II = 1, NEW2
CALL RANDU(P)
T = TMIN + DDALFA*(P + FLOAT(J-1))
CALL RANDU(P)
RNEM = RMAX - PXDR
CALL RANDU(P)
TEM = FSN2(4, J, KR+1)
VTER2 = SQRT(2. * BOLTZ * TEM / SPEC2(J, 1))
B = VTER2 * SQRT(-ALOG(P))
CALL RANDU(P)
BB = 2. * PI * P
VELX = FSN2(2, J, KR+1) + BB * COS(BB)
VELY = FSN2(3, J, KR+1) + BB * SIN(BB)
CALL RANDU(P)
VELZ = VTER2 * SQRT(-ALOG(P))
C
C FIND A NEW MOLECULE TO BE ACTIVATED
DO 454 IACT = 1, NMOL2
IF(P2(4, IACT).EQ.-99) GO TO 456
454 CONTINUE
IF(IAct.EQ.NMOL2) GO TO 3004
456 P2(4, IACT) = RNEM
P2(5, IACT) = T
89
\begin{verbatim}
P2(1,IACT)=VELX
P2(2,IACT)=VELY
452 P2(3,IACT)=VELZ
460 CONTINUE

REARRANGE MOLECULES IN THEIR CELLS
C INITIALIZATION
5000 CONTINUE

KIP=NMOL1+NMOL2+NMOL3
DO 1001 I=1,KIP
1001 IP(KADD)=0

DO 1010 KADD=O,KIP
N1A=O
N2A=O
N3A=O
NIA=O
N2A=N3A ARE THE NUMBER OF ACTIVE MOLECULES (COUNTED NEXT)
DO 1100 I=1,NRD
 DO 1100 J=1,NAD
 DO 1005 K=1,4
1005 CONTINUE

SET SPECIES 1
N1C=O
N2C=O
N3C=O
NTC=O
DO 1020 K1=1,NMOL1
IF(P1(4,K1).EQ.-99.)GO TO 1020
RLOC=ABS(C(19,I,J)-P1(4,K1))
TLOC=ABS(C(20,I,J)-P1(5,K1))
IF(RLOC.GT.DR*.5)GO TO 1020
IF(TLOC.GT.DDALFA*.5)GO TO 1020
NiC=NIC+1
NTC=NTC+1
N1A=N1A+1
IF(NTC.EQ.1)IC(4,I,J)=KADD
IC(1,I,J):IC(1,I,J)+1
KADD=KADD+1
IP(KADD)=K1
1020 CONTINUE

SET SPECIES 2 MOLECULES ........................................
DO 1040 K2=1,NMOL2
IF(P2(4,K2).EQ.-99.)GO TO 1040
RLOC=ABS(C(19,I,J)-P2(4,K2))
TLOC=ABS(C(20,I,J)-P2(5,K2))
IF(RLOC.GT.DR*.5)GO TO 1040
IF(TLOC.GT.DDALFA*.5)GO TO 1040
N2A=N2A+1
NTC=NTC+1
IC(1,I,J):IC(1,I,J)+1
KADD=KADD+1
IP(KADD)=K2
1040 CONTINUE

WRITE(6,1021)N1A,N2A
1021 FORMAT(' NUMBER OF ACTIVE MOLECULES SPEC1= ',I5,' SPEC2=',I5)

CALCULATE COLLISIONS .................................................. BLOCK
EXTERNAL LOOPS ARE OVER CELLS I,J

\end{verbatim}
DO 999 I=1,NRD
DO 999 J=1,NAD
999 NCOL(I,J)=0
C
DO 900 I=1,NRD
DO 900 J=1,NAD
C
NM(1)=IC(1,I,J)
NM(2)=IC(2,I,J)
NM(3)=IC(3,I,J)
NTOT=NM(1)+NM(2)+NM(3)
DO 900 L=1,3
DO 900 M=1,3
C NUMBER OF SPECIES IN THE PROGRAM IS 2 (3)

KV=(L-1)*3+M
KT=KV+9
C KV, KT ARE THE ADDRESSES OF RELATIVE VELOCITY AND COLLISION TIMERS
920 IF(C(KV,I,J).GE.TIME) GO TO 900
C C(KV,I,J) IS THE INTEGRATED TIME FOR L-M COLLISION

KSEL=0
KREJ=0
IF(NM(L).GT.1.AND.NM(M).GT.1)GO TO 912
C NO COLLISIONS ARE CALCULATED IF THERE ARE NO MOLECULES
911 C(KT,I,J)=C(KT,I,J)+DTM
GO TO 900
C SELECT NOW THE MOLECULES FOR COLLISION
912 IF (KSEL.GE.100)GO TO 911
CALL RANDU(P)
MOL1=P*NMCL)+.999999
IF(MOL1.EQ.0)MOL1=1
C
CALL RANDU(P)
MOL2=P*NMCM)+.999999
IF(MOL2.EQ.0)MOL2=1
C
KSEL=KSEL+1
C
C CHECK IF THE SAME MOLECULE HAS BEEN SELECTED TWICE
IF(L.EQ.1)KI=0
IF(L.EQ.2)KI=NM(1)
IF(L.EQ.3)KI=NM(1)+NM(2)
IF(M.EQ.1)K2=0
IF(M.EQ.2)K2=NM(1)
IF(M.EQ.3)K2=NM(1)+NM(2)
KADI=MOL1+KI+IC(4,I,J)
KAD2=MOL2+K2+IC(4,I,J)
C KAD1, KAD2 ARE THE LOCATION OF SELECTED MOLECULES IN IPC
DO 930 Nl,3
IF(L.EQ.1)VNIPCN,MAD1)
IF(L.EQ.2)VNI=P2CN,MAD1)
IF(L.EQ.3)VNI=P3(N,MAD1)
IF(M.EQ.1)VN2zPI(N,MAD2)
IF(M.EQ.2)VN2zP2CN,MAD2)
IF(M.EQ.3)VN2:P3(N,MAD2)
C
VRC(N):VN1-VN2
VR=SQRT(VRCC1(NVRCC1)+VRC(2)*VRC(2)+VRC(3) VRC(3))
C VR IS THE RELATIVE SPEED IN A SPECIFIC COLLISION
IF(C(KV,I,J).LT.VR)C(KV,I,J)=VR
C LAST STATEMENT RESETS THE MAXIMUM RELATIVE VELOCITY FOR FURTHER CALCULATIONS
C
IF(KREJ.GT.100)GO TO 911
C
930 VRC(N):VNI-VN2
C VR(N) CONTAINS THE THREE RELATIVE VELOCITY COMPONENTS
C VR IS THE RELATIVE SPEED IN A SPECIFIC COLLISION
C LAST STATEMENT RESETS THE MAXIMUM RELATIVE VELOCITY FOR FURTHER CALCULATIONS
C
IF(KREJ.GT.100)GO TO 911
C
995 CONTINUE
C
920 CONTINUE
C
900 CONTINUE
C
900 CONTINUE
C
900 CONTINUE
CALL RANDU(P)
AVR=VR/C(KV,I,J)
KREJ=KREJ+1
IF(AVR.LT.P)GO TO 912
L  
LAST STATEMENT REJECTS THE CALCULATED COLLISION
NOW A SPECIES L-M COLLISION HAS BEEN SELECTED
CALCULATE NOW THE PROBABILITY THAT SUCH A COLLISION WILL BE COUNTED
FOR THE L AND M SPECIES RESPECTIVELY
LP=1
LM=1
CALL RANDU(P)
ANM=FLOAT(NMCL)/FLOAT(NM(M))
IF(ANM.GT.1.)GO TO 950
IF(ANM.LT.P)MP=0
GO TO 955
C  
950 ANM=1./ANM
IF(ANM.LT.P)LP=0
C  
955 CXS=PI*(SPEC(L,2)+SPEC(M,2))**2/4.
ALP=LP
ALM=LM
C  
VOLUME=REG(4,KR,KS)*VOL(I)
DNL=FLOAT(NM(L))/VOLUME
DNM=FLOAT(NM(M))/VOLUME
C  
USE EQ.10.3
TOC(L,M)=ALP/(CXS*DNM*VR*NMCL))+ALM/CCXS*DNL*VR*NM(M)
C  
SET THIS VALUE INTO C(KT,I,J)
C(KT,I,J)=C(KT, I,J)+TOC(L,M)
C  
C SAMPLE THIS COLLISION
NCOL(I,J)=NCOL(I,J)+1
C  
FIND RELATIVE MASSES
CALL RANDU(P)
BB=1.-2.*P
AA=SQRT(1.-BB*BB)
VR(1)=BB*VR
CALL RANDU(P)
BB=2.*PI*P
VR(2)=AA*COS(BB)*VR
VR(3)=AA*SIN(BB)*VR
C  
FIND RELATIVE MASSES
SM=SPEC(L,1)+SPEC(M,1)
RML=SPEC(L,1)/SM
RMM=SPEC(M,1)/SM
C  
CALCULATE HERE THE ACTUAL ADDRESSES OF COLLIDING MOLECULES AND SET
THEIR NEW VELOCITIES (NEW VELOCITY COMPONENTS ARE ADDED TO THE
VELOCITY OF THE CENTER OF MASS VCCM)
DO 960 N=1,3
IF(L.EQ.1)V1=PI(N,MAD1)
IF(L.EQ.2)V1=P2(N,MAD1)
IF(L.EQ.3)V1=P3(N,MAD1)
IF(M.EQ.1)V2=PI(N,MAD2)
IF(M.EQ.2)V2=P2(N,MAD2)
IF(M.EQ.3)V2=P3(N,MAD2)
VCCM=RML*V1+RMM*V2
VCCM1=VCCM+VR(N)*RMM
VCCM2=VCCM-VR(N)*RML
C CHANGE IN VELOCITY IS INPUTTED ONLY IF PROBABILITY OF COLLISION.GT.1
IF(LP.NE.1)GO TO 961
IF(LE.EQ.1)P1(N,MADI)=VCCM1
IF(LE.EQ.2)P2(N,MADI)=VCCM1
C
961 IF(LM.NE.1)GO TO 960
IF(LM.EQ.1)P1CN,MAD1)=VCCM1
IF(LM.EQ.2)P2CN,MAD1)=VCCM2
IF(LM.EQ.3)P3(N,MAD1)=VCCM2
C
960 CONTINUE
GO TO 920
900 CONTINUE
WRITE(6,4545)TOC(1,1),TOC(1,2),TOC(2,1),TOC(2,2),TIME
4545 FORMAT(' TIME',5.E10.3)
C END OF COLLISIONS
C NOW NEW TEMPERATURES MAY BE CALCULATED IN EACH CELL
C AVERAGE VELOCITY IN CELLS
C
WRITE(6,4547)
4547 FORMAT('0 I J NIE N2E TEMPR1 TEMPR2 VAVX1 VAVY1 VAVX2 VAVY2 NCOL',/)
C
DO 1110 I=1,NRD
DO 1110 J=1,NRD
NIE=IC(1,1,J)
N2E=IC(2,1,J)
KAD1=IC(4,1,J)
KAD2=IC(4,1,J)+NIE
IF(NIE.LT.1)GO TO 1112
VX1=0.
VX2=0.
VY1=0.
VY2=0.
C
DO 1111 IM=1,NIE
MADI=KAD1+IM
IAD=IP(MADI)
VX=VX1+P1(1,IAD)
1111 VY=VY1+P1(2,IAD)
1112 IF(N2E.LT.0)GO TO 1110
C
DO 1115 IM=1,N2E
MAD2=KAD1+IM
IAD=IP(MAD2)
VX=VX2+P2(1,IAD)
1115 VY=VY2+P2(2,IAD)
C
THE AVERAGE VELOCITIES IN THE CELL WILL RESULT-
VAVX1=VX1/NIE
VAVY1=VY1/NIE
VAVX2=VX2/N2E
VAVY2=VY2/N2E
IF(I.NE.1)GO TO 1116
C
FSN1(2,J,KR)=VAVX1+FSN1(2,J,KR)
FSN1(3,J,KR)=VAVY1+FSN1(3,J,KR)
FSN2(2,J,KR)=VAVX2+FSN2(2,J,KR)
FSN2(3,J,KR)=VAVY2+FSN2(3,J,KR)
C
1116 IF(I.NE.NRD)GO TO 1117
FNN1(2,J,KR)=VAVX1+FNN1(2,J,KR)
FNN1(3,J,KR)=VAVY1+FNN1(3,J,KR)
FNN2(2,J,KR)=VAVX2+FNN2(2,J,KR)
FNN2(3,J,KR)=VAVY2+FNN2(3,J,KR)
C
1117 IF(I.NE.1)GO TO 1118
FEN1(2,I)=VAVX1+FEN1(2,I)
FEN1(3,I)=VAVY1+FEN1(3,I)
FEN2(2, I) = VAVX2 + FEN2(2, I)
FEN2(3, I) = VAVY2 + FEN2(3, I)

1118 IF (.NE. NRD) GO TO 1119
FNN1(2, I) = VAVX1 + FNN1(2, I)
FNN1(3, I) = VAVY1 + FNN1(3, I)
FNN2(2, I) = VAVX2 + FNN2(2, I)
FNN2(3, I) = VAVY2 + FNN2(3, I)
1119 CONTINUE

C THERMAL VELOCITIES AND TEMPERATURES

ENRG1 = 0.
ENRG2 = 0.
IF (NIE .LT. 1) GO TO 1131
DO 1130 IM = 1, NIE
MADI = KAD1 + IM
IAD = IP(MADI)
CX1 = P1(1, IAD) - VAVX1
CY1 = P1(2, IAD) - VAVY1
CZ1 = P1(3, IAD)
1130 ENRG1 = ENRG1 + CX1 * CX1 + CY1 * CY1 + CZ1 * CZ1

1131 IF (N2E .LT. 1) GO TO 1150
DO 1140 IM = 1, N2E
MAD2 = KAD2 + IM
IAD = IP(MAD2)
CX2 = P2(1, IAD) - VAVX2
CY2 = P2(2, IAD) - VAVY2
CZ2 = P2(3, IAD)
1140 ENRG2 = ENRG2 + CX2 * CX2 + CY2 * CY2 + CZ2 * CZ2

1150 TEMPR1 = (ENRG1 / NIE) * SPEC(1, I) / (3.*BOLTZ)
TEMPR2 = (ENRG2 / N2E) * SPEC(2, I) / (3.*BOLTZ)

C IF (.NE. 1) GO TO 1151
FSN1(4, J, KR) = TEMPR1 + FSN1(4, J, KR)
1151 IF (.NE. NRD) GO TO 1152
FNN1(4, J, KR) = TEMPR1 + FNN1(4, J, KR)
1152 IF (.NE. 1) GO TO 1153
FNN1(4, I) = TEMPR1 + FNN1(4, I)
FNN2(4, I) = TEMPR2 + FNN2(4, I)

1153 IF (.NE. NAD) GO TO 1154
FEN1(4, I) = TEMPR1 + FEN1(4, I)
FEN2(4, I) = TEMPR2 + FEN2(4, I)
1154 CONTINUE

C WRITE(6, 4548) I, J, NIE, N2E, TEMPR1, TEMPR2, VAVX1, VAVY1, VAVX2, VAVY2, NCS
1110 CONTINUE

4548 FORMAT (* , 4I5, 6F12.3, I7)

6000 CONTINUE
C CALCULATE AVERAGED PARAMETERS, WEIGHTED BY DFI
DO 6010 I = 1, NRD
DO 6020 KPAR = 1, 4
6010 DO 6020 J = 1, NAD
DO 6020 KPAR = 1, 4
FSN1(KPAR, J, KR) = FSN1(KPAR, J, KR) / NIS
FSN2(KPAR, J, KR) = FSN2(KPAR, J, KR) / NIS
FEN1(KPAR, J, KR) = FEN1(KPAR, J, KR) / NIS
FEN2(KPAR, J, KR) = FEN2(KPAR, J, KR) / NIS
6020 CONTINUE

94
6020 FNN2(KPAR,J,KR)=FNN2(KPAR,J,KR)/NIS
C TO PREPARE FLOWS FOR THE NEXT REGION OR SECTOR, DIVIDE F(N) BY LOCAL
C DFI AND MULTIPLY BY NEXT DFI WHEN STARTING NEW REGION
C CALCULATE HERE THE MEAN FREE PATH AND STORE INTO REG(,,)
C
C STOP PROGRAM IF FLOW BECOMES COLLISIONLESS OR NUMBER DENSITY IS EQUAL
C TO THE AMBIENT NUMBER DENSITY. STORE FOE1,FOE2 IN A SEPARATE FILE TO
C BE USED IN A DIFFERENT PROGRAM.
C
C PRINT AVERAGED RESULTS
WRITE(6,6029)
6029 FORMAT(' ,//,')
WRITE(6,6030)NIS,KR
6030 FORMAT(' AVERAGED OUTPUT FLOWS AFTER ',I5, ' TIME INCREMENTS IN REGI')
WRITE(6,6031)I
6031 FORMAT(' I FEN1(I,I) FEN2(I,I) FSN1(I,I) FSN2(I,I)')
DO 6032 I=1,NRDI
WRITE(6,6032)I,FEN1(I,I),FEN2(I,I),FSN1(I,I),FSN2(I,I)
6032 CONTINUE
WRITE(6,6033)
6033 CONTINUE
WRITE(6,6034)
6034 FORMAT(' I FNN1(1,J,KR) FNN2(1,J,KR) FSN1(1,J,KR) FSN2(1,J,KR)')
DO 6035 J=1,NAD
WRITE(6,6035)J,FNN1(1,J,KR),FNN2(1,J,KR),FSN1(1,J,KR),FSN2(1,J,KR)
6035 CONTINUE
6036 CONTINUE
C
START A NEW REGION
IF(KR.EQ.10) GO TO 7000
KR=KR+1
GO TO 2000

7000 CONTINUE
C
FIND IF FLOW BECAME COLLISIONLESS IN THE WHOLE SECTOR
IF POSITIVE, STORE FOE1,FOE2 IN A SEPARATE FILE AND STOP PROGRAM

PREPARE DATA FOR THE NEXT SECTOR
KR=1
STOP PROGRAM IF KS WAS BOUNDED BY THE WALL
KS=KS+1
GO TO 1000

IF THERE IS BACK FLOW (FWN1,FWN2) NONZERO CALCULATE NEXT ITERATION
ITER=ITER+1
KS=KR=1
GO TO 3000

WRITE(6,6099)
6099 FORMAT(' I DATA FOR TEN MOLECULES SPEC.2')
DO 3003 I=1,10
WRITE(6,3002)P2(1,I),P2(2,I),P2(3,I),P2(4,I),P2(5,I)
3002 FORMAT(' ,4F10.3,E18.10)
3003 CONTINUE
GO TO 3009
3004 WRITE(6,3005)
3005 FORMAT('NO PLACE FOR ADDITIONAL MOLECULES')
3009 CONTINUE
STOP
END

C
C SUBROUTINE RANDU(P)
COMMON IX
IY = IX*65539
IF (IY) 5,6,6
5 IY = IY+2147483647+1
6 P = IY
P = P*.4656613E-9
IX = IY
RETURN
END
B.5 Program SIMUL - User's Guide

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

ALFA - The averaged angle for the continuum breakdown

\[ (P \approx 0.05) \]

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 \( Spec(I,1) \)
Molecular diameter of each species \( Spec(I,2) \)
Mean free path along \( (ALFA) \) \( FPR \)
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 AXSYH * (XTYPE)
```

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

The temperature, pressure and density of the ambient gas are shown in Table I. 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 (SIIUL) supply the number flux, flow velocity components 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 Boundaries. 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 reflection' (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.
Figure 25. The Low Density Region in the Jet
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 SIMUL 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 SIMUL 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


## INITIAL DISTRIBUTION LIST

<table>
<thead>
<tr>
<th>No.</th>
<th>Copies</th>
<th>Name</th>
<th>Address</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>2</td>
<td>Defense Technical Information Center</td>
<td>Cameron Station, Alexandria, VA 22314</td>
</tr>
<tr>
<td>2.</td>
<td>2</td>
<td>Library, Code 0142</td>
<td>Naval Postgraduate School, Monterey, CA 93943-5100</td>
</tr>
<tr>
<td>3.</td>
<td>1</td>
<td>Chairman, Department of Aeronautics, Code 67</td>
<td>Naval Postgraduate School, Monterey, CA 93943-5100</td>
</tr>
<tr>
<td>4.</td>
<td>1</td>
<td>Distinguished Professor A. E. Fuhs</td>
<td>Naval Postgraduate School, Monterey, CA 93943-5100</td>
</tr>
<tr>
<td>5.</td>
<td>3</td>
<td>Dr. Neil Griff</td>
<td>SDIO/DEO, Washington, D. C. 20301-7100</td>
</tr>
<tr>
<td>6.</td>
<td>1</td>
<td>Mr. Bruce Pierce</td>
<td>SDIO/DEO, Washington, D. C. 20301-7100</td>
</tr>
<tr>
<td>7.</td>
<td>3</td>
<td>Dr. Joseph Falcovitz</td>
<td>Naval Postgraduate School, Monterey, CA 93943-5100</td>
</tr>
<tr>
<td>8.</td>
<td>1</td>
<td>Associate Professor O. Biblarz</td>
<td>Naval Postgraduate School, Monterey, CA 93943-5100</td>
</tr>
<tr>
<td>9.</td>
<td>4</td>
<td>Dr. Shaul Abramovich</td>
<td>Ministry of Defence, Haifa, ISRAEL 31021</td>
</tr>
</tbody>
</table>
10. Dr. P. Avidonis  
Air Force Weapons Laboratory  
Kirtland Air Force Base, NM 87117

11. Research Administration Office  
Naval Postgraduate School  
Monterey, CA 93943-5100