School on
"Use of Synchrotron Radiation in Science and Technology"

14 October - 8 November 1991

Molflow
User's Guide

R. Kersevan
Sincrotrone Trieste
Trieste, Italy
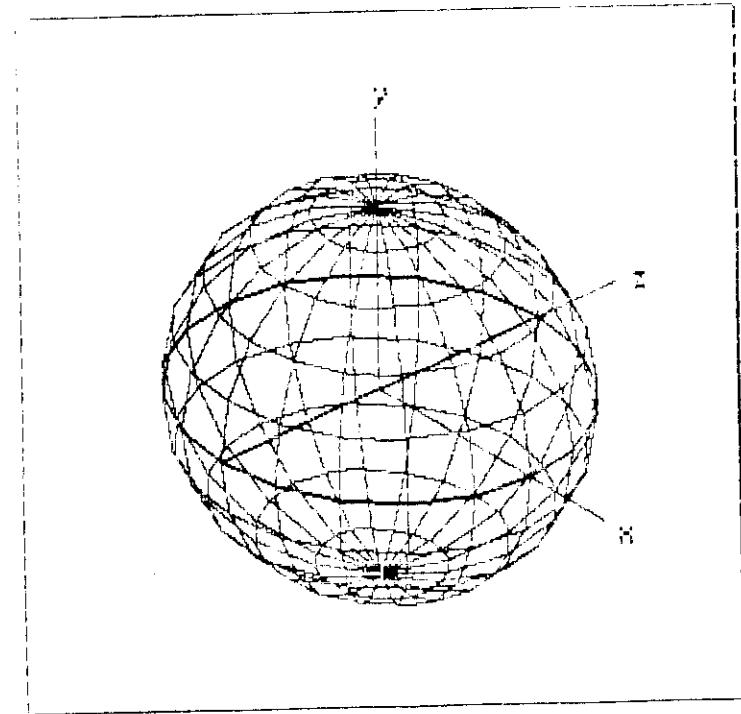
SINCROTRONE TRIESTE

ST/M-91/17

MOLFLOW

User's Guide

Roberto Kersevan

September 1991

to Luigi, my father

4. The Monte Carlo Program (MOLFLOWR)

5. Examples and Applications

6. Acknowledgements

7. References

Appendices

1.Introduction

MOLFLOW (for molecular flow) is a software tool written for the calculation of several quantities relevant to ultra-high vacuum (UHV) technology, namely conductances, pumping speeds, efficiency of cryopumping chevrons and baffles and many others. The algorithm herein implemented is the well-known Monte Carlo (MC) method, the power of which is recently increased due to the drop of hardware prices in the EDP market .

The application of the MC method under UHV conditions is justified by the analogy between molecular paths and random walks. For rather simple vacuum ducts, such as cylindrical pipes, analytical formulae do exist, but their application is very tedious (see appendix A2 for details): in fact, these formulae are usually given as nomograms, and the conductance of a tube is usually obtained graphically. In addition to that, special assumptions on the gas sources, as for instance effusion from a bigger volume, have to be made in order to get the results, and this assumptions are often unrealistic. Unfortunately vacuum systems rarely resemble a straight tube, just think about a curved bellow, an angle valve, a tube with a varying cross section, etc. In these cases the MC method is the only practical alternative: it can be tailored to the specific problem under consideration, taking into account all the different aspects and the real 3-D geometry. Obviously, one has to pay for such a flexibility: early MC calculations were very time-consuming, and powerful mainframes were mandatory. In the recent years, PC-based workstations equipped with 32-bit microprocessors and coprocessors have become very common. Their computing power is sufficient to simulate the molecular flow and photon trajectories under UHV conditions of complex 3-D geometries in reasonably short times, with great accuracy (compared to the correct analytical values, when existing), giving the user the possibility of checking the vacuum performance of a vacuum system without the need of making a prototype or a mockup. In the case of a synchrotron radiation source like ELETTRA, this allowed a considerable reduction in the development and data analysis of many different parts of its vacuum system, as will be shown in a separate paper.

2.Program Lay-out

MOLFLOW originally consisted in two programs written in Turbo Pascal, one to be used as an editor (MOLFLOWE) to create the structures to be analysed, and one to perform the MC simulation (MOLFLOWR). This program lay-out has been maintained due to many different reasons which will be outlined in the following paragraphs.

From now on, we will name *structure* a collection of *points* and *facets* . A point is defined by its three x_i, y_i and z_i cartesian coordinates, while a facet is defined by identifying the points which occupy the vertices of a polygon. Figure 1 shows an example of such a facet.
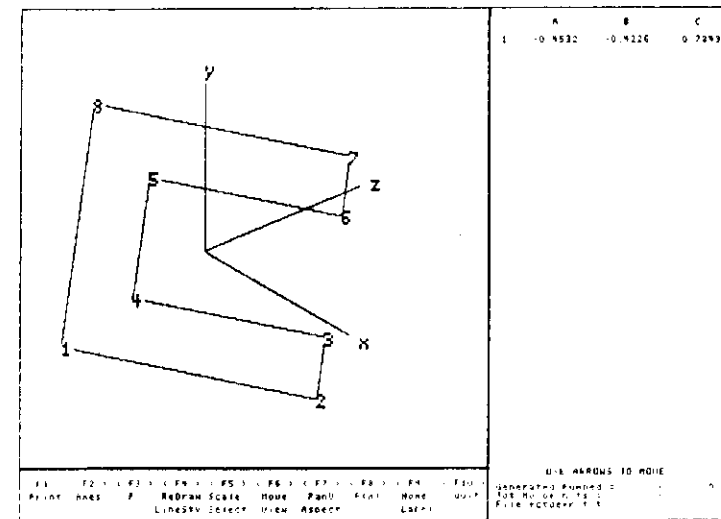
Fig.2 Example of definition of a facet in the 3-D space

Each facet is oriented in the 3-D space and has some properties like a *sticking coefficient*, s, (or a *reflectivity* R=1-s if photons are concerned), a *transparency*, T, *desorption* and *reflection* coefficients.

2.1 Database Structure

The organisation of the database, i.e. the set of data which are used by the programs, both the editor and the MC, is given.

The database contains the information about the points, the facets and other parameters used during the MC simulation.

As already said, a point is defined by its three cartesian coordinates, x_i, y_i and z_i.

A facet is defined by 23 real numbers, call it *components*, namely:

#	Definition
1	A, in the facet equation: $Ax + By + Cz + D = 0$;
2	B, " " " "
3	C, " " " "
4	D, " " " "
5	cosalfa, defining the orientation of the facet;
6	cosbeta, " " " "
7	sinalfa, " " " "
8	sinbeta, " " " "
9(*)	Sticking, the sticking coefficient S (for molecules), or R=(1-S), the reflectivity (for photons);
10(*)	Transparency, the transparency coefficient;
11(*)	Area, the facet's surface, in cm^2;
12(*)	Desorption, the desorption coefficient, i.e.(number of desorbed molecules+1);
13	Xmin, used in the program;
14	Lx, "
15	Ymin, "
16	Ly, "
17(*)	Hits, the number of intersections between the trajectories of the molecules (or photons) and the facet;
18(*)	Adsorb.Mol., the number of molecules adsorbed by the facet;
19	alfa, one of the two angles defining the orientation of the facet;
20	beta, " " " " " "
21(*)	Des.Type, the type of desorption from the facet;
22(*)	Refl.Type, the type of reflection from the facet;
23(*)	(free, for custom extensions).

Only the components marked with an asterisk, i.e. no. 9, 10, 11, 12, 17, 18, 21, 22 and 23, called *attributes* of the facet, are saved on disk, while the others are obtained by the programs starting from the points' coordinates and the definition of the facet.

When you save a data file (ASCII format) on disk, three constants are written at the beginning of it:

nmp, the maximum number of points defining a structure: nmp=200;

nmf, the maximum number of facets: nmf=80;

nmp_fc, the maximum number of points defining a facet plus 1: nmp_fc=20.

These three constants should not be changed.
Then the program writes:

n_tot, the number of molecules generated in the structure;
n_mlcl, the number of molecules to be generated (i.e. generated before the MC program stops automatically. Usually n_mlcl is a very large number);
n_p, the number of points defining the structure;
n_fc, the number of facets defining the structure;

From now on, an array will be identified by the notation A[i,j], following the notation used by the Pascal language.

At this point the cartesian coordinates of the n_p points are written:
v[1,1]=X-coordinate of the first point, v[1,2]=Y-coordinate of the first point, v[1,3]=Z-coordinate of the first point, etc..:

v[1,1]	v[1,2]	v[1,3], XYZ-coordinates of the first point
v[2,1]	v[2,2]	v[2,3] " 2-nd point
...	...	... "
v[n_p,1]	v[n_p,2]	v[n_p,3] " last point

After the coordinates of the points, the definition of each facet follows:
Poly[i,j] is an array of dimension nmf times nmp_fc containing all the information. For each facet, index i, Poly[i,nmp_fc] gives the number of points defining the i-th facet, while Poly[i,1], Poly[i,2], ..., Poly[i,n] identify the n points defining the i-th facet:

Poly[1,nmp_fc]	Poly[1,1]	Poly[1,2]	...	Poly[1,Poly[1,nmp_fc]]
Poly[2,nmp_fc]	Poly[2,1]	Poly[2,2]	...	Poly[2,Poly[2,nmp_fc]]
Poly[n_fc,nmp_fc]	Poly[n_fc,1]	Poly[n_fc,2]	...	Poly[n_fc,Poly[n_fc,nmp_fc]]

Then the attributes of each facet are written:

P[1,9]	Sticking coefficient of facet no.1
P[1,10]	Transparency
P[1,11]	Area
P[1,12]	Desorption
P[1,17]	Hits
P[1,18]	Adsorb.Mol.
P[1,21]	Des.Type
P[1,22]	Refl.Type
P[1,23]	(not used)

(Same for the other (n_fc-1) facets)

...

Finally, the two pressure vectors Pr[i,1] and Pr[i,2], i=1,..,100 are written (refer to section 3.2.2.8 (Pressure Profiles) for details):

Pr[1,1]	**Pr[1,2]**
Pr[2,1]	**Pr[2,2]**
...	...
Pr[100,1]	**Pr[100,2]**

3 The Editor Program (MOLFLOWE)

This program is divided in two sections. There is a *graphic* session where a structure can be visualised together with some of the properties of its facets and points, and a *screen* session used for inputting the data and listing some other properties of the structure. Switching between the two sessions is frequently required during the definition of a structure. The screen session will be examined first.

You're sometimes asked to enter some data: throughout this manual the underscore symbol "_" means that you are expected to enter a value, numeric or alpha-numeric. We will refer to the screen templates using a bold typeface.

In the following, please refer to 2.1 (Database Structure), and A1 (Hardware and Software).

After installing the programs on your hard-disk (say the C disk), you may run MOLFLOWE simply issuing the command molflowe from the DOS prompt 'C>'. The first thing appearing on the screen is the template recalling you which program is going to be executed.

You should set the printer parameter according to the printer connected to your computer (see Appendix A1 (Hardware and Software)).

3.1 Main Menu

The Main Menu is the following:

3.1 - MAIN MENU -	
GRAPHIC SESSION	**: (0)**
LOAD/MERGE DATA FROM DISK	**: (1)**
MODIFY DATA IN MEMORY	**: (2)**
INPUT NEW DATA	**: (3)**
SAVE DATA ON DISK	**: (4)**
LISTING OF DATABASE	**: (5)**
ENTER YOUR OPTION :	

Entering a number between 0 and 5 lets you move to other sub-menus, corresponding to the different features of the program. We will now review all these options.

3.1.1. Load/Merge Data from Disk

This option loads data previously saved on disk:

```
         3.1.1. - LOAD/MERGE OPTIONS MENU -
         LOAD DATA FROM DISK                 : (1)
         MERGE DATA WITH EXISTING DATA   : (2)
                 ENTER YOUR OPTION :
```

You should specify the correct *drive*, *directory* and *filename*. Failing to do so the program beeps and the message

       File *drive:\ directory \ filename* NOT FOUND !!!

is displayed, and you are asked again to enter a new filename. If you want to quit this menu, simply press the Enter key and you'll be back to the Main Menu.

If the filename is correctly specified, the data are read from the disk and loaded in the program's database. The suggested extension *.TXT is not compulsory. You can specify your own extension, for instance to distinguish between different groups of files.

If the Merge option is selected, data read from disk are loaded into the program's database and placed at the end of already existing data. You should not invoke the Merge option if the database is empty.

3.1.2. Modify Data Menu

There are several possibilities of modifying the database of the structure:

```
           3.1.2. - MODIFY DATA OPTIONS MENU -
    ADD/REMOVE/CHANGE POINT(S)              : (1)
    ADD/REMOVE/CHANGE FACET(S)              : (2)
    MODIFY THE COORDINATES OF POINT(S)      : (3)
    MODIFY A FACET                          : (4)
    TRANSLATE (AND COPY)                    : ,(5)
    ROTATE (AND COPY)                       : (6)
    MAGNIFY (AND COPY)                      : (7)
                ENTER YOUR OPTION :
```

The coordinates of the points and the definitions of the facets can be modified as follows.

3.1.2.1. Add/Remove/Change Point(s)

The sub-menu is the following:

```
3.1.2.1. - ADD/REMOVE CHANGE POINT(S) OPTIONS MENU -
ADD A SINGLE POINT TO THE DATABASE           : (1)
ADD POINTS ON AN ARC OF ELLIPSE              : (2)
FIND THE INTERSECTION BETWEEN 3 PLANES       : (3)
REMOVE POINT(S) FROM THE DATABASE            : (4)
EXCHANGE POSITIONS IN THE DATABASE           : (5)
ADD POINTS ON SEGMENT                        : (6)
                ENTER YOUR OPTION :
```

We will now outline the different features:

3.1.2.1.1. Add a Single Point to the Database

```
3.1.2.1.1. ADD A SINGLE POINT TO THE DATABASE
ADD A NEW POINT TO THE DATABASE (0 to exit)
    AS THE LAST POINT        : (1)
    AT A SPECIFIC POSITION    : (2)
          ENTER YOUR OPTION :
```

If there are N points in the database, the Last Point option prompts you for entering the $X_{N+1}, Y_{N+1}, Z_{N+1}$ coordinates of the (N+1)-th point. The Specific Position option creates a new point at the i-th position and shifts downward the remaining (N-i) points in the database. You can check this by means of the 3.1.5. option (Listing of Database).

3.1.2.1.2. - Add Points on an Arc of Ellipse

Selecting this option you first get the file info message:

```
3.1.2.1.2. - ADD POINTS ON AN ARC OF ELLIPSE -
THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS
```

then the following questions will appear:

```
Enter the (X0,Y0) coordinates of the center of the ellipse (polygon) :
X0=_; Y0=_; Z-coordinates of the points : Z0=_
Horizontal semi-axis, R1=_; Vertical semi-haxis, R2=_
How many sides, N1, has the polygon ? _
Now enter the two angles (in degrees) alfa1 and alfa2 corresponding to the
first and N1-th point:
alfa1=_; alfa2=_
```

Suppose that N=0 and M=0, neither points nor facets in the database, and that you answer to the above questions entering the following numbers

X0=3.0, Y0=2.0, Z0=2.5, R1=2.5, R2=2.0, N1=11, alfa1=0.0, alfa2=180.0

then you create 10 new points in the database as shown in the following figure:
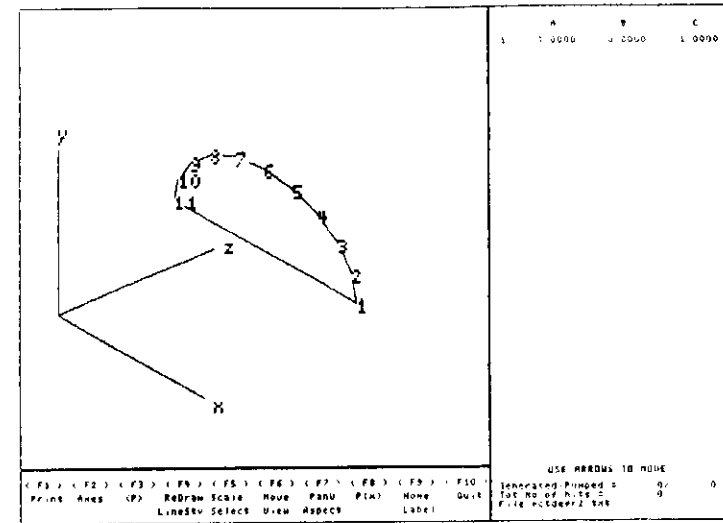
Fig.3.1.2.1.2 Add Points on an Arc of Ellipse

The points are always created in a plane parallel to the XY plane, at Z=Z0. You can then use options 3.1.5 (Translate (and Copy)), 3.1.6 (Rotate (and Copy)) and 3.1.7 (Modify (and Copy)) to move these points to the required position and orientation.

3.1.2.1.3 - Find the Intersection Between 3 Planes

There is the possibility of finding the intersection between 3 planes: all of them, or two only, should be planes already existing in the database, i.e. planes identifying facets in the database, while the third one could optionally be a plane whose A, B, C and D coefficients are entered from keyboard:

```
3.1.2.1.3 - FIND THE INTERSECTION BETWEEN 3 PLANES -
THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS
You can now select 3 planes:
Enter  0 as the first plane to exit ...
Enter -1 to input plane coefficients from keyboard ...
Enter -2 to find a plane passing through 3 given points ...
```

All these options are useful when you have, for instance, two round tubes connected to form an elbow. An example is given in section 5.1.2.

Entering 0 you simply leave this sub-menu and go back to the Main Menu;
if you enter 3 positive integers then the program finds the intersection (if any) between the planes identified by these numbers.
If there is an intersection (with a 1E-5 approximation) then the A,B,C and D coefficients of the 3 planes are listed (refer to section 2.1 for details) and the following question appears:

Assign these coordinates to a point (Y/N) ? _

If your answer is Y then the point number, i.e. the position in the database, is asked. You can overwrite the coordinates of an existing point, between 1 and N, or create a new point , the (N+1)-th.

If you enter -1 as the *third* plane number, then the program allows you to find the intersection between 2 already existing planes (facets in the database) and a plane whose A,B,C and D coefficients are entered from keyboard.

Entering -2 as the *third* plane number allows you to find the intersection between 2 already existing planes and a plane identified by 3 points whose coordinates are entered from keyboard (these points are not stored in the points' database).

3.1.2.1.4 Remove Point(s) from Database

Sometimes one or more points in the database become useless due to modifications or redefinition of the structure. This option is used to remove, i.e. *delete*, such points.

3.1.2.1.4 - REMOVE POINT(S) FROM DATABASE -
THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS
Remove unused points (1) or selected (2) ? _

If you answer 1, then the facets' database is scanned and all the points which are not contributing to the definition of any facet are removed from the points' database. If you answer 2, then the following question appears

Select point to be removed (0 to exit) : No._

The last question will be asked until you enter a 0 and go back to the Main Menu.

11

Suppose you enter a 1, and suppose that point no.1 defines facets no.3, 5 and 10. Then the following message is displayed:

WARNING !! The point you*re going to remove defines facet no. 3
WARNING !! The point you*re going to remove defines facet no. 5
WARNING !! The point you*re going to remove defines facet no. 10
Remove point anyway (Y/N) ? _

Should you answer Y, then point no.1 will be deleted.

Entering an integer, i, removes the i-th point from the database, i.e. moves the (i+1)-th, ..., N-th point upward one position and decreases N to (N-1). Therefore if you want to delete 3 points at positions (in the database) 10, 15 and 22, you should enter the integers 10, 14, 20. After using this option you better verify the correctness of the operation using the < Alt - F5 > (Select (Facet)) option running the graphic session (see section 3.2).

3.1.2.1.5 - Exchange Positions in the Database

The positions of two groups of points in the database may be exchanged:

3.1.2.1.5 - EXCHANGE POSITIONS IN THE DATABASE -
THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS
The positions of two groups of points in the database will be exchanged.
Select the first point of the first group (0 to exit) :
First point no. _ , and now the first point of the second group _
How many points to move in each group ? _

Suppose you enter the following 3 numbers

3, 20, 7

then the position in the database of the 7 points 3,4,5,6,7,8 and 9 will be exchanged with points 20, 21, 22, 23, 24, 25 and 26. This option doesn't really change the structure definition, only the way it is displayed is changed, see for instance section 3.1.5 (Listing of Database)). It's practical usefulness is therefore limited.

12

3.1.2.1.6 - Add Points on Segment

There is the possibility of creating points in the database which lay on a straight segment connecting two points whose (x_1,y_1,z_1) and (x_2,y_2,z_2) coordinates must be entered. The points are evenly spaced. An example:

3.1.2.1.6 - ADD POINTS ON SEGMENT -

THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS
How many points (0 to exit) ? 4
X-coord of first point : 0.0 ;   X-coord of last point : 1.0
Y-coord of first point : 0.0 ;   Y-coord of last point : -1.0
Z-coord of first point : 1.0 ;   Z-coord of last point : 2.0

Suppose N=72, then the program lists the X, Y, Z coordinates of the 4 new points created in the database:

#	X	Y	Z
73	0.000E+000	0.000E+000	1.000E+000
74	3.333E-001	-3.333E-001	1.333E+000
75	6.667E-001	-6.667E-001	1.667E+000
76	1.000E+000	-1.00E+000	2.000E+000

3.1.2.2. Add/Remove/Change Facets

We will now examine the possibility of creating facets in the database. The sub-menu is

3.1.2.2. - ADD/REMOVE/CHANGE FACET(S) OPTIONS MENU -
ADD A SINGLE FACET   : (1)
DEFINE THE FACETS OF A POLYGONAL SOLID   : (2)
REMOVE A FACET FROM THE DATABASE   : (3)
EXCHANGE POSITIONS IN THE DATABASE   : (4)
MODIFY FACET ATTRIBUTES ON RANGE   : (5)
REVERSE ORIENTATION OF FACET(S)   : (6)
                ENTER YOUR OPTION :

The first option is the following:

3.1.2.2.1. Add a Single Facet

Refer to section 3.1.3 for the coordinates of the following 8 points.

3.1.2.2.1. - ADD A SINGLE FACET -

THIS DATA FILE REPRESENTS A STRUCTURE WITH 11 POINTS AND 0 FACETS
FACET DEFINED BY N1 POINTS
Enter the number of points defining facet no. 1
Enter the number identifying facet no. 1, moving clockwise or counter-clockwise:
Point No.1   Point No.2   Point No.3   ....   Point No.8

Referring to the following figure, the program displays the lines

Is it facet no.1 properly oriented (Y) or reverse it (N) <DEFAULT=Y>
(0.000E+000,0.000E+000,4.000E+000)   D=0.000E+000
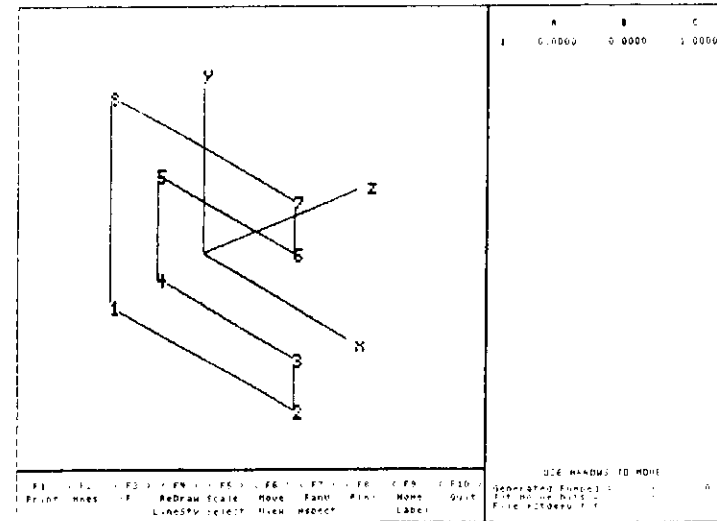

Fig.3.1.2.2.1 Definition of a facet

where the values shown for (A',B',C') and D' are related to the coefficients A,B and C identifying the orientation of the vector perpendicular to the facet currently being defined. If you answer Y (default value), then the facet is oriented as shown by the vector (A',B',C'), while if you answer N the orientation is reversed, $(-A', -B',-C')$.

Note that each facet should be oriented so as to point inside the structure. If this is not the case then the MC simulation program might not run properly. Refer to Appendix A3.

At this point the following lines are displayed:

EQ. FACET 1 : 0.000E+000 X + 0.000E+000 Y + 4.000E+000 Z +0.000E+000 = 0
Enter the sticking coeff. S of this facet:
S=0.0   --> the facet is not pumping (DEF) ;
0.0<S<=1.0--> the facet has a probability S of pumping the molecules;
S>=1.0   --> used to connect together many structures (TR=0.0);
Enter the sticking coeff. of facet no. M1 : S=0.000E+000 _
TR=-1.0   --> selects a facet to visualize pressures;
TR=0.0   --> facet is totally transparent to molecules;
TR=1.0   --> facet is totally opaque to molecules (DEF);
TR>1.0   --> double-sided opaque facet;
Enter the transparency TR of this facet : TR=1.000E+000 _
Desorption from this facet (Y/N) ? _

If you answer Y to the last question then the following line appears:

Desorption is diffuse (0) or uniform (2) ? (DEF=0) _

Reflection is diffuse (0), mirror (1) or uniform (2) ? (DEF=0) _

For informations about the meaning of *diffuse, mirror* and *uniform* for the desorption and reflection of the particles, please refer to Appendix A3 (The Monte Carlo Algorithm), and A4 (Comments about Functions and Procedures).

At this point the surface area of this facet is displayed and all of the facets and their sticking coefficient and transparency values are listed.

Finally, you go back to the Main Menu.

3.1.2.2.2. Define Facets of a Polygonal Solid

The situation is as follows: suppose you want to create an elliptical tube (its sidewall). For this task you can use twice option 3.1.2.1.2 (Create Points on an Arc of Ellipse). Suppose each set has 11 points as already seen before. Then you may define the sidewall by selecting the 3.1.2.2.2 option:

Now, referring to the elliptical tube example, suppose N=22 and M=1: if you enter,the values

3.1.2.2.2. - DEFINE FACETS OF A POLYGONAL SOLID -
THIS DATA FILE REPRESENTS A STRUCTURE WITH 22 POINTS AND 1 FACETS
(0 to exit) ...
First polygon defined by point no. 1 through no. 11
Second polygon defined by point no. 12 through no. 22

then the following 11 lines, already seen in 3.1.2.2.1, are displayed:

Is it facet no.2 properly oriented (Y) or reverse it (N) <DEFAULT=Y>
(-1.24E+000,-2.45E-001,0.000E+000)   D=7.288E+000

· · ·

· · ·

Is it facet no.12 properly oriented (Y) or reverse it (N) <DEFAULT=Y>
(1.436E-008,1.00E+001,0.000E+000)   D=-2.000E+001

As before, you should specify the orientation of each facet. The attributes of each facet are set to their default values, i.e. S=0.0, Tr=1.0, no desorption, diffuse reflection. To change these settings please refer to section 3.1.2.2.5 (Modify Facet Attributes on Range) and 3.1.2.4 (Modify Facet(s)). The structure you've created looks like this:
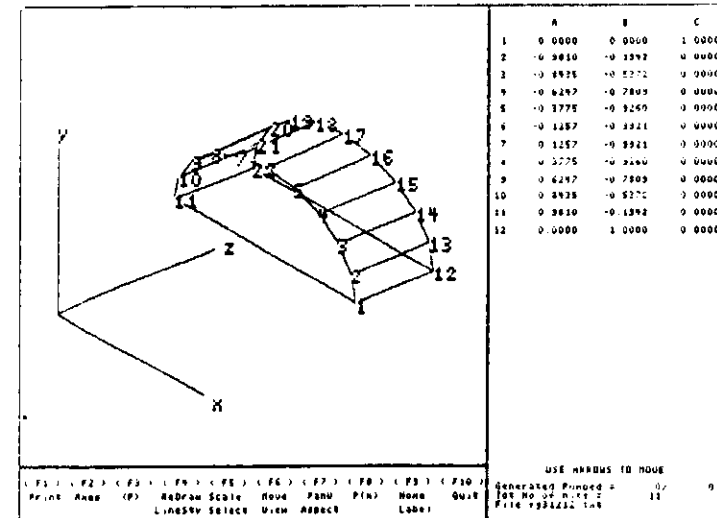

Fig.3.1.2.2.2 Define facets of a polygonal solid

Reversing the data input, i.e. entering

First polygon defined by point no. 12 through no. 22
Second polygon defined by point no. 1 through no. 11

all of the 11 facets will be oriented the other way, pointing outside the structure.

3.1.2.2.3. Remove Facet(s) from Database

One or more facets may result unnecessary: you can remove them from the database:

3.1.2.2.3. - REMOVE FACET(S) FROM DATABASE -
THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS
Facet to be removed (0 to exit) _

This question is asked until you enter a 0 and leave this option going back to the Main Menu.

3.1.2.2.4. Exchange Positions in the Database

Sometimes one needs to move (in the database) some facets in order to visualize better the structure: for instance, suppose you create a new facet, say the 50-th, which is placed close to facet no.1. Exchanging facet no.50 with no.2, you can analyse better your structure when you go in the Graphic Session. The usefulness of this option is limited.

3.1.2.2.4. - EXCHANGE POSITIONS IN THE DATABASE -
THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS
The positions of two groups of facets in the database will be exchanged.
Select the first facet of the first group (0 to exit) :
First facet _, and now the first facet of the second group _
How many facets to move in each group ? _

Now suppose that N=50, M=20, and you enter the numbers

1, 5, 4

to answer the 3 questions: then the program displays the following lines

Swapping facet # 1 with facet # 5
Swapping facet # 2 with facet # 6
Swapping facet # 3 with facet # 7
Swapping facet # 4 with facet # 8
... DONE! <ENTER> to continue ...

The positions of the two groups of facets are exchanged in the database. Also the utility of this option is limited.

3.1.2.2.5 Modify Facet Attributes on Range

You can now change the attributes of one or more facets in the database. Selecting this option you get the following sub-menu

3.1.2.2.5. - MODIFY FACET ATTRIBUTES ON RANGE OPTIONS MENU -
THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS

- CHANGE STICKING COEFFICIENT OF FACET(S)   : (9)
- CHANGE TRANSPARENCY COEFF. OF FACETS   : (10)
- CHANGE DESORPTION OF FACET(S)   : (12)
- CHANGE DESORPTION TYPE OF FACET(S)   : (21)
- CHANGE REFLECTION TYPE OF FACET(S)   : (22)
ENTER YOUR OPTION : _

Depending on your choice, a message is displayed: if you enter 9 then

S=0.0   --> the facet is not pumping;
0.0<S<=1.0 --> the facet has a probability S of pumping the molecules;
S>=1.0   --> used to connect together many structures (TR =0.0);
Change selected attribute of facet no. _ through facet no. _
Enter new value for attribute : _

If you answer

1, 10, 0.5

then the sticking coefficient of facets no. 1, 2, ..., 10 is set equal to 0.5.

This option is useful after you've created many facets by means of the option 3.1.2.2.2 (Define Facets of Polygonal Solid).

3.1.2.2.6 Reverse Orientation of Facet(s)

It is sometimes useful to have the possibility of reversing the orientation of a group of facets in the database: instead of using option 3.1.2.4 (Modify Facet(s)) many times, you may use the following option:

3.2.2.2.6 - REVERSE ORIENTATION OF FACET(S) -

THIS DATA FILE REPRESENTS A STRUCTURE WITH 11 POINTS AND 0 FACETS

Reverse orientation of facet no. _ through no. _

Entering, for instance 1 and 11, you reverse the orientation of facet no.1, 2, ..., 11.
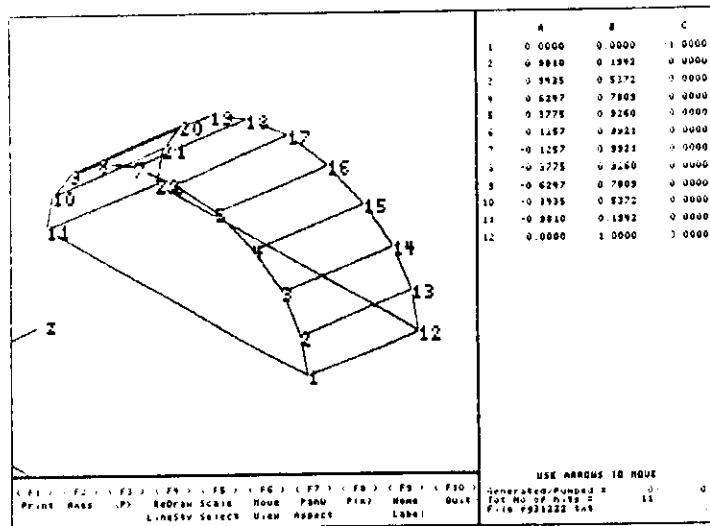
Fig.3.1.2.2.6 Structure as in fig.3.1.2.2.2 after reversing 11 out of 12 facets. The A, B, C and D coefficients are just the opposite.

3.1.2.3 Modify Coordinates of Point(s)

If necessary, the coordinates of one or more points in the database can be changed:

3.1.2.3 - MODIFY COORDINATES OF POINT(S) -

THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS
You can now modify the coordinates of existing points:
the database WILL BE UPDATED, so please be sure that the facets are defined properly.
Select the point to be modified (0 to exit) ? _

If you enter 10, then the program asks you the (x_{10}, y_{10}, z_{10}) coordinates of the 10-th point:

x(10)= _   y(10)= _   z(10)= _

The database is not updated, i.e. the facets' coefficients A, B, C and D are not re-calculated following the modification. You can update the database running option 3.1.5.2 (Listing of Database (Facets' Definition)) in the Screen Session, or command 3.2.2.5.2 (Select a Facet) in the Graphic Session.

3.1.2.4 Modify Facet(s)

Facets in the database can be modified.

3.1.2.4. - MODIFY FACET(S) -

THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS

At this point refer to section 3.1.2.2.1 (Add a Single Facet), and 3.1.3 (Enter New Data). The procedure for entering the data is the same.

Now a set of options to translate, rotate and magnify the coordinates of already existing points in the database is described. They can also be used to create new points in the database.

3.1.2.5 Translate (and Copy)

The possibility of translating some points in the database turns out to be very useful. You can translate independently along the X, Y and Z direction. The sub-menu is

3.1.2.5 - TRANSLATE (AND COPY) -

THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS
Points to be translated in X (1), Y (2) or Z (3) direction (0 to exit) ? _

Suppose you enter 3, then the you get the following question

The (x,y) coordinates of points in the database will be translated:
TRANSLATE on range (1) or selected points (2) (DEF=2) ? _

If you enter 1, then the program displays

Copy coordinates of point no._ through point no._

if you enter 1, 10, then you've selected points no.1, 2, ..., 10:

and translate along Z-direction by amount delta = _
Create new points (Y) or overwrite old ones (N) ? _

If you enter 10 and y, then the coordinates of these points in the database are translated in Z direction by 10 cm, and assigned to 10 new point, the (N+1)-th, ..., (N+10)-th.

If the last answer is n, then the coordinates of the selected points are changed, and any new point is created.

A final question is

Update database (Y/N) ? _

if you answer y, then the parameters of all facets in the database are updated, i.e re-calculated, following the alterations you've just made, otherwise they are left unchanged. Sometimes you'll have to answer n to this question.

If you enter 2 (Selected Points option), then the situation is as follows: Suppose you want to translate point no.1, 13 and 25 by the same amount in the Z-direction: then you enter

Select point (0 to exit) : 1
Select point (0 to exit) : 13
Select point (0 to exit) : 25
Select point (0 to exit) : 0

and you're brought back to the request for the translation amount, the creation, or not, of 3 new points, and database updating.

3.1.2.6 Rotate (and Copy)

Option 3.1.2.1.2 (Add Point on Arc of Ellipse), for instance, can create points in the database in a plane parallel to XY. In this case an option to rotate the points to the desired orientation is very useful.

3.1.2.6. - ROTATE (AND COPY) -

THIS DATA FILE REPRESENTS A STRUCTURE WITH 40 POINTS AND 20 FACETS
The (x,y,z) coordinates of selected points will be rotated (0 to exit):
Select: point no._ up to point no._
ROTATE ABOUT ONE OF THE AXIS (1) OR COMBINE ALFA-BETA ROTATION (2) _

Now, there are two distinct possibilities: the first allows a rotation about an axis parallel to the X, Y and Z axes, while the other combines two rotations in one single step.

If you choose the first option, entering a 1, then you get the following lines

Points to be rotated about an axis parallel to the X (1), Y (2) or Z (3) axis ? _
Enter the (x_,z_) coordinates of the rotation axis: x_=_ ; z_=_
Rotate about Y_-axis by an angle alfa=_
Create new points (Y) or overwrite old ones (N) ? _
Update database (Y/N) ?_

Suppose that, as a first step, you've created 20 points on a circle in the XY plane using option 3.1.2.1.2 (Add Points on Arc of Ellipse), with X0=0.0, Y0=0.0, Z0=0.0, R1=1.0, R2=1.0, N1=20, alfa1=0.0, alfa2=360.0. The second step is to create 20 more points in a plane parallel to XY, using the same option, with X0=0.0, Y0=0.0, Z0=5.0, R1=1.41421356, R2=1.0, N1=20, alfa1=0.0, alfa2=360.0.

At this point you use option 3.1.2.2.2 (Define Facets of Polygonal Solid), entering the following four numbers, 1, 20, 21, 40, and accept the orientation of the 20 facets

(simply press <ENTER>). If you now go in the graphic session (option 0 in the Main Menu), then the following structure is displayed:
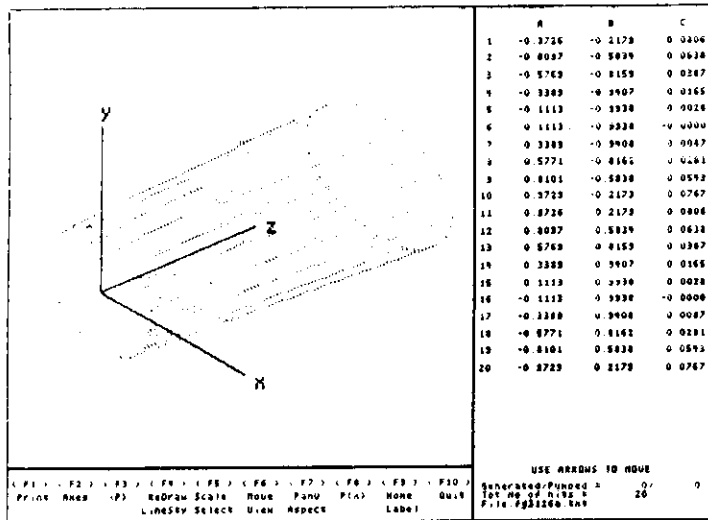
Fig.3.1.2.6 a) Rotate (and Copy)): situation before rotation ...

If you use option 3.1.2.6 and enter the numbers 21, 40.0, 1, 2, 0.0, 5.0, 45.0, n, y, you get the rotation
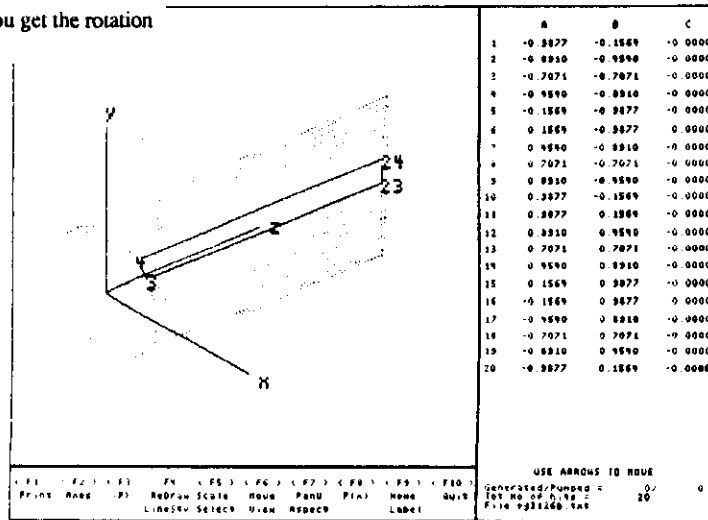
Fig.3.1.2.6 b) ... and after rotation. Facet no.3 is selected

Note that before the rotation, the facets are not defined properly. In fact, if you use option 3.1.5 (Listing of Database (Facets' Definition)), then all of the facets have a point (the fourth) which doesn't belong to the plane defining the facets' orientation.

The structure shown in fig.3.1.2.6.b) is the first part of the data file DAVIS53.TXT.

The other option, α–β Rotation, is connected to the two angles α and β defining the orientation of a facet in the 3-D space. Referring to the structure just shown, if you set α=45, β=90 (the two angles orienting facet no.3, shown with a solid line), then selecting all 40 points for the α–β rotation, you orientate the whole structure perpendicularly to facet no.3 (the Z-axis becomes the perpendicular to facet no.3).

Just select option 3.1.2.6 and enter 1, 40, 2, 90.0, 45.0, n, y. The α–β rotation is always performed about the origin, therefore you would possibly need to translate the structure before using this option
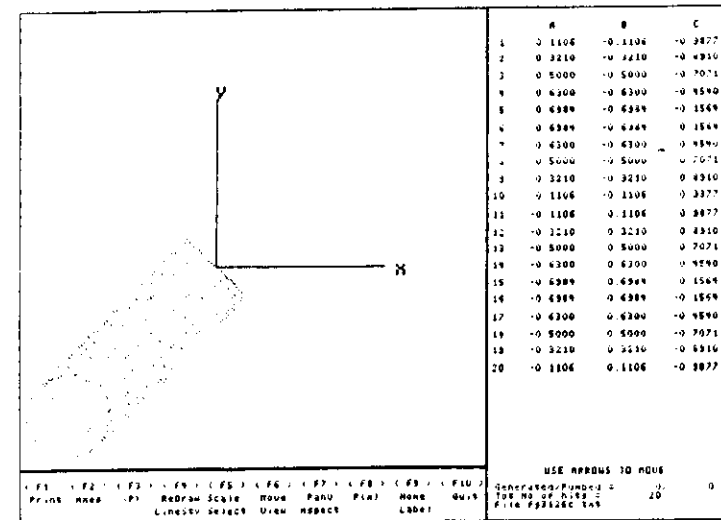
Fig.3.1.2.6.c) X-Y view of the structure after an α–β rotation, with α=45° and β=90°

3.1.2.7 Magnify (and Copy)

Consider the 20-facets structure already shown. This option is the following:

3.1.2.7. - MAGNIFY (AND COPY)

THIS DATA FILE REPRESENTS A STRUCTURE WITH 40 POINTS AND 20 FACETS
Points to be magnified in X (1), Y (1) or Z (3) direction (0 to exit) ? _
The (x,y) coordinates of selected points will be copied:
Copy coordinates of point no._ up to point no._
and magnify in Z-direction by a factor delta = _
Create new points (Y) or overwrite old ones (N) ? _

Select this option and then answer as follows: 1, 1, 40, 2.0, n, 0 (to exit), y (update)
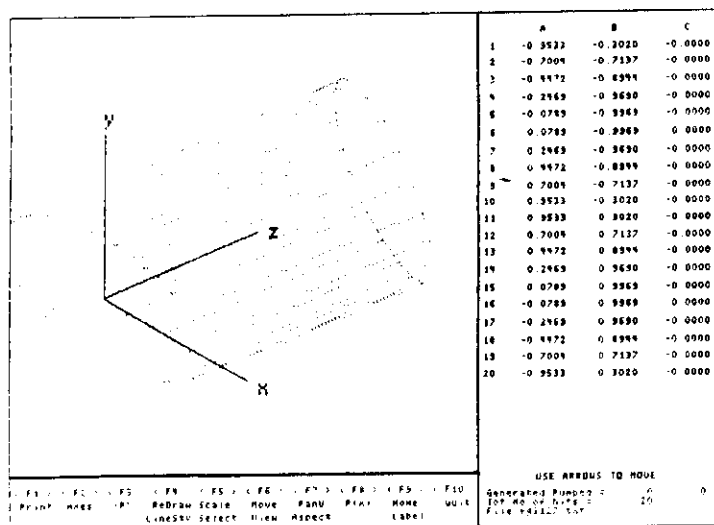
Fig.3.1.2.7 Magnification in the X-direction

and suppose you want to study the transmission probability for molecules as a function of the ellipticity (i.e. horizontal/vertical dimensions). You can use this option to simply magnify in the horizontal (X) direction to obtain elliptical profiles. In this case the X-coordinates of all points have been multiplied times 2.0.

Another application of this option is shown in section 5.1.4 (Transmission Probability of Butterfly and Angle Valves).

3.1.3 Enter New Data

This is the option to be used when you have to create a new structure from the beginning:

3.1.3 - ENTER NEW DATA -
Enter number of points defining the structure, Np (0 < n_p <=200) : _

The default value, n_p=0, is used just to reset the database. If you enter a number greater than 0, say 8, the points' coordinates are asked.

The following coordinates have been entered to create the facet shown in fig.3.1.2.2.1:

Now enter the (x,y,z) coordinates of each point ...
x(1)= -2 y(1)= -2 z(1)= 0
x(2)= 2 y(2)= -2 z(2)= 0
x(3)= 2 y(3)= -1 z(3)= 0
x(4)= -1 y(4)= -1 z(4)= 0
x(5)= -1 y(5)= 1 z(5)= 0
x(6)= 2 y(6)= 1 z(6)= 0
x(7)= 2 y(7)= 2 z(7)= 0
x(8)= -2 y(8)= 2 z(8)= 0

Then the number of facets of the structure is asked:

How many facets in the structure ? (0 <= n_fc <=80) : _

If you enter a number greater than 0, say 1, then you have to specify the definition of the facet as follows: suppose that the this facet is defined by 8 points, no.1, ..., no.8, as in the following figure

Fig.3.1.3 Definition of a facet in terms of its points

REMEMBER: A MAXIMUM OF 19 POINTS/FACET IS ALLOWED ...
Now define each facet ...
FACET no.1 DEFINED BY N1 POINTS
Enter number of points defining facet no.1 (0 to exit)
Enter numbers identifying facet no.1
 Point No.1 Point No.2 Point No.3 Point No.4 Point No.5 Point
No.6 Point No.7 Point No.8

Now, you're in a situation similar to that described in section 3.1.2.4 (Modify
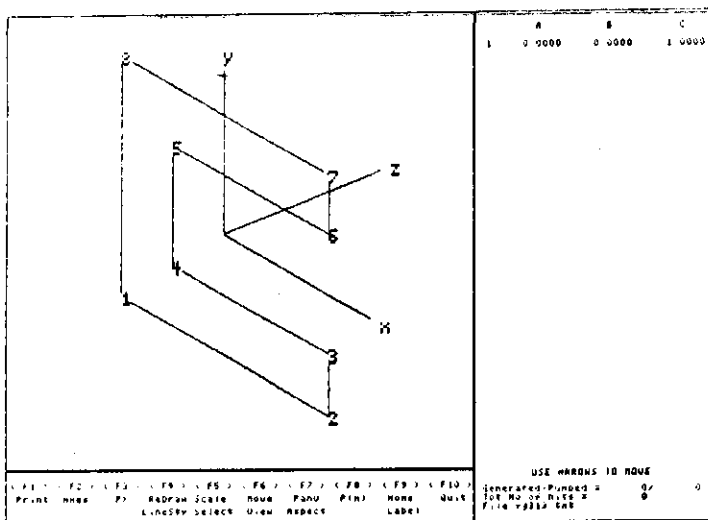Facet(s)), that is you have to accept or reverse the orientation of the facet (the vector
(A',B',C') should point inside the structure):

Is it facet no.1 properly oriented (Y) or reverse it (N) <DEFAULT=Y>
(0.000E+000,0.000E+000,4.000E+000)   D=0.000E+000 (Y/N) _

        ...   .

        ...   .

3.1.4 Save Data on Disk

This option allows you to save on disk your structure or part of it:

Do you want to save data on disk (Y/N) ? _

If you answer N (default value), then you simply go back to the Main Menu, otherwise

THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS

Save full database (1) or part of it (2) ? _

Entering 1 you're allowed to save the whole database, while entering 2 makes the
following questions to appear on the screen:

You can now select the facets to be saved on disk. REMEMBER that the whole
POINT database will be saved. You should run option 3.1.2.1.4 (Remove
Point(s) from the Database) to remove unused point(s).
SELECT FACETS on range (1) or choose (2) (DEF=2) ? _

Suppose you want to save on disk only facets no.6, 7, 8, 9 and 10: then you should
enter a 1 and then specify

Select facets from no. 6 up to no. 10

If, on the other hand, you want to delete facet s no.6, 8 and 10, then you should enter a
2 and then specify

Select facet no. (0 to exit) : 6
Select facet no. (0 to exit) : 8
Select facet no. (0 to exit) : 10
Select facet no. (0 to exit) : 0   (to exit)

Finally, the name of the file is asked:

Enter the name of the file to be saved (*.TXT) : _

If you specify a non existing filename (at least in the current directory), then data are
stored on disk and you go back to the Main Menu, otherwise if the file already exists,
you are warned

File filename ALREADY EXISTS: OVERWRITE (Y/N) ? _

If your answer is Y, then you overwrite the existing data: be sure that you really want this, since the old data file cannot be recovered.

If you answer N, the default value, then the file name is asked again.

3.1.5 Listing of Database

There is the possibility of listing on the screen the coordinates of the points in the database, the definition of each facet, the two pressure profile vectors and to evaluate the running sum of some quantities related to the facets, such as the number of hits, the surface area, the number of adsorbed and desorbed molecules.

The sub-menu is the following:

THIS DATA FILE REPRESENTS A STRUCTURE WITH N POINTS AND M FACETS

3.1.5.1 - LISTING OF DATABASE (0 to exit) -	
LIST POINT(S) COORDINATES	: (1)
SHOW FACET(S) DEFINITION	: (2)
LIST PRESSURE PROFILE VECTORS	: (3)
EVALUATE RUNNING SUM OF SELECTED COMPONENTS	: (4)
SET NUMBER OF MOLECULES TO BE GENERATED	: (5)
ENTER YOUR OPTION : _	

We will now examine all different possibilities:

3.1.5.1.1.List Point(s) Coordinates

Suppose that the data file DAVIS53 is loaded in the database, then selecting this option you get the following output

#	X	Y	Z
1	1.0000	0.0000	0.0000
2	0.9511	0.3090	0.0000
3	0.8090	0.5878	0.0000
..	....	....	....
60	3.0000	-0.3090	4.0489

listing the X, Y and Z coordinates of the 60 points in the database.

3.1.5.1.2 Show Facet(s) Definition

This option shows how each facet has been defined, i.e. the list of points (at least three) defining the facet with the proper orientation (refer to fig.2.1).

In the case of DAVIS53.TXT, you firstly get on the screen a message: it remainds you that a check is performed on the definition of each facet. In fact, the equation of the plane containing a facet is obtained simply calculating the vector product of the two vectors connecting the 3rd point and the 2nd point, and that connecting the 2nd point with the first. Therefore the other points defining the facet could not lay in that plane. The real variable SUM in the program shows the running sum of the quantity

$$A_i x_j + B_i y_j + C_i z_j + D_i = 0$$

for the i-th facet, where j identifies the points defining this facet. When SUM is higher than a default value, 10E-6 in the program, a warning message is displayed

POINT No.j DOES NOT BELONG TO THIS FACET !!.

That means that the MC program might lock, i.e. the intersection of the particle trajectories with this facet might not be found during the simulation, thus causing the traced particle to be lost. In this case unpredictable results could be obtained. See the sections referring to the MOLFLOWR program for further information (section 4.1 (Screen Session)).

It should be noted that, sometimes, values of SUM of the order of 1.0E-4 didn't cause any problem during the MC simulation. In any case, you should try to make SUM as low as possible. Values of the order of 1.0E-8 or lower are simply due to round-off errors in the calculation of the plane/facet equation.

After the warning message the output is

Points identifying the facets ...

Facet # 1	4 POINTS:	1 21 22 2 SUM=0.000E+000
Facet # 2	4 POINTS:	2 22 23 3 SUM=8.882E-016
...	...	... ...
Facet # 44	11 POINTS:	60 59 58 57 56 55 54 53 52 51 41

SUM=3.597E-014

Total surface (real facets)=5.62394E+001

<ENTER> to continue ...

The 'Total surface (real facets)' value equals the sum of the areas of all the *real* facets, i.e. those with transparency greater than 0. Double-sided facets (i.e. those facets with transparency coeff. Tr>1.0) are taken into account. The Total surface value should represent the geometrical surface of the real structure.

3.1.5.1.3 List Pressure Profile Vectors

This option lists the content of the two pressure vectors, i.e. the (maximum) two test facets used for measuring the pressure profiles. These facets should be rectangular (four points per facet): each of them is divided into 100 smaller parts as explained in sections 3.2.2.8 and 4.2.2.8). The test facets are identified by a transparency coefficient Tr=-1.0 and a sticking coefficient S=0.0: suppose that these facet are no.23 and 27, then the list is

#	Pr[#23]	Pr[#27]
1	1.939E+003	2.933E+003
2	3.876E+003	2.877E+003
...	....	....
100	1.760E+002	2.345E+002

Running sum=7.18022E+005 ; Running sum=8.12345E+005

<ENTER> to continue ...

The above list is to be interpreted in the following way:

The first part of the first test surface, Pr[1,1] in the program, has been traversed 1939 times by the particle trajectories (as specified in sections 3.2.2.8 and 4.2.2.8 the size of the first and 100-th section is one half of the others), the second Pr[1,2] 3876, ..., the last one Pr[1,100] 176 times, and so on for the second test surface. The running sums reported at the end of the listing are the total number of hits received by the two test facets.

If there is only one facet then the first vector is shown twice, while if no facets have been selected as test facets, then both of the vectors are shown as a list of zero's.

Pressing <ENTER> takes you back to the 3.1.5.1 sub-menu.

3.1.5.1.4 Evaluate Running Sum of Selected Components

When you select this option, you may obtain some useful informations about the geometry of a structure, such as the surface area, the number of desorbed and adsorbed molecules, and the number of hits. In the following refer to section 2.1 (Database Organisation).

THIS DATA FILE REPRESENTS A STRUCTURE WITH 56 POINTS AND 25 FACETS

Select component (11=Area; 12=Des.; 17=Hits; 18=Ads.; 0=EXIT) : _

If, for instance, you want to know the surface area then enter 11.

Sum selected component of facet no. _ through facet no. _

You can specify the whole structure, simply selecting the first and last facet, 1 and 25: then you get the answer

Running sum of component no. 11 = 1.381E+004

To exit this sub-menu you have to enter 0, to go back to the 3.1.5.1 sub-menu.

3.1.5.1.5 Set Number of Molecules To Be Generated

You can set the maximum number of molecules to be generated before the MC simulation program stops automatically:

No. of molecules to be generated = 1000000 : n_mlcl=_

The default value is 1,000,000.

3.2 Graphic Session

After you've entered new data or read existing data, you may run the graphic session just selecting the option no.0 in the Main Menu.

3.2.1 Graphic Screen Organisation

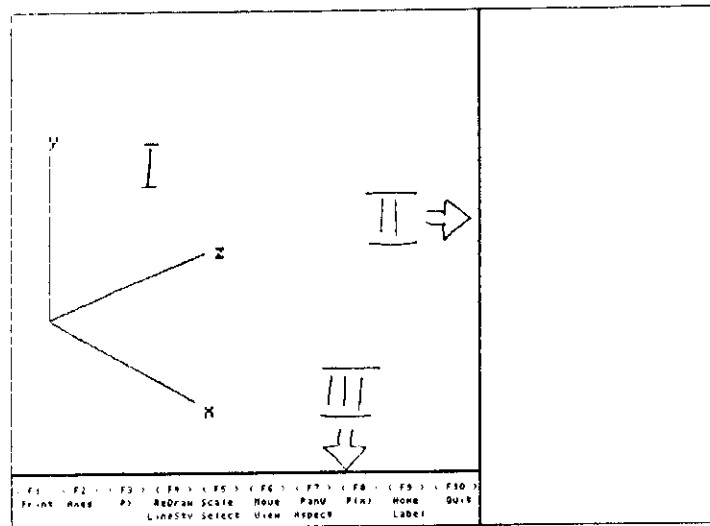The PC screen, during the graphic session, is divided in 3 windows as follows:

Fig.3.2.1 Graphic screen organisation

The first window is the biggest one: it is used to visualize the structure and show the pressure profiles. There are several possibilities: the structure can be viewed in quasi-axonometric mode or you can select one out of 3 projections in the coordinate planes, X-Y, X-Z, Y-Z. Refer to the following sections for additional informations.

The second window is used to look at the parameters and attributes of all of the facets in the database defining the structure (refer to 2.1 (Database Structure)), or if the

< Alt-F5 > option is invoked, only the ones of a selected facet. You may 'move' in the facet's database, thus viewing the 23 parameters and attributes of all facets, just using the arrow-keys.

The third window is a *command window*, recalling the user which action is taken by the program when a function key < F# >, or the combination < Alt - F# > keys are pressed (combination means that you have to hold down the < Alt > key and then press one of the function keys < F# >). It looks like this:

< F1 > < F2 > < F3 > < F4 > < F5 > < F6 > < F7 > < F8 > < F9 > < F10 >
Print   Axes   <P>   ReDraw Scale   Move   PanV   P(x)   Home   Quit
LineSty Select   View   Aspect

The first line shows the function-keys, the second line shows the action taken by the program when you press the corresponding function key (i.e. the F4 function key corresponds to an option called ReDraw).

The third line shows the action taken by the program when you press the Alt key and the corresponding function key at the same time (or, better, *first* Alt *then* F#).

3.2.2. Graphic Session Commands

An overview of all different options available during the graphic session is given.

3.2.2.1 < F1 > Print (Print Screen)

Pressing the function key F1 during the graphic session causes a hardcopy of the screen to be sent to the line printer connected with your PC (if any). Please be sure that the printer is properly connected and ready to accept data, otherwise an MS DOS error-handling routine is invoked and the program could be aborted.

For informations on the compatibility of this command with the printer connected to your PC, please refer to appendix A1 (Hardware and Software).

The following figure has been obtained using this option.
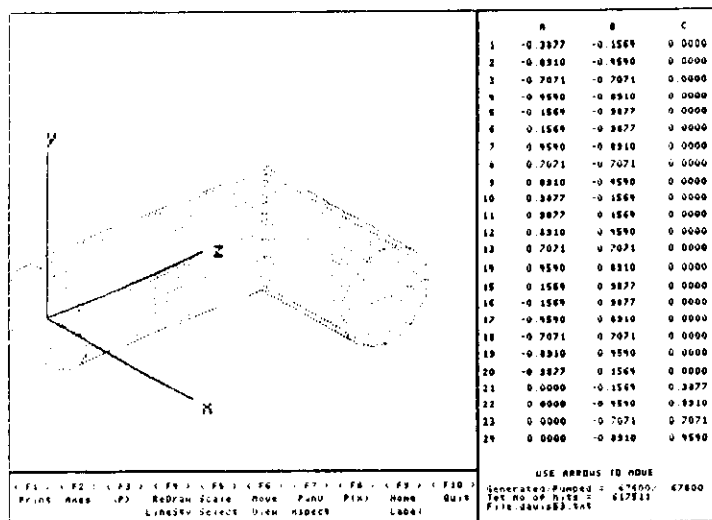
Fig.3.2.2.1 < F1 > Print command. Set the printer parameter at program start-up (see Appendix A1 (Hardware and Software)).

3.2.2.2 < F2 > Axes (Show/Hide Axes)

The action issued by this command is simply to toggle between the visualization of the XYZ axes and their hiding.
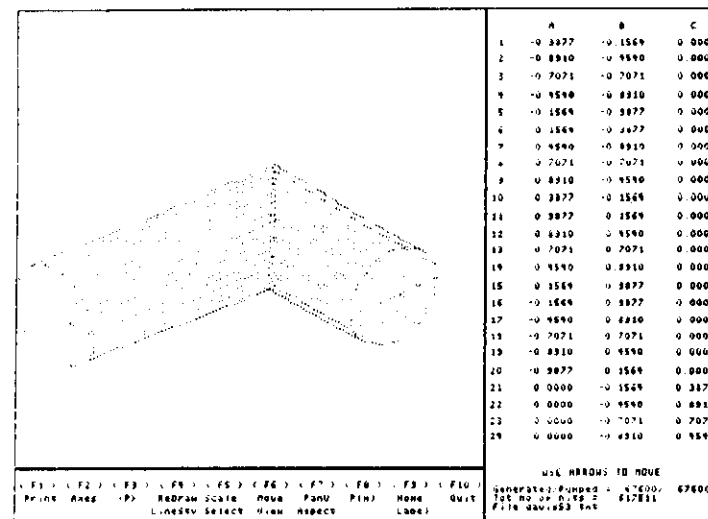
Fig.3.2.2.2 < F2 > Axes command. The reference frame is hidden

3.2.2.3 < F3 > <P> (Mean Values On Facets)

This command is used to visualize the average values of several quantities related to the facets in the database, such as:

1) the average pressures exerted by the molecules on the facets defining the structure;

2) the adsorption profile, i.e. the number of molecules pumped by each facet or the number of photons adsorbed if photons are concerned, weighted by the surface area of each facet;

3) the desorption profile, i.e. the same as 2) but for the desorbed molecules.

Pressing < F3 > you get the following message:

Show profile of:
Pressure (1), adsorption (2) or desorption (3) ? _

We now review these 3 options.

3.2.2.3.1 Average Pressure on Facets

The following formulae, according to the free-molecular range here assumed (UHV conditions) and assuming a Maxwellian distribution of the velocities for the molecules, give the average pressure P_i on the i-th facet having a surface A_i [cm^2] [29]:

$$P_i = \frac{4\,k\,T\,Z_i}{c} = \frac{4\,Q\,v_i}{c\,A\,N}$$

where:
$$c = \sqrt{\frac{8\,R}{\pi}\frac{T}{M}} = 1.455 \times 10^4 \sqrt{\frac{T}{M}} \ [cm/s]$$

is the average speed of the gas molecules, R is the universal gas constant, T is the gas temperature in $^{\circ}$K and M its molecular weight; k is Boltzmann's constant, Q is the gas load (if you give it in torr l/s then you get pressures expressed in torr); Z_i is the impingement rate, in collisions/cm^2, given by

$$Z_i = \frac{v_i}{A\,N}$$

and v_i is the number of collisions. N is the number of traced molecules.

Note that while you are using the < F3 > option the command window changes: only the < F1 > option (Print Screen) can be used, and the arrow keys are not effective.

You can go back to the main screen just pressing < F10 > (Exit), thus exiting this option.

Some comments:

1) the numbers written below the horizontal axis identify the facets;

2) the vertical scale is linear, ranging from 0 up to a maximum value (referred to as 'FULL-SCALE VALUE' in the graph) corresponding to the highest average pressure exerted on the facets of the structure being analysed;

3) the FULL-SCALE VALUE (FSV) can sometimes be used to obtain an estimate of the pumping speed of a facet as follows.

One of the most important equations of UHV technology is

$$P = \frac{Q}{S}$$

where P is the pressure, Q the gas load and S the pumping speed, therefore an estimate of S, the pumping speed, can be obtained just taking the reciprocal of the numerical coefficient multiplying Q. Similar considerations hold also for the < F8 > option (P(x)).
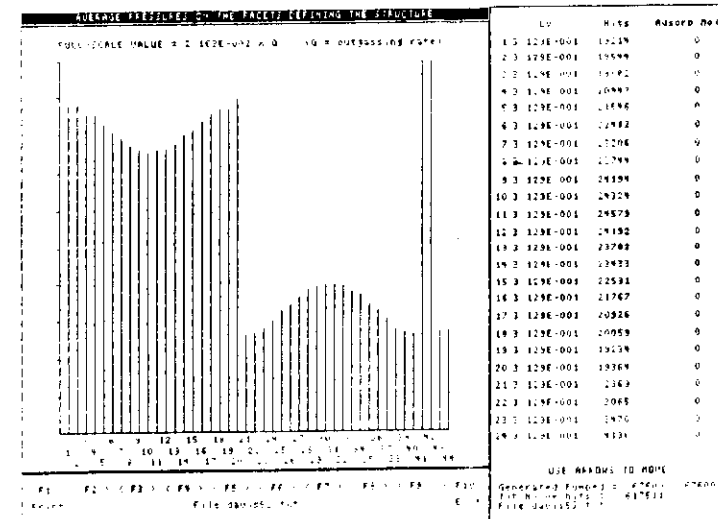
Fig.3.2.2.3.1 Average Pressure on Facets. It is proportional to the number of hits received by each facet weighted by its surface area (twice if double-sided)

3.2.2.3.2 Adsorption Profile

As before, the numbers below the horizontal axis refer to the facets:

In this case only the four facets with sticking coefficient greater than zero are shown: the first two, no.41 and 42, are the two making-up the entrance surface (see also next section), while the other two, no.43 and 44, constitute the exit surface.
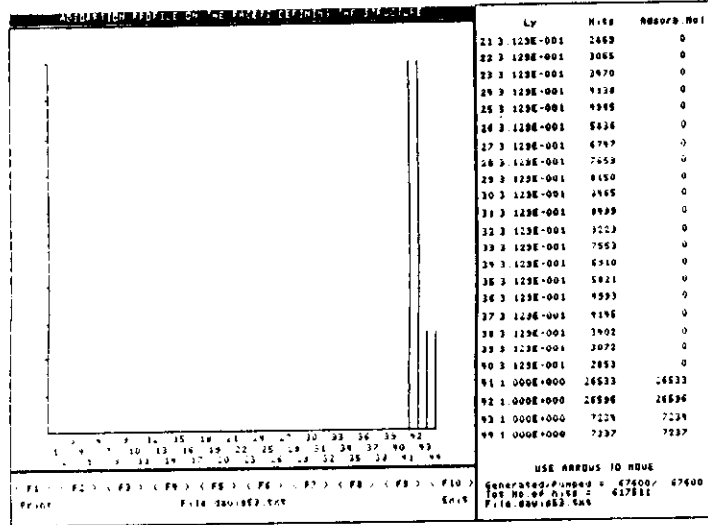
Fig.3.2.2.3.2 Adsorption Profile. The number of particles adsorbed by each facet, weighted by the facet's surface area, is shown

3.2.2.3.3 Desorption Profile

The facets with desorption coefficient greater than one are shown here:

Fig.3.2.2.3.3 Desorption Profile. The number of particles desorbed by each facet, weighted by the facet's surface area, is shown

3.2.2.4.1 < F4 > ReDraw (Re-Draw Structure)

This command refreshes the screen, i.e. draws again the structure and de-selects all the selected facets (see 3.2.2.5.1 (Select)). The same view as shown in figure 3.2.2.1 is obtained.

3.2.2.4.2 < Alt - F4 > LineSty (Set Line Style)

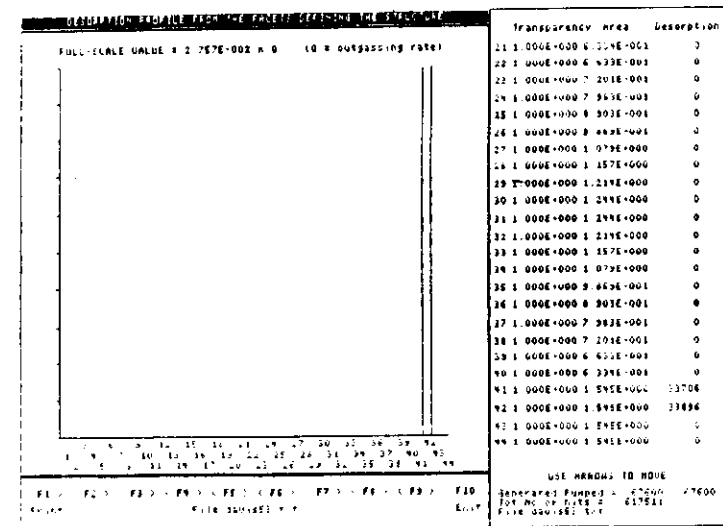The so called 'line style' of the lines corresponding to the edges of the facets of the structure can be changed. Each line is made up of sequences of 8 points, as follows:

0	************	(solid)
1	* * * * * * *	(dotted)
2	***** *****	(long dash)
3	*** * *** *	(dot and dash)
4	*** *** ***	(short dash)

An integer greater than 4 is treated using the mod function. The most significant byte is ignored and the low significant byte determines the line style.

As an example, consider the number 100 (decimal)=01100100 (binary): each line drawn with Line_style =100 is of the kind   ** *   ** *   ** *   ** ....

The following figure shows the structure drawn with Line_style set equal to 0:
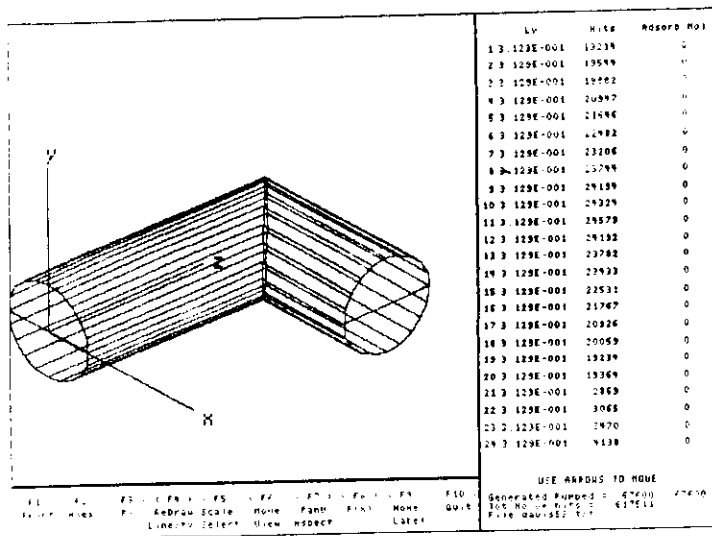
Fig.3.2.2.4.2 Effect of changing the line style. Line stile = 0 means a solid line

3.2.2.5.1 < F5 > Scale (Set Drawing Magnification)

The scale used to draw the structure can be changed so as to fit in the graphic window regardless of the real structure's dimensions.

The current value of the scale is shown (and taken as default value), and a new value is accepted.

The following figure shows the effect of doubling the scale from 4.5 to 9.0: the structure is displayed smaller, its actual dimensions being unchanged
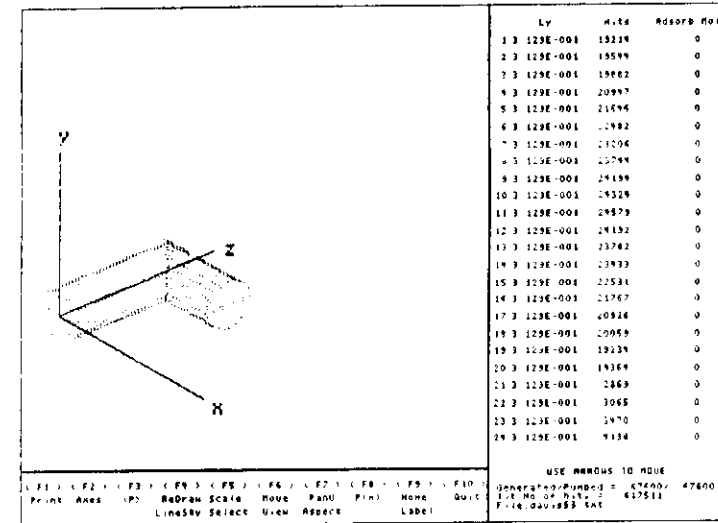
Fig.3.2.2.5.1 Drawing scale magnification set equal to 9.0

3.2.2.5.2 < Alt -F5 > Select (Select a Facet)

Each facet in the database can be selected, i.e. highlighted

The question SELECT A FACET : _ is asked: if you enter an integer between 1 and n_fc, the number of facets in the database, then all parameters and attributes of the selected facet are displayed on the right (window no.2 on the screen).Suppose you enter 44. Using the 'up' arrow-key you go to the next facet in the database, while pressing the 'down' arrow-key you select the previous one. If you press the 'right' arrow-key then the corresponding polygon, i.e. the contour of the selected facet in its X"Y"Z" frame of reference is shown on the screen superimposing the existing drawing. Note that the polygon is shown using an arbitrary scale, i.e. it is stretched vertically and/or horizontally in order to fit the graphic window, which is approximately square, see fig. 3.2.2.5.1.b). The 'left' arrow-key, or any function key, leaves a facet selected (i.e. drawn with a solid line).

Note that when the < Alt - F5 > command is issued, the command window is changed: you can only have a hardcopy of the screen, label the points (< Alt - F9 >), or Exit < F10 > this option.
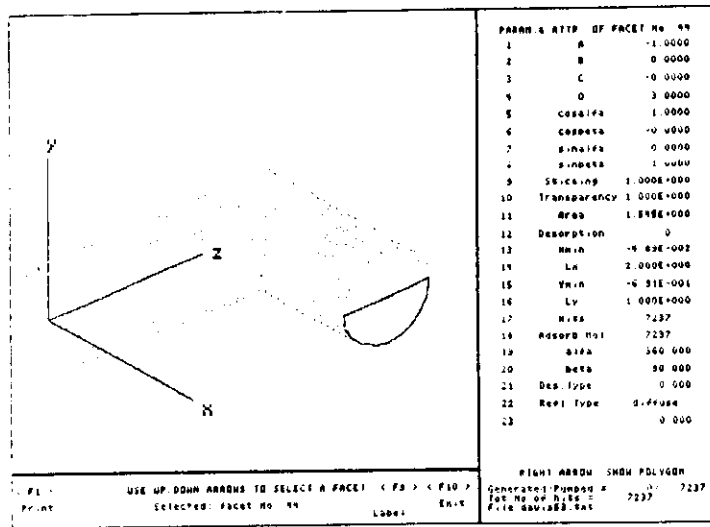
Fig.3.2.2.5.2.a) < Alt - F5 > option, selection of facet no.44
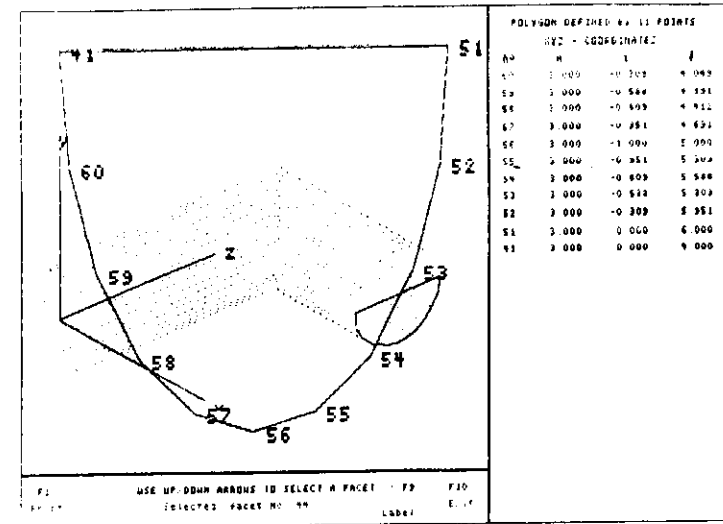
Fig.3.2.2.5.2.b) < Alt -F5 > option: pressing the 'right' arrow key the coordinates of the points defining the selected facet are listed in the graphic window no.2, and the facet's polygon in the X"Y"Z" frame of reference is displayed in the first graphic window. The size of the points' labels has been set equal to 2 using command < Alt - F9 > before entering the < Alt - F5 > option

Note that the polygon drawing is not to scale: the horizontal/vertical scales (i.e. in the X" and Y"-directions) are changed in order to fit the square window.

3.2.2.6.1 < F6 > Move (Move View-Point)

This option is used to move the graphic window in order to be able to visualize a structure, or part of it, which is not positioned in the neighbourhood of the XYZ origin.

The effect of this command is to display the question **Move = _**: if you enter **-2** then the structure is re-drawn as follows, moving the view-point in the -Z direction
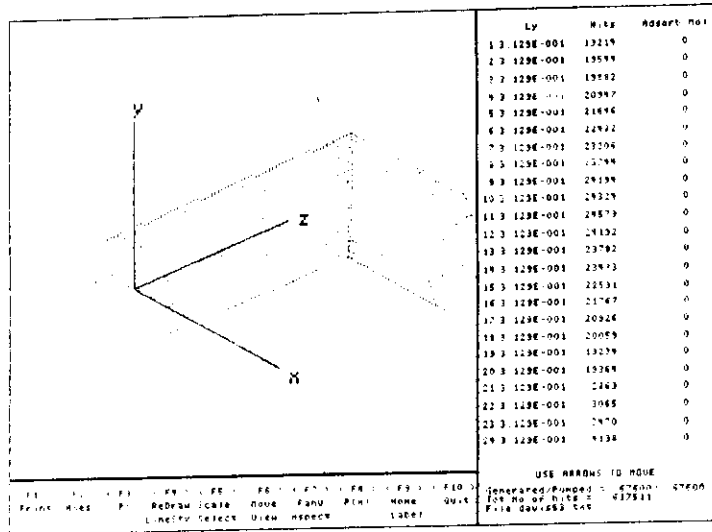
Fig.3.2.2.6.1 Effect of moving the view-point

3.2.2.6.2 < Alt - F6 > View (Select View-mode)

Sometimes the possibility of displaying the projections on the coordinate planes (X-Y, X-Z and Z-Y) of a structure turns out to be very useful.

This can be done issuing the < Alt - F6 > command:

Select view mode:
AXONOMETRIC (1); X-Y (2); Z-X (3); Z-Y (4) : _

The default value is '1', and this corresponds to the view-mode already seen, while the other possibilities lead to the views shown in figures 3.2.2.6.1 a), b) and c).

For view-modes 2, 3 and 4, the effect of the < F6 > command, Move, is to move horizontally, i.e. in the direction of the horizontal axis being displayed (X, Z and Z respectively).
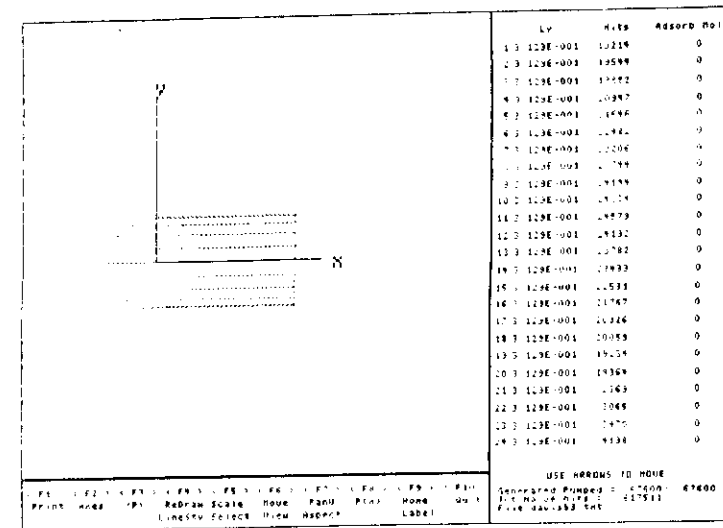
Fig. 3.2.2.6.1 a) X-Y view of the structure
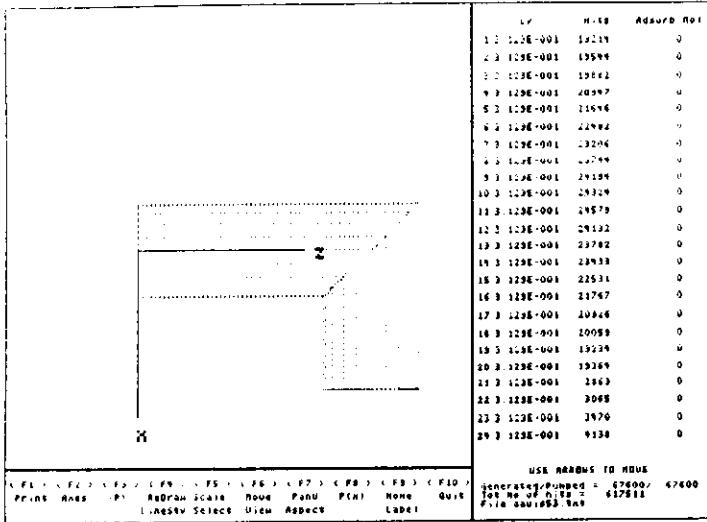
Fig.3.2.2.6.1 b) Z-X view of the structure
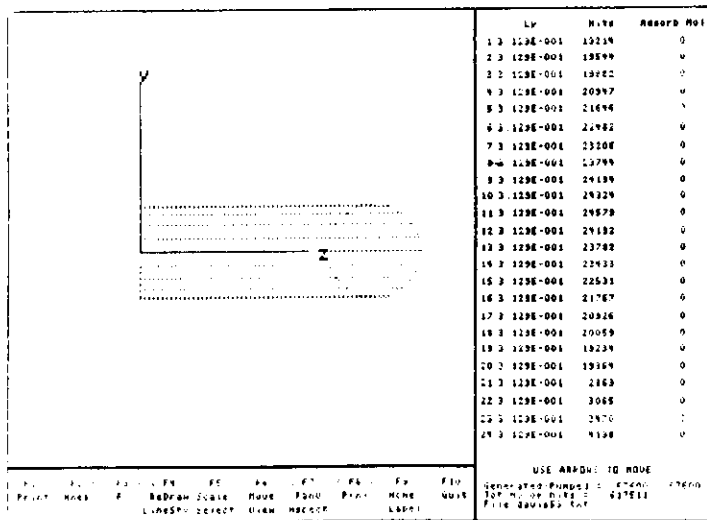
Fig. 3.2.2.6.1 c) Z-Y view of the structure

3.2.2.7.1 < F7 > PanV (Pan Vertically)

This command allows you to move *vertically* the graphic window; what *vertically* means depends upon the selected view-mode (< Alt - F6 > command). If, for instance, you are in axonometric view-mode, and if the graphic window is as that in fig.3.2.2.1, then the question **Pan vert.** = _ is asked: answering -1.5 you get a display like the following, i.e. you move the view-point downward in the -Y direction:
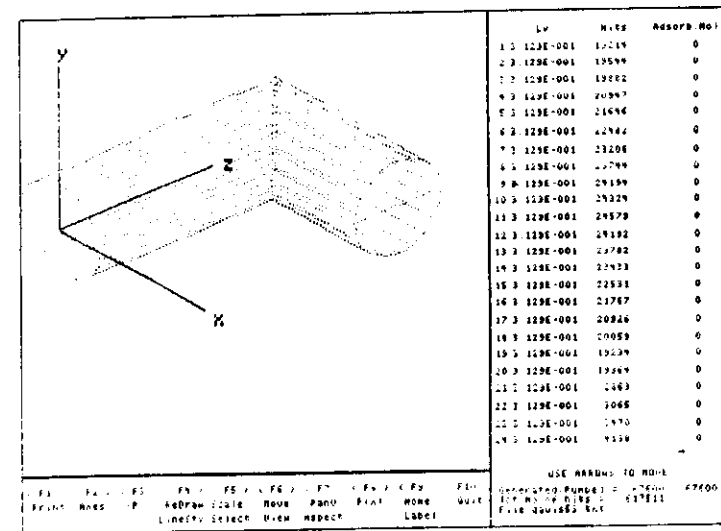
Fig. 3.2.2.7 Effect of the < F7 > PanV command

3.2.2.7.2 < Alt - F7 > Aspect (Aspect Ratio)

Depending on the PC monitor or the graphic printer you're using, all of the previous graphic displays and hardcopies could look like being *squeezed* or *stretched* : in this case you can modify the value of a variable called ar (Aspect ratio) in order to get a satisfying output.

The question **Aspect ratio = 1.3276E+000 : _** is displayed: 1.3276E+000 is the default value, i.e. the one which should make look like *round* a circumference. If you enter **1.0**, then the following display is obtained:
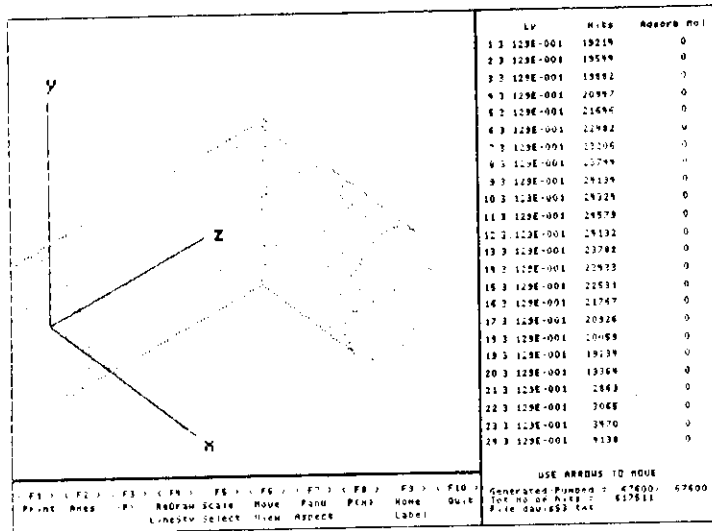
Fig.3.2.2.7.2 Effect of changing the aspect ratio

3.2.2.8 < F8 > P(x) (Pressure Profiles)

Especially in the particle accelerator field, the possibility of calculating the pressure distribution in the vacuum chamber turns out to be very useful.

The following example of application of this option will refer to the data file ALSID4.TXT (see section 5.3.1 (Pressure Profiles in Accelerator Vacuum Chambers)). Two *test facets* (i.e. facets with transparency coeff.= -1.0) parallel to the Z-axis have been selected. Facet no.32 is the one situated where the electron beam goes through, while facet no.41 is in the so-called antechamber [31]:

The question **Lin (1) or log (2) scale ? _** is displayed. This lets you choose between a linear and a logarithmic vertical scale. The default value is logarithmic.

3.2.2.8.1 Linear Scale

Suppose you choose the linear scale option, then you have to answer to two more questions,

Gas Load Q=_ ; Traced molecules, n_tot=_.

The gas load is the quantity of gas, in torr l/s for instance, desorbed by the structure: if you are analysing a structure which is a part of a so-called *superstructure* (see section 4.3 (Multiple Structures: Superstructures)), then you should enter the total gas load desorbed in the superstructure.

Accordingly, the number of traced molecules should be set equal to the number of molecules adsorbed in the structure or equal to the total number of molecules adsorbed in the superstructure. Therefore, if for instance you have a superstructure made up of 5 structures then, in order to get correct results for the pressure profiles, you should count the number of molecules generated in all of the 5 structures and assign this number to n_tot. Failing to do so, the 5 pressure profiles that you obtain will not have the same vertical scale.

The default value for both Q and n_tot is 1.0. In this case you have to scale properly the pressure values shown on the vertical scale. The graph of fig.3.2.2.8 a) is obtained.

In our case [31], the gas load is 8.177E-7 torr l/s.
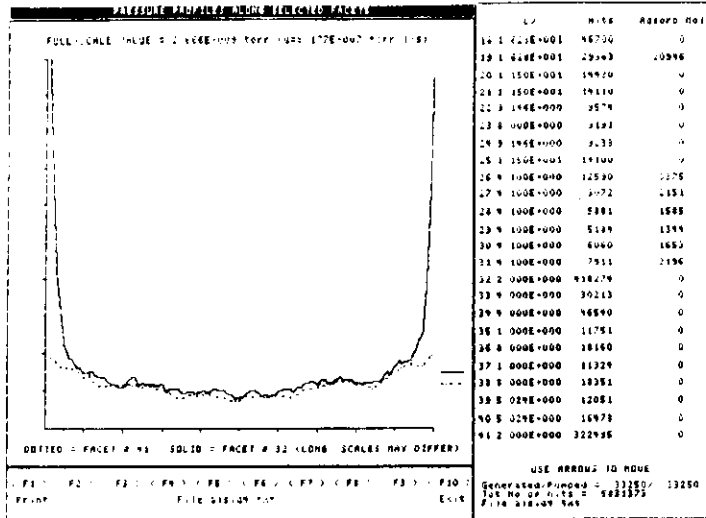
Fig. 3.2.2.8 1 < F8 > P(x) option. Longitudinal pressure profile, linear scale

3.2.2.8.2 Logarithmic Scale

If you select the log scale option, then after entering the values for Q and n_tot as before, the program automatically calculates the maximum and minimum pressure (for both test facets), and displays the decimal logarithm of these values (default values)

MAX_PRESSURE=-8.574 ; MIN_PRESSURE=-9.710 .

Enter new max_pressure: _

Enter new min_pressure: _

If you simply press enter twice, i.e. you accept the default values, you obtain the graph of fig.3.2.2.8 b), while entering -8 and -10, respectively, you let only the pressure values between 10E-10 and 10E-8 to be displayed, fig. 3.2.2.8 c).

Fig. 3.2.2.8 2 < F8 > option P(x). Longitudinal pressure profile, log scale, automatic scaling
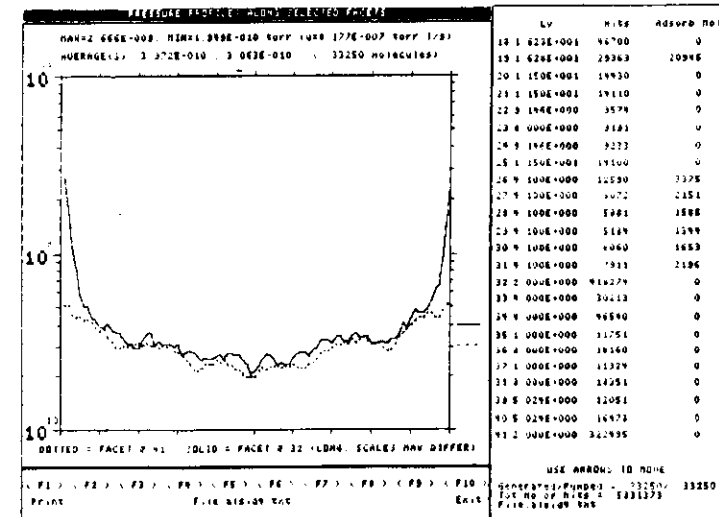

Fig. 3.2.2.8 c) < F8 > P(x) option. Longitudinal pressure profile, log scale, selected range scaling

Note that, for all of the above mentioned possibilities, values lower than, or equal to, zero are set equal to a very small number, 1.0E-30, in order to avoid problems when calculating the decimal logarithms.

3.2.2.9.1 < F9 > Home (Default View-Point)

This command simply takes the view-point back to the default value, i.e. the XYZ frame of reference shown on the left side of the graphic window.

3.2.2.9.2 < Alt - F9 > Label (Show/Hide Point no.)

There are two distinct actions taken by the editor program when issuing the < Alt - F9 > command, depending on where you are in graphic session: if you are simply looking at the structure, i.e. you haven't selected neither options < F3 >, nor option< Alt - F5 >, nor < F8 >, then the following qestion will appear:

Enter size of labelled points:_

You should enter an integer value: this will set the font size for the points being selected. At program start-up, this size is set equal to 1.
Another question is:

Label all points (Y/N) ? _

If you answer $\underline{Y}$, then all facets in the database are selected and therefore all points defining at least a facet are labelled and shown. Unused points are not shown.

If you invoke < Alt - F9 > while you are in the Select mode,< Alt - F5 > command, then you can toggle between two different statuses, that is you can show or hide the point number of the selected a facet(s).

3.2.2.10 < F10 > Quit (Quit Graphic Session)

To quit the graphic session simply press < F10 >. You are then taken back to the Main Menu, Screen Session.

---

4. The Monte Carlo Program (MOLFLOWR)

This section and its sub-sections will be devoted to the explanation of how the Monte Carlo simulation program works. The *environment* of this program is very similar to that of the editor program, i.e. we have tried to keep the two graphic sessions to look alike. Unfortunately, due to memory limitations of the 3.02 version of the Turbo Pascal compiler used here, some of the options of the editor program couldn't be implemented. This results in a different command window. Refer also to Appendix A3.

4.1 Screen Session

The screen session of the MC simulation program MOLFLOWR is much simpler than that of the editor program.

As you invoke the program, entering **molflowr** from the DOS prompt, a template recalling the program and asking for the printer parameter is printed on the screen. Then, you are asked to enter the seed for the random number generator (see section 4.4 (Comments About Functions and Procedures)).

Set idum equal to a negative integer value (-32768<idum<0) : idum=_

The same seed, the integer variable called **idum** in the program, always generates the same simulation: this is useful for debugging, i.e. when a structure has some problems such as non well-defined facets, missing facets ('holes' in the structure), etc.

Afterwards, you should enter the number of structures to be analysed or making-up the so called superstructure (see section 4.3 (Multiple Structures: Superstructures)).

How many files to be analysed (MAX 15) ? No_of_struct=_

A maximum of about 15 structures is allowed, this number being limited by the dimension of the stack/heap area (refer to a Turbo Pascal User's Manual). As you enter the filenames, the program allocates some space on the heap area for the structure database, usually 1552 paragraphs per structure (24352 bytes). A standard Turbo Pascal variable called **memavail** shows you the remaining free space on the heap, which is displayed.

Then the name of the directory where the data files have to be read from (and written in) is asked:

Read data from directory (DEFAULT=current directory) : _

The file names of the No_of_struct structures should then be entered:

File # 1 = filename 23913 paragraphs free on the heap.

    ...   .

Failing to specify correctly the filenames and/or directory generates another request for the file names.

The drawing magnification factor is then asked: the default value is 120, but you may change it afterwards, during the graphic session, issuing the command < F5 > (see section 4.2.1.5 (Set Drawing Magnification)):

Set drawing magnification factor: Scale=_

An important parameter for the MC simulation is asked. It's the number of molecules to be generated before the data of all No_of_struct structures are saved on disk, not to be counfused with the total number of molecules to be generated before the program stops, n_mlcl:

Save on disk after n_mlcl_save molecules pumped (DEF=100):n_mlcl_save=_

This number may affect strongly the speed of the simulation, especially if you read/write data from/to the floppy disk drive, which is quite slow. Usually a pre-run of the program is necessary in order to find the correct value for n_mlcl_save. Remember that **you should not set n_mlcl_save>32767, otherwise an error will be generated.**

In some cases data have to be saved just after few molecules have been generated, say 5, sometimes 1000 is a good value. You will find a good compromise after experiencing for a while with the program.

You're then asked to re-direct the error messages generated by the program. You can select between printer and screen:

Send error messages to printer (1) or screen (2) (DEF=2) : _

In the first case be sure that the printer is connected, in the other case the error messages (if more than one) will overlap on the screen, and therefore you will see only the last one.

The output of these error messages has the following format:

x1 y1 z1   Facet no. Struct.no.   Struct.Prec.no.   Tipo_L   No.bad

where x1, y1 and z1 are the coordinates of the source point which generated the *bad hit*, Facet no. is the facet's number, Struct.no. is the number identifying the structure (always equal to one if there is not a superstructure), Struct.Prec.no. is the number identifying the structure where the hit before the bad hit occurred (useful only for superstructures), Tipo_L is connected to the kind of facet (useful to find which part of the procedure Find_Length calculated the intersection in the previous hit), No.bad is the number of bad hits which occurred since the beginning of *this* simulation (it always starts from 0 every time you read data from disk).

Using this information you should be able to find what caused the error, for instance a missing facet in a structure.

Please note that an error message (bad hit) after many thousands hits may be generated even if your structures are defined properly: this is believed to be due to round-off errors in the calculations, especially in the routine which tries to find if the intersection point is inside a facet or not (see Appendix A3 (The Monte Carlo Algorithm) for details). The number of these round-off errors should be very small compared to the number of molecules generated in the structures.

For instance, running the simulation of the data files LEPQ.TXT, LEPB1.TXT, LEPB2.TXT and LEPB3.TXT (refer to section 5.3.1), an error message has been issued after about 10 million hits (!!).

The last message is

<ENTER> to start the Monte Carlo simulation ...

and after that the program automatically activates the graphic session and starts the Monte Carlo simulation. You should see the particle trajectories being drawn on the screen if your structures are not too large or small compared to the drawing magnification.

The MOLFLOWR.EXE version of the program, i.e. the one compiled by version 5.5 of the Turbo Pascal compiler, has a slightly different set of questions compared to what we've just seen.

The output of MOLFLOWR.EXE is simply the following:

<filename>   <total number of hits>   <total number of generated molecules>

all on the same line, after about 1000 hits have been done. You can stop the program
just pressing < Ctrl - Break >.

4.2 Graphic Session

The graphic session of MOLFLOWR closely resembles that of the editor program. The
different options will be outlined in the following. The PC screen is divided in three
windows, as already seen for MOLFLOWE, but the command window is different:

< F1 > < F2 > < F3 > < F4 > < F5 > < F6 > < F7 > < F8 > < F9 > < F10 >
Print   Axes   <P>   ReDraw Scale Move PanV   P(x)   Home   Quit
                     LineSty   View Aspect   Trace

4.2.1 Graphic Session Commands

As already mentioned, some of the commands available running the editor program
MOLFLOWE have been not implemented here due to memory limitations of the 3.02
version of the Turbo Pascal compiler. Some of the remaining commands are very
similar to those already described in section 3.2 and its sub-sections. The division of
the PC screen into three separate windows, as in the MOLFLOWE editor program, is
maintained (refer to section 3.2.1 (Graphic Screen Organisation)).

4.2.1.1 < F1 > Print (Print Screen)

Same as before. The printer parameter is to be set at the beginning of the MC simulation
run. Refer to Appendix A1 (Hardware and Software) for details. Be sure that the
printer is connected, otherwise an MS DOS error will be generated, and you'll be
forced to quit the program loosing everything you've made after the last data save on
disk.

4.2.1.2 < F2 > Axes (Show/Hide Axes)

Same as before. You can show/hide the XYZ frame of reference.

4.2.1.3 < F3 > <P> (Mean Values On Facets)

Only the average pressures on the facet of the structure currently being selected are
shown. For informations about the desorption/adsorption profiles you should use the
arrow-keys to move in the database.

4.2.1.4.1 < F4 > ReDraw (Re-draw Structure)

This command simply re-draws the structure(s) on the screen. It is used mainly to
refresh the image when a lot of particle trajectories have been drawn.

4.2.1.4.2 < Alt - F4 > LineSty (Set Line Style)

The line style can be changed in order to visualize better the structure(s).
Refer to section 3.2.2.4.2 (Set Line Style) for details.

4.2.1.5 < F5 > Scale (Set Drawing Magnification)

Same as before. You can zoom in and out just changing the value of the variable Scale.

4.2.1.6 < F6 > Move (Move View-Point)

This command is useful to visualize those parts of the structure(s) which do not fit the
output screen due to their dimensions and/or the selected drawing magnification.
Note that only the axonometric view-mode is available.

4.2.1.7.1 < F7 > PanV (Pan Vertically)

Same as before. The panning is vertical, i.e. in the Y-direction, downward for positive
values and upward for negative values.

4.2.1.7.2 < Alt - F7 > Aspect (Set Aspect Ratio)

As before, you should set this value in order to fit the size of the image on the screen of your PC. The default value is ar=1.3276.

4.2.1.8 < F8 > P(x) (Pressure Profiles)

Only the linear scale option is available. You can visualize the pressure profile along the (maximum) two rectangular facets which have been selected as test facets for measuring the 'longitudinal' pressure, i.e. those facets with transparency coefficient Tr=-1.0 and sticking coefficient S=0.0.

Each of the two facets is divided in 100 smaller sections. The length of sections no.2, 3, ..., 99 is given by Lx/100, while sections no.1 and 100 are half this value long (Lx is the 14-th component of the test facet, see section 2.1 (Database Organization). The following figure shows you the two test facets of file ALSID4.TXT. Refer also to section 5.3.1.
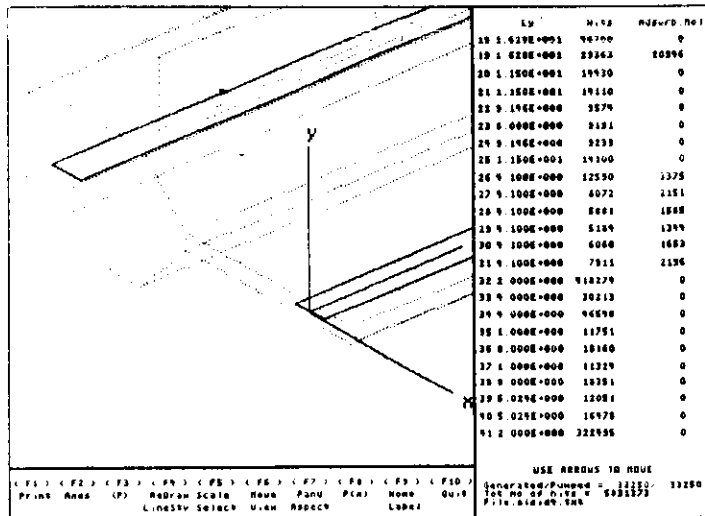

Fig.4.2.1.8 Test facets in data file ALSID4.TXT: the < Alt - F5 > option (Select a Facet) of the editor program has been used to highlight them (no.32 and 41)

4.2.1.9.1 < F9 > Home (default View-Point)

The effect of this command is to take the structure view-point back to the initial value, i.e. the XYZ frame of reference is shown in the first graphic window.

4.2.1.9.2 < Alt - F9 > Trace (Show/Hide Trajectories)

This option allows you to show/hide the trajectories of the particles during the MC simulation. A slight improvement in speed is effective when the trajectory drawing is hidden, but only for structures with a small number of facets.
In fact, for the data file DAVIS53.TXT the program made 2080 hits with trajectory drawing and 2400 with no drawing, yielding an improvement of about 15%.

4.2.1.10 < F10 > Quit (Quit Graphic Session)

This command let's you quit the MC simulation session, taking you back to the DOS prompt. There is no data save, therefore you should be careful in using this command.

4.3 Multiple Structures: Superstructures

Let's discuss now about an important issue, the *superstructure*.

A superstructure will be intended in the following as a set of structures interconnected together, i.e. the particles generated in the superstructure are allowed to pass from one structure to the others.

Superstructures are necessary if the structure you're going to create exceeds the dimensions of the database (see section 2.1 (Database Structure)), i.e. if you need more than 200 points and/or 80 facets to describe a vacuum system.

For instance, consider the data files PIPE1.TXT, PIPE2.TXT and PIPE3.TXT (see section 5.1.3, fig.5.1.3.a), b), c) and d)): in this case there are 66, 88 and 33 points and 48, 68 and 26 facets, respectively. Therefore such a superstructure couldn't be stored in a single structure, and the analysis couldn't be done.

It will now be described how to tell the program that a molecule leaves a structure to enter another structure.In order to understand better the following descriptions, you should run the editor program and look at the three structures separately.

Molecules are desorbed from facet no.23 (inlet), file PIPE3.TXT: they are considered as transmitted by the superstructure when they reach facet no.1, file PIPE1.TXT.

Once a molecule is generated in PIPE3.TXT, then either it is rejected by the superstructure (i.e. it is pumped by facet no.23), or it is transmitted to the structure following PIPE3.TXT, that is PIPE2.TXT. In order to do that, the sticking coeff. of facet no.26 (outlet) in PIPE3.TXT is set equal to 2.0 and its transparency coeff. is set equal to zero: this tells the program that data corresponding to the second structure in the superstructure have to be loaded in the database (after saving, on the heap, PIPE3.TXT).

Also in the second structure, the molecule has two possibilities: either it goes back to the first structure or it enters the third. In the first case the molecule hits facet no.68 (inlet) whose sticking coeff. is equal to 3.0: this tell the program to load again the data corresponding to the third structure. In the second case the molecule hits facet no.67 (outlet) whose sticking coeff. is equal to 1.1: data corresponding to the first structure are loaded in the database.

If the molecule is transmitted to the first structure, PIPE1.TXT, then there are two possibilities, as before: either it is pumped by facet no.1 (outlet), and in this case another molecule is generated, or it goes back to the second structure. If this is the case, then it hits facet no.48 whose sticking coeff. is equal to 2.0 (inlet).

Please note the following **important consideration**: when running the MC program MOLFLOWR on a superstructure, the way you enter the file names is important: if for instance you specify the three mentioned files PIPE1.TXT, PIPE2.TXT and PIPE3.TXT in the reversed order PIPE3.TXT then PIPE2.TXT and finally PIPE1.TXT, in this case it happens that a molecule desorbed by the first structure PIPE3.TXT can be transmitted to PIPE2.TXT, but afterwards it cannot go to any other structure since the sticking coeff. of the outlet facet (no.67). is equal to 1.1 and the program loads the data corresponding to PIPE3.TXT while it should load PIPE1.TXT. The same thing happens if the molecule tries to leave PIPE2.TXT to reach PIPE3.TXT: the sticking coeff. of the inlet facet (no.68) is equal to 3 and therefore the data corresponding to PIPE1.TXT are loaded instead of PIPE3.TXT.

In this case an error message is issued (refer to section 4.1 (Screen Session)): this kind of errors are easily discovered since their generation rate is high compared to the number of molecules generated in the superstructure.

If you have more than one input file for MOLFLOWR but these files do not *interact*, i.e. they describe structures which are not communicating, then in this case we do not call it a superstructure.

In fact, if you run at the same time 14 out of the 25 data files DAVISab.TXT (see section 5.1.2 (Transmission Probability of Curved Elbows)), then all of the structures are shown on the screen, and they seem to overlap. Molecules are generated randomly in each structure but they cannot leave one structure for another since there are not facets with sticking coefficient greater than one.

Therefore you can obtain the Monte Carlo simulation for several different structures at the same time. At the end, you should use the editor program MOLFLOWE to look at each structure separately.

5. Examples and Applications

The following sections will be devoted to show some of the possible applications of MOLFLOW, for both molecules and photons.

5.1 Molecular Flow Calculations

The first part of the examples concerns the calculation of some quantities relevant to UHV technology.

5.1.1 Transmission Probability of a Straight Round Tube

Figure 5.1.1 a) shows a structure, BENCH.TXT, representing a cylindrical round pipe with a radius R=5 cm and a length L=200: therefore the ratio R/L=40. The sidewall of the cylinder is approximated by 20 facets, and the inlet and outlet by two polygons with 11 sides (each of them has sticking coeff.=1.0). Each sidewall facet, therefore subtends an angle of 18 degrees. This approximation is sufficiently good: in fact, the ratio between the polygonal inlet area and the πR^2 real value is 0.9837. Molecules are assumed to enter the tube diffusely, i.e. a $\cos\theta$ emission from facet no.19 is assumed.

The transmission probability is 0.0583 compared to a value of about 0.06 as reported in [2, 21]. This value has been obtained generating 10100 molecules and 404247 hits with MOLFLOWR.EXE in about 24 minutes.

Figure 5.1.1 b) shows a different way of representing the same physical structure, BENCH5.TXT.

Everytime a structure has some symmetry properties (in this case there is a rotational symmetry about the Z-axis), then you can introduce one or more *mirror facets*: they are identified by a reflection coefficient equal to 1 (the 22nd component of the facets, see section 2.1 (Database Organisation)). In this case there are two such facets, and most of the hits (more than 86% of the total 322270) are made on them (the smaller you take the angle between the mirror facets the better you approximate the triangle to the circle but the slower becomes the MC simulation). This results in a lowered computing speed for BENCH5.TXT (about 3.3 times slower than BENCH.TXT), even if the value computed for the transmission probability is about the same, 0.06.

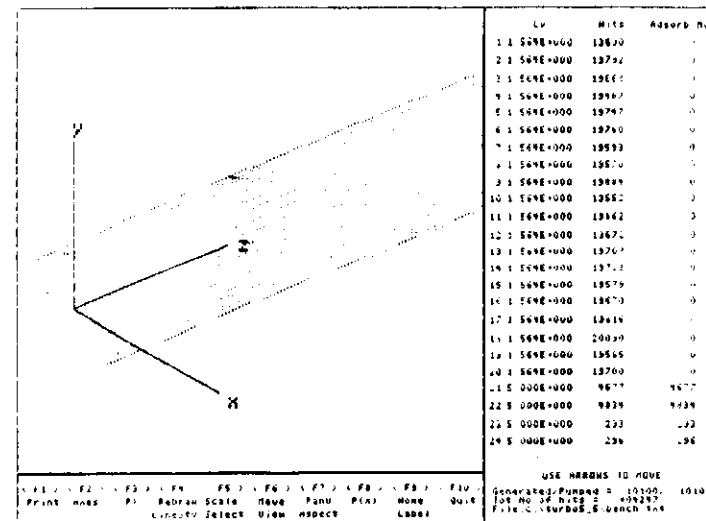The concept of *mirror facet* will be extensively used in the following examples.

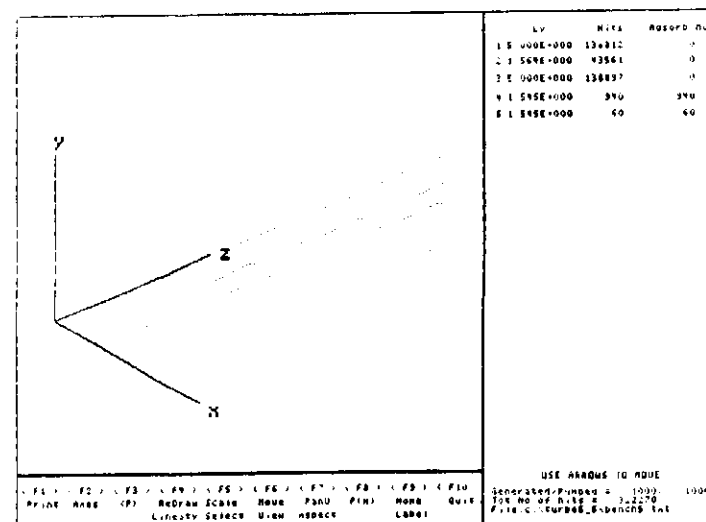Fig.5.1.1 a) Transmission probability of a round tube.

Fig.5.1.1 b) Same physical structure represented using mirror facets. Only 5 facets are necessary to simulate a straight round tube.

63

64

5.1.2 Transmission Probability of: Curved Elbows, Cylindrical Pipes With Restricted Openings and a Blocking Plate, and Coaxial Pipes

This second example is relevant from an historical point of view. The first applications of the Monte Carlo method concerned this kind of structures [1,3].

First we have created several data files called DAVISab.TXT, where 'a' and 'b' represent the length of the two arms of the cylindrical elbows. The same set of values for a and b as in [1] has been studied, just for comparison: the following figure shows the data file DAVIS53.TXT which has already been used extensively.
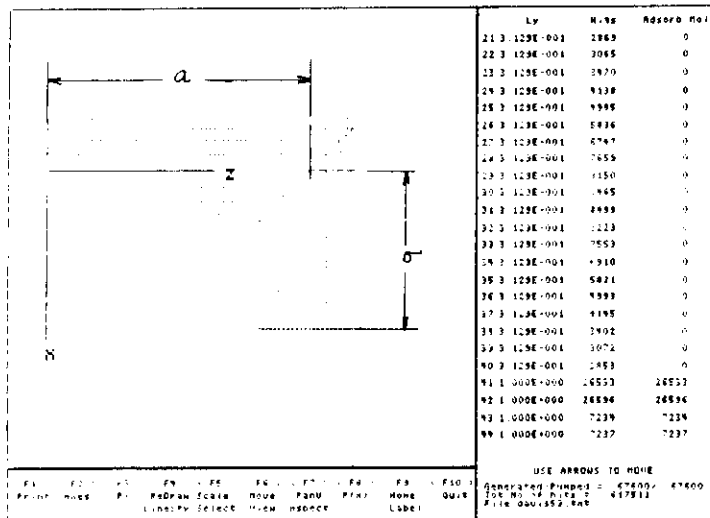
Fig.5.1.2.a) File DAVIS53.TXT: X-Z view defining the parameters a and b. Compare with values in table II, ref. [1].

You can verify, just reading all the data files on the attached diskette, that the results obtained by Davis [1] are well reproduced and, in some cases, have a better behaviour.

Another historically important device of high-vacuum technology is the so called cylindrical pipe with restricted openings and blocking plate [1]. Its utilization was mainly understood as a meaning for reducing the backstreaming of vapours from diffusion pumps.

The data file BLK1.TXT represents a 'slice' of $10°$ (i.e. there are two mirror planes (four mirror facets), and the symmetry around the Z-axis is 36-fold). Fig.5.1.2.b) shows the structure. The 'real' facets have been selected with the < Alt - F5 > Select option, and drawn as solid lines. This data file refers to the case $(R/R_0)^2=2$, $L/R_0=2.8284$, where R, R_0 and L are, respectively, the outer radius, the inner radius and the length.

The transmission probability is $8001/21760=3.6769E-1$, compared to about 0.37 as reported in fig.6 of ref. [1].
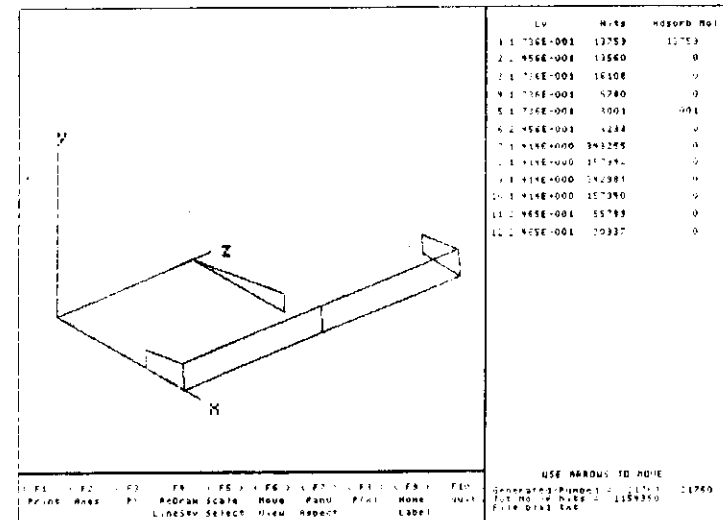
Fig.5.1.2.b) Cylindrical pipe with restricted openings and a central blocking plate.

The blocking plate is represented by two facets, no.3 and 4 (each side). If you remove them, then you get a cylindrical pipe with restricted openings [1].

The last data file represents a so called cylindrical annulus, i.e. a vacuum system consisting in the space between two coaxial cylinders, inner radius R_0, outer radius R, length L[1]; the file name is COAX10.TXT.

Here, again, the concept of mirror facet has been used. Also in this case the subtended angle is 10°, while $R_0/R=0.25$, $L/R=10$:
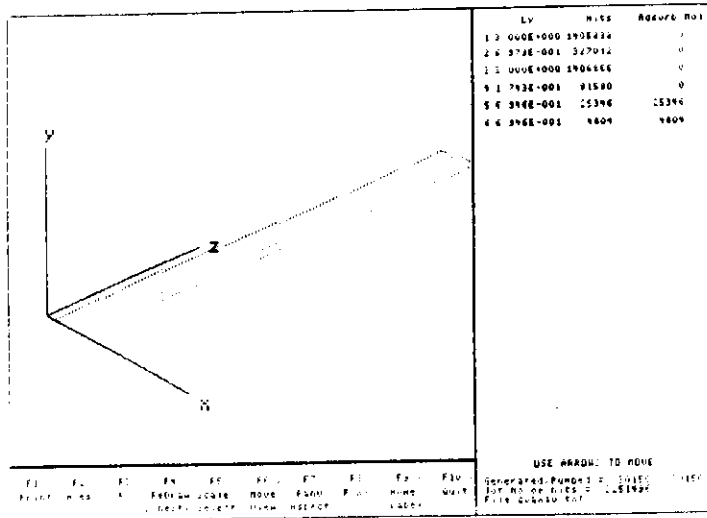
Fig.5.1.2.c) Cylindrical annulus

The transmission probability is 4804/30150=1.5934E-1, compared to about 0.16 as derived from fig.4 of ref.[1].

5.1.3 Transmission Probability and Conductance of a Compound Tube

A superstructure consisting of the three data files PIPE1.TXT, PIPE2.TXT and PIPE3.TXT is used in order to find the conductance of a compound tube, i.e. a non-straight tube with a varying cross-section, as found in document PM 800 062 PE (8802) 'Turbo-Molecular Pumps' by Balzers AG, Balzers (FL):

The concept of mirror facet has been used here also: there is a symmetry plane represented by the XZ plane in the following figures.

The four figures show the three structures separately, and the superstructure:
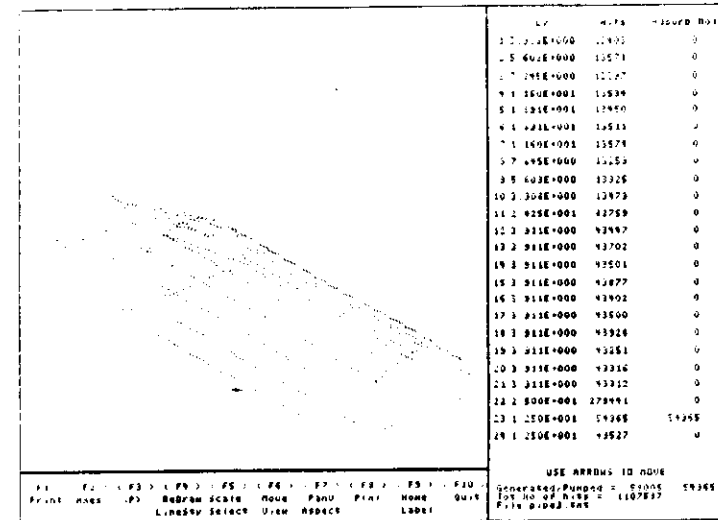
Fig.5.1.3 a) First structure, PIPE3.TXT, a cylinder and a cone connected in series: molecules are desorbed by the round facet on the right hand side (facet no.23).
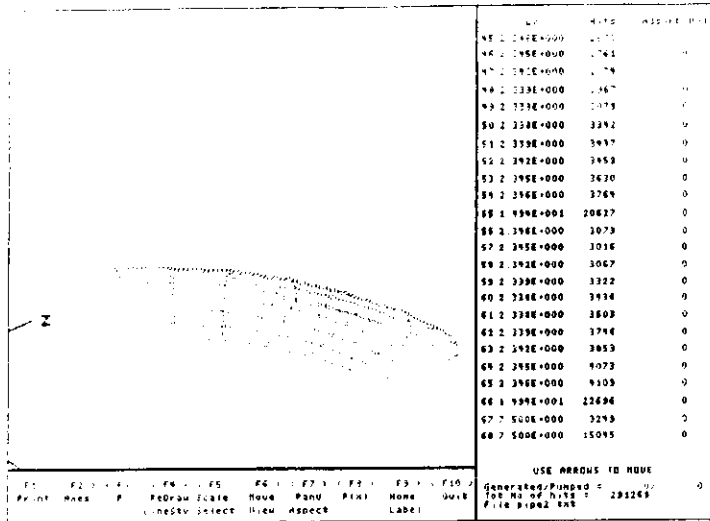
Fig.5.1.3 b) Second structure, PIPE2.TXT. It is a 60° -bent round pipe.

Fig.5.1.3 c) Third structure, PIPE1.TXT, a 30° elbow and a cone connected in series. Molecules are considered to be transmitted when they hit the round facet on the XY plane.

Fig.5.1.3 d) Overall view of the superstructure as obtained running the MC simulation

The conductance C of the superstructure, in l/s, is given by the transmission probability, T=3040/58005=0.0524 in the present simulation, times a factor of 5682.6 l/s given by

$$C = 11.77 \times 2.0 \times A \times T \ [l/s]$$

The factor 11.77 is the conductance of a 1 cm^2 orifice for N_2 at 20° C, A is the inlet surface area in cm^2, 2.0 accounts for the mirror facet (half of the real structures); substituting, we get

$$C = 297.8 \ l/s.$$

This value should be compared to that reported in the referenced publication. There the superstructure is considered as made up of four parts, namely:

1) a cylinder d_1=25 cm, length l_1=50 cm, resistance W_1 [sm^{-3}];

2) a cone inlet d_1=25 cm, outlet d_2=15 cm, length l_2=20 cm, resistance W_2 [sm^{-3}];

3) a 90° elbow, d_2=15 cm, length l_3=74.6128 cm, resistance W_3 [sm^{-3}];

4) a cone inlet d_2=15 cm, outlet d_3=20 cm, length l_4=20 cm, resistance W_4 [sm^{-3}];

If the following standard formulae of vacuum technology are used

$$W_{tot} = W_{Omin} - W_{Op} + W_1 + W_2 + W_3 + W_4$$

$$W_{Omin} = 0.011 \frac{1}{d_2^2} = 0.489 \ [sm^{-3}]$$

$$W_{Op} = 0.011 \frac{1}{d_3^2} = 0.069 \ [sm^{-3}]$$

$$W_1 = 0.00826 \frac{1}{d_1^2} = 0.264 \ [sm^{-3}]$$

$$W_2 = 0.00826 \ l_2 \frac{\frac{d_1 + d_2}{2}}{d_1^2 d_2^2} = 0.235 \ [sm^{-3}]$$

$$W_3 = 0.00826 \frac{l_3}{2} R \frac{1}{d_2^3} = 1.538 \ [sm^{-3}]$$

$$W_4 = 0.00826 \ l_4 \frac{\frac{d_2 + d_3}{2}}{d_2^2 d_3^2} = 0.321 \ [sm^{-3}]$$

$$W_{tot} = 2.778 \ [sm^{-3}]$$

where W_{Omin} is the resistance of the smallest cross-section along the superstructure, and W_{Op} is the resistance of the inlet opening, then the theoretical conductance C_{th} is obtained taking the reciprocal of W_{tot}:

$$C_{th} = 360 \ l/s$$

which is about 20% higher than calculated by the MC simulation (it is not clear at which temperature the previously reported quantities have been calculated, but this should not affect appreciably the results).

This shows clearly the magnitude of the variations to be expected between conductance and pumping speed data obtained by application of standard analytical formulae.

71

5.1.4 Transmission Probability of Butterfly and Angle Valves

Now 2 different structures will be shown: both are related to vacuum valves, namely an angle valve and a butterfly valve [14,15,16].

The first data file is LH68025R.TXT that is the following structure:
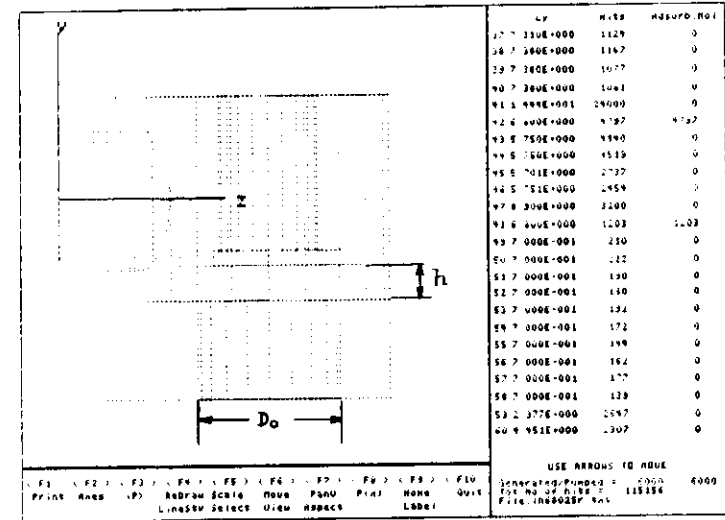
Fig.5.1.4 a) Angle valve, ID D_0=68 mm, relative lift h/D_0=0.25

The inlet facet is no.42, the one on the left (on the XY plane), the outlet is no.48, the one on the bottom. A mirror facet has been used. Its shape has been set rectangular in order to minimise the time necessary to find the trajectory intersections on it: in fact, see Appendix A3, the CPU time taken by the algorithm finding if a point is inside a facet or not, increases almost linearly with the number of points/facet.

Figure 5.1.4 b) shows the MC simulation running. You can change the valve's lift, h, and therefore create new data files, using option 3.1.2.5 Translate (and Copy): the points to be translated in the Y-direction are no.78 through 114 included, i.e. the valve's plate.

If w is the transmission probability, w=1203/6000=2.0050E-1 then the reported *measured* transmission probability $w^*=(1/w-1)^{-1}$ [14] is about 0.27 while that calculated in the present simulation is 0.2508 (1203 transmitted molecules out of 6000).

72

The first file, LH68LEFT.TXT, has been obtained in the following way:

1) using option 3.1.2.7 (Magnify (and Copy)), magnifying all of the points of LH68025R.TXT by a factor of -1.0 in the X-direction; the structure obtained in this way is the mirror image of LH68025R.TXT, but all of the facets are oriented outward;

2) using option 3.1.2.2.6 (Reverse Orientation of Facet(s)), reversing all of the facets in order to correct the orientation;

3) setting the sticking and transparency coefficients of the mirror facet equal to 2.0 and 0.0, respectively, in order to let the molecules go in the right half of the valve (LH68RIGT.TXT).

The second file, LH68RIGT.TXT has been obtained from LH68025R.TXT simply changing the sticking and transparency coefficients to 1.1 and 0.0, to let the molecules go in the left half of the valve (LH68LEFT.TXT).

The transmission probability is : w=(5056+5032)/51120=0.1973, and w*=0.2458.

This last result clearly indicates the validity of the mirror facet concept even when applied to complex structures.

Another kind of vacuum valve has been studied, a butterfly valve [15].

Fig.5.1.4.d) shows the geometry of the valve: the configuration with α=50° is shown here, but you could easily obtain other angles of rotation simply rotating points no.39 through 76 using option 3.1.2.6 (Rotate (and Copy)), selecting the rotation about an axis parallel to the X-axis at coordinates Z=0.83, Y=0.0: positive angles of rotation increase the angle α, negative values decrease it. You should not increase α, otherwise a part of the valve disc 'exits' through the inlet facet.

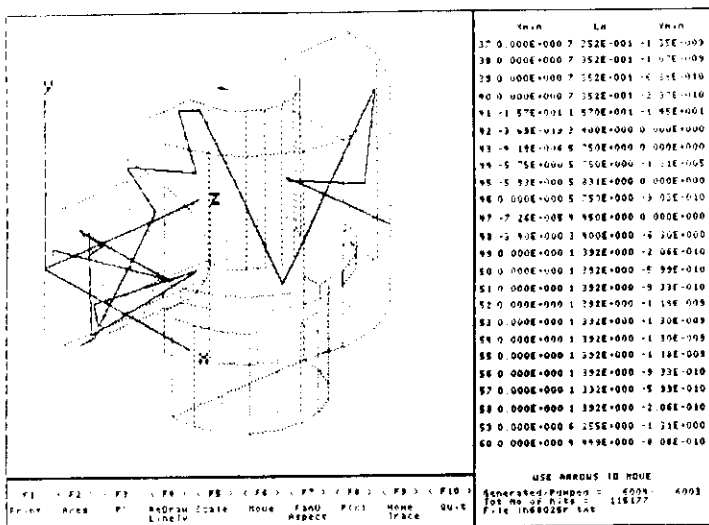Fig.5.1.4.e) shows the axonometric view of the structure.

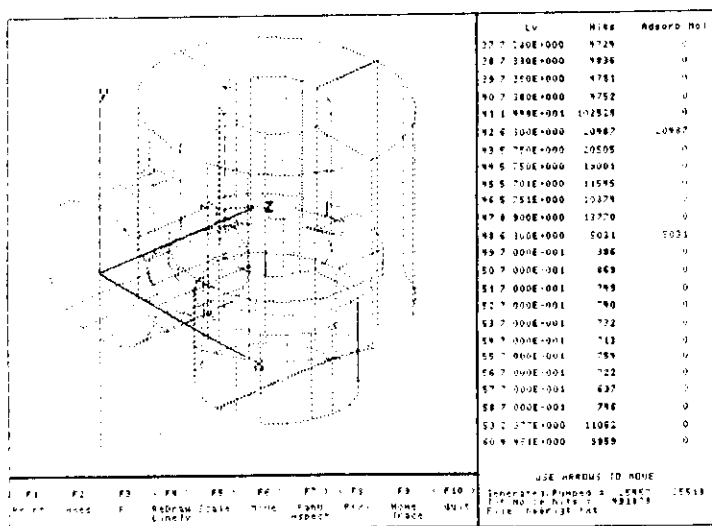

Fig.5.1.4.b) MC simulation running data file LH68025R.TXT

Fig.5.1.4.c) MOLFLOWR running a superstructure made up of two files, LH68LEFT.TXT (left half of the angle valve) and LH68RIGT.TXT (right half)
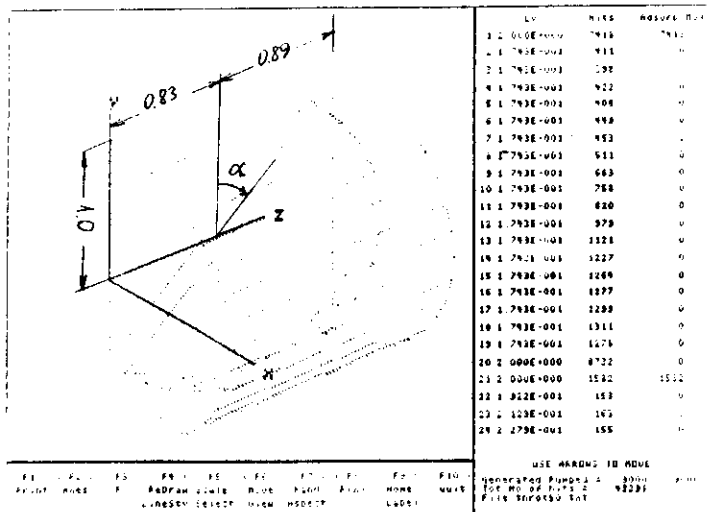
Fig.5.1.4.e) Butterfly valve: the concept of mirror facet has been applied again

5.1.5 Molecular Transmissivity of a Chevron Type Baffle

Chevron-type baffles are commonly used to protect the cold heads of cryopumps from the incident radiation. Therefore the ideal chevron baffle should have a very high molecular transmissivity and a very low radiation transmissivity. This subject has been studied extensively in the past years [6,8,9,10], in order to reduce LHe consumption and compressors' power.

The molecular transmissivity will be treated here, that for radiation in section 5.2.2.

The data file is BENVEM.TXT, and refers to the case when the chevrons do not overlap (P=0) and form an angle of 120°, the diameter of the chevron is d=13.6 cm, its height is h=4 cm, and therefore d/h=3.4 (refer to fig.1 and 2 of ref. [9]). Molecules enter the baffle diffusely, i.e. a cosθ emission from facet no.19 is assumed.

The situation is as follows
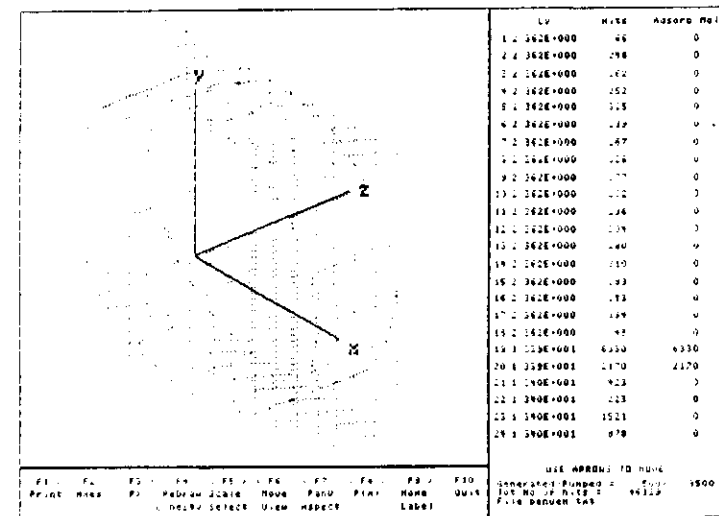
Fig.5.1.5.a) Chevron-type baffle.

The molecular transmissivity is given by $T_M = 2170/8500 = 2.5529E-1$, compared to a value of about 2.6E-1 as reported in [9]. Note that some of the chevrons 'overflow' the round flange: this was done in order to have a simpler data input (only one chevron has

been created and then copied and translated). This fact does not affect the results of the simulations.

The following figure shows the top-view, XZ projection, of the chevron-type baffle.

As you can see there is not overlapping of the chevrons (P=0 case in ref.[9]), and the angle formed by the chevron's blades is 120°.
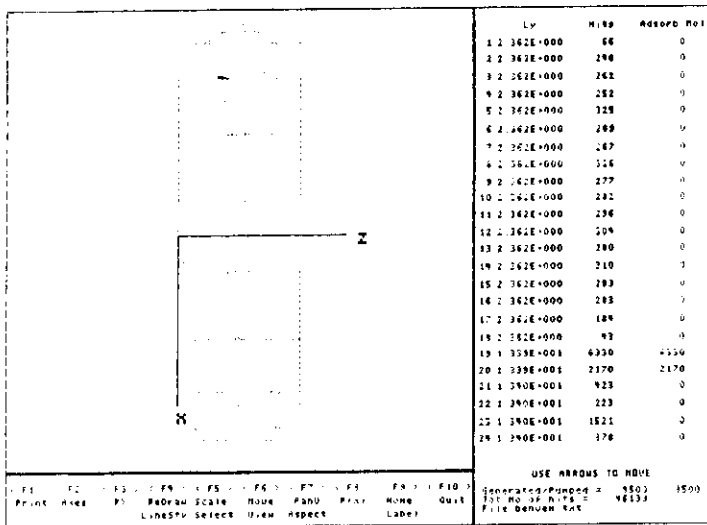
Fig.5.1.5.b) Chevron-type baffle: top view

The given transmissivity T_M has a standard deviation of

$$\sigma_T = [T_M (1 - T_M) / 8500]^{1/2} = 4.512E-3$$

5.1.6 Specific Conductances of the Vacuum Chambers of Particle Accelerators

One of the most challenging tasks to fulfil in modern particle accelerators is to have a very low base pressure in order to obtain sufficiently long beam lifetimes and/or small backgrounds in the experimental areas. Usually a small bore diameter in the magnetic elements, bendings, quadrupoles etc., dictates very stringent requirements for the dimensions of the vacuum chamber, and this, in turn, requires a careful choice for all of the various parts of the vacuum system. In addition to that, very high outgassing rates are involved, especially in electron/positron machines.

The theoretical conductance of the vacuum chamber, C_{th}, is a factor strongly affecting the average pressure. It depends on the dimension and shape (cross-section) of the vacuum chamber. Usually the following formula is applied

$$C_{th} = \frac{4}{3} 10^{-3} \frac{\langle v \rangle}{\int_0^L \frac{H}{A^2} dl} \ [l/s]$$

with <v> the average molecular speed, $\langle v \rangle = \sqrt{\frac{8R}{\pi}\frac{T}{M}} = 1.455 \times 10^4 \sqrt{\frac{T}{M}}$ [cm/s]

H is the vacuum chamber perimeter in cm, A is the cross-sectional area in cm^2, L is the length of the vacuum chamber in cm, T is the gas temperature in °K and M the molecular weight. This formula gives approximate results: the more the cross-section is regular, read *circular*, the more it gives good results.

Nowadays, several particle accelerators, mainly synchrotron radiation light sources [29,31,35-37], use or plan to use multi-chambered vacuum systems, where most of the vacuum chamber consists in the beam-chamber *and* an attached ante-chamber, usually connected by means of slots. In this case the application of the above formula is not allowed, since it assumes that particles enter the cross-sectional area uniformly. This is not certainly the case, since molecules are desorbed in one of the two chambers only.

It will now be shown the application of MOLFLOW to the calculation of the specific conductance of several vacuum chamber configurations, and the results will be compared with those obtained by application of the mentioned formula.

In the following L=100 cm, to get the specific conductance in [l*m/s], and M=28 (N2). For a constant cross-section $C_{th}=0.6277 \ A^2/H$ [l/s].

Data file ELETTRA.TXT, Sincrotrone Trieste vacuum chamber. A=30.34 cm^2, H=20.78 cm, L=100 cm.
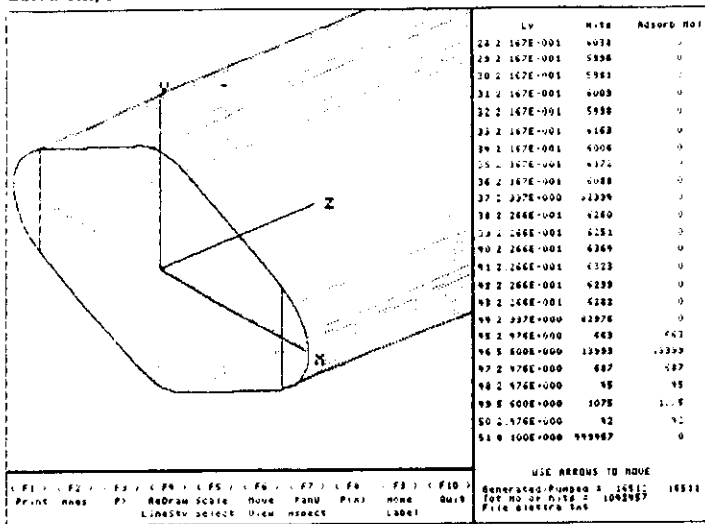
Fig.5.1.6.a) ELETTRA vacuum chamber [34].
C=11.77*A*(45+1075+42)/16511=25.132 [l*m/s], compared to C_{th} = 27.81 [l*m/s].
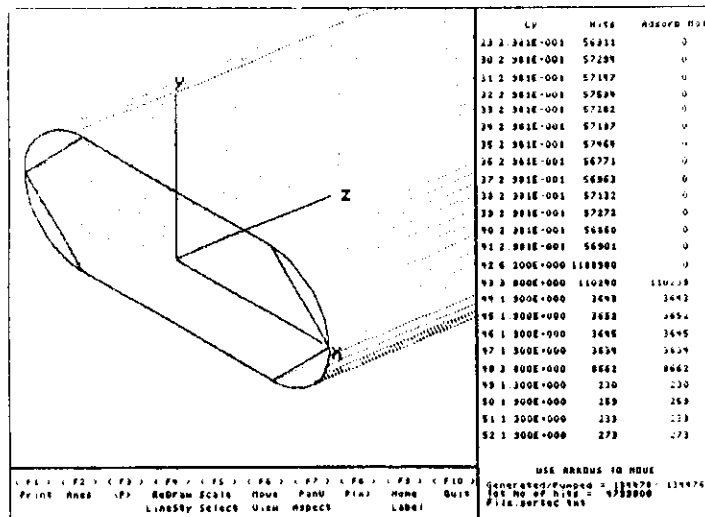
Fig.5.1.6.b) SORTEC vacuum chamber [39]: A=34.85 cm^2, H=24.33 cm;
C=11.77*A*(8662+230+259+239+273)/134476=29.47 [l*m/s], C_{th}=31.33 [l*m/s]
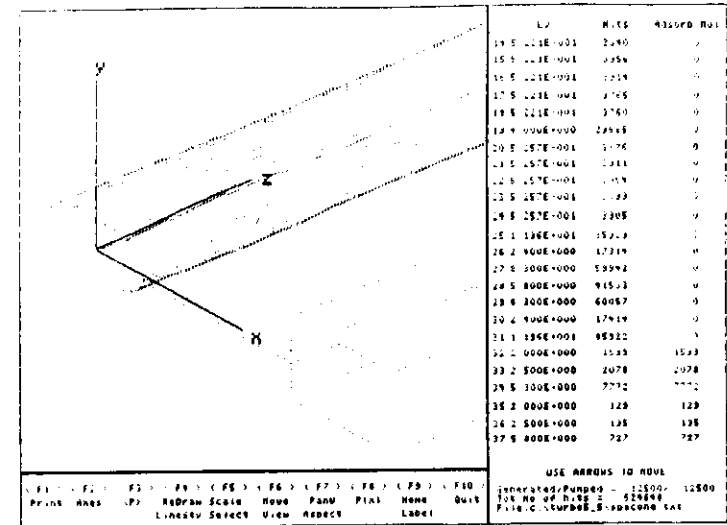
Fig.5.1.6.c) SPring-8 vacuum chamber (straight sec.)[39]: A=88.50 cm^2, H=70.65 cm, C=11.77*A*(129+195+727)/12500=87.58 [l*m/s], C_{th}=69.59 [l*m/s]
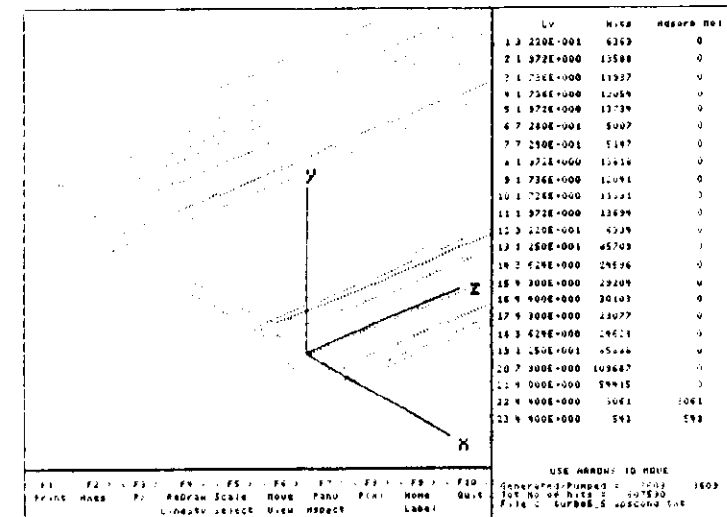
Fig.5.1.6.d) APS vacuum chamber (straight sec.)[35]: A=62.19 cm^2, H=63.38 cm, C=11.77*A*548/8609=46.59 [l*m/s], C_{th}=38.30 [l*m/s]
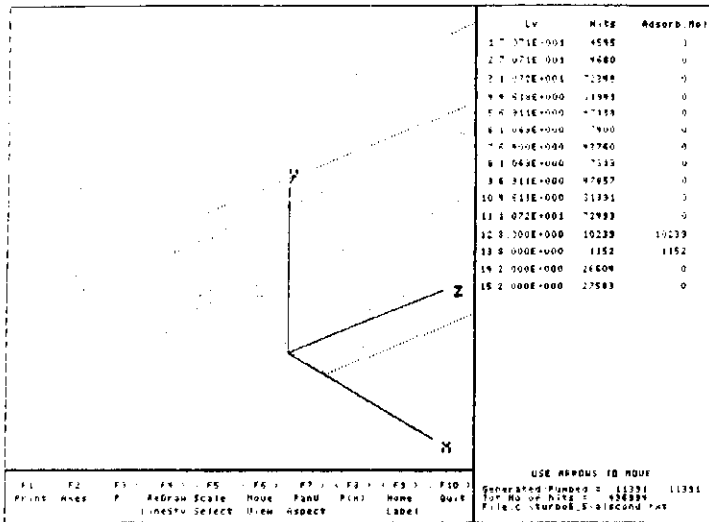
Fig.5.1.6.e) ALS U5.0 insertion device vacuum chamber [31]: A=84.92 cm^2,
H=54.46 cm, C=11.77*A*1152/11391=101.08 [l*m/s], C$_{th}$=83.12 [l*m/s]

Note that for all of the shown accelerator vacuum chambers, the beam direction is along
the Z-axis.

5.1.7 Pumping Speed Calculations for Lumped NEG Pumps

In the last years, Non-Evaporable Getters (NEG) have increasingly been used in the
UHV systems of many particle accelerators [12,29,30,34-37,41], among many other
applications.

NEGs for particle accelerators are usually under the form of strips, and the user has to
find a convenient way of 'packing' these strips to increase both the pumping speed and
the pumping capacity, and therefore the time interval between NEG regenerations.
'Module' configurations, a folded strip, are available on the market and frequently
used.

The following application of MOLFLOW shows how to get an estimate of the pumping
speed of a so called Lumped NEG Pump (LNP) proposed for installation in the 8 GeV
SPring-8 synchrotron light source to be built in Japan [30,39].

The purpose is to obtain the pumping speed of a LNP made up of 14 NEG modules
arranged vertically inside a cylindrical body. The pump's flange is a CF 250.

The idea is to study the LNP pumping speed vs NEG sticking coefficient, s: only the
case where s=0.17, in comparison with the results given in [30], will be shown.

In order to minimise the CPU time, since the geometry of the proposed LNP has a 14-
fold symmetry axis, the concept of mirror facets has been applied again. There are two
such facets making an angle of 2π/14 radians. There are 3 data files in the
superstructure: LNP017.TXT represents the pump's body, and has 5 facets with
sticking coeff. set equal to 2.0 and 5 more facets with sticking coeff. equal to 3.0, in
order to let the molecules go in the 2-nd structure and in the 3-rd. The second structure
represents the first half of the NEG module (it has been divided in two halves since its
total number of facets exceeded 80, the maximum number allowed), and the third the
second half. Their file names are WP1017.TXT and WP2017.TXT.

The pumping speed obtained with MOLFLOW is:
S=14*11.77 *A*(10897+17815)/50500=3258.41 [l/s], compared to a calculated value
of 2200 [l/s] and a measured value of 4000 [l/s] as given in ref.[30].

Fig.5.1.7.a) shows the LNP body, with the position of the NEG module, while the
other figure shows the adsorption profile on the first half of the NEG module.
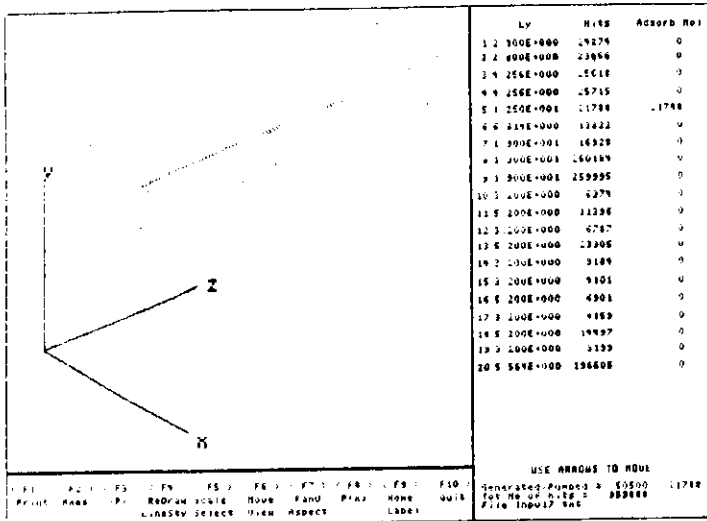
Fig.5.1.7.a) LNP body with a NEG module (1/14-th). Two mirror facets are used
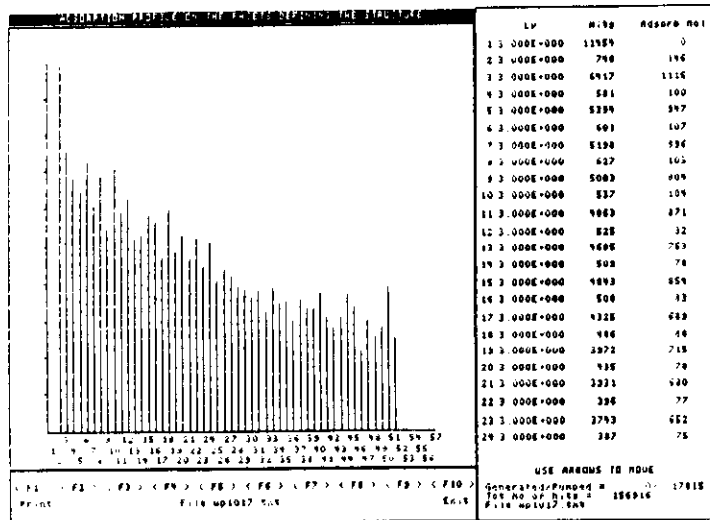
Fig.5.1.7.b) First half of the NEG module. Adsorption profile showing the non-uniform saturation of the getter module. The higher the NEG sticking coefficient, the more non-uniform is the adsorption profile

The following graph shows a summary of the results which have been obtained by varying the sticking coefficient of the NEG strip: the effective pumping speed S_{eff} for CO at pump's inlet flange is plotted against the NEG sticking coefficient, together with an estimate of the conductance of the body of the pump, C.

The latter can be obtained by the following formula:

$$\frac{1}{C} = \frac{1}{S_{eff}} - \frac{1}{S_{nom}}$$

where S_{nom} is the nominal pumping speed of the folded NEG strip, i.e. the product of the 11.77 [l/s/cm^2] times the strip's surface [cm^2] times the sticking coefficient.
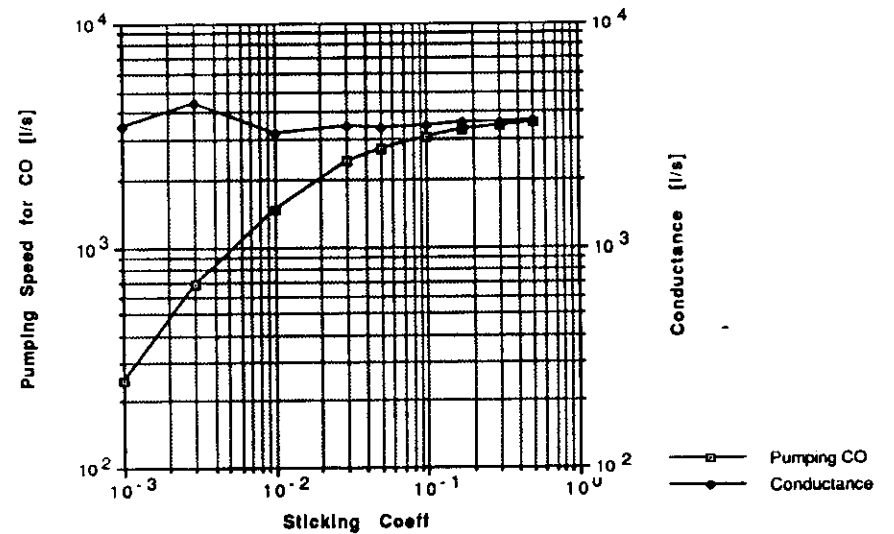
Fig.5.1.7.c) Pumping speed at pump's inlet flange and conductance of the body of the pump for a mass 28 gas

5.1.8 Pumping Efficiency of 3-D Cryopumping Structures

3-D cryopumping structures have been studied in order to increase the pumping speed available in experiments with neutral injectors for fusion research [8]. Several different configurations of cryopanels protected by louvre-blind elements cooled to LN_2 temperature have been studied. Here one of these configurations has been studied, see fig.5 of ref. [8]. The data file HEMM12.TXT corresponding to a spacing a=12 cm between the pumping structures is shown. An overall pumping efficiency $\eta(a)=0.377$ is obtained, thus suggesting a 'lower limit' for it, as reported in [8].

LN_2 surfaces are assumed to be as non pumping: molecules are reflected following a cosine law; LHe cryosurfaces trap molecules with a probability of 1.

The louvre elements are represented by the double-sided facets no.1, 2, ..., 17 and 24. The cryosurface is facet no.20. Facets no.18, 19, 21 are mirror facets (mirror symmetry in the X and Y directions).
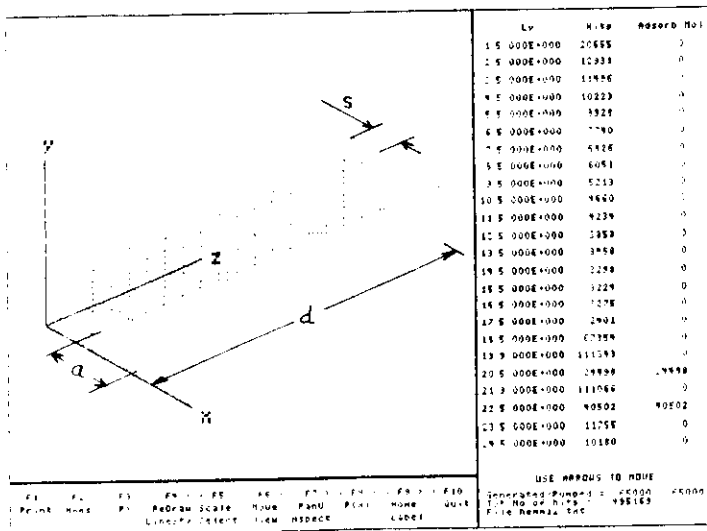
Fig.5.1.8 Well consisting of louvre-blind elements. Depth d=30 cm, width s=6 cm, distance a=12 cm. Pumping efficiency $\eta(a)=0.377$.

5.1.9 Sputter-Ion Pump

A 120 l/s sputter-ion pump has been simulated. The two rectangular facets, no.30 and 31, represent the two cathode-anode 'pockets', where actual pumping occurs. Assigning a sticking coefficient of 0.04 to the two facets, one gets a pumping speed, S, of

$$S=11.77*48.45*2.0*(1132+1019)/21100 \text{ [l/s]} = 116.267 \pm 2.376 \text{ [l/s]}$$
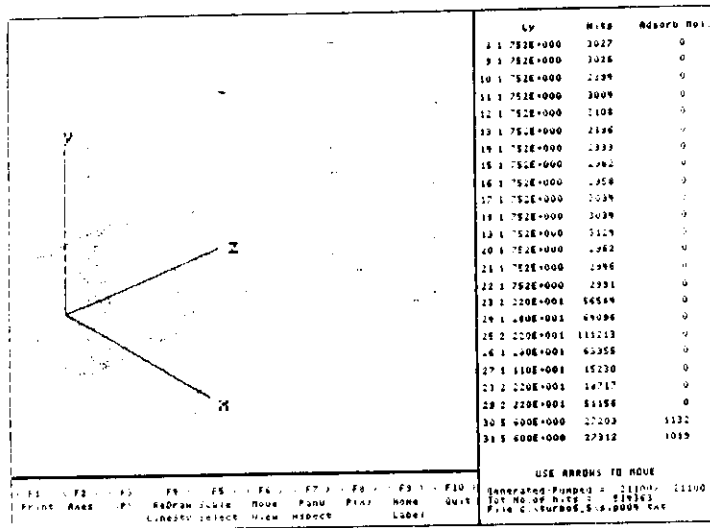
Fig.5.1.9 A 120 l/s sputter-ion pump (VARIAN StarCell).The actual geometry inside the two 'pockets', where the pumping Penning cells are situated, is not taken into account

5.2 Photon Trajectory Calculations

This section is devoted to the application of MOLFLOW to problems which do not involve molecular trajectories, but instead photon trajectories.

The main difference is that photons are usually assumed to undergo mirror reflection instead of diffusive reflection. Moreover, the ability of surfaces to reflect or absorb photons is usually described by a factor called *reflectivity*, r.

In MOLFLOW this reflectivity is treated as a sticking coefficient: r=1 is obtained setting the sticking coeff.=0, while r=0 requires a sticking coeff.=1.0.

5.2.1 Transmission Probability of a Straight Round Tube

The first structure to be studied is a straight round tube [6]. The data file BLECHD20.TXT represents the case of a tube with radius R=1, diameter D=2, length L=40, with reflectivity r=0.5, and a diffuse initial photon distribution.
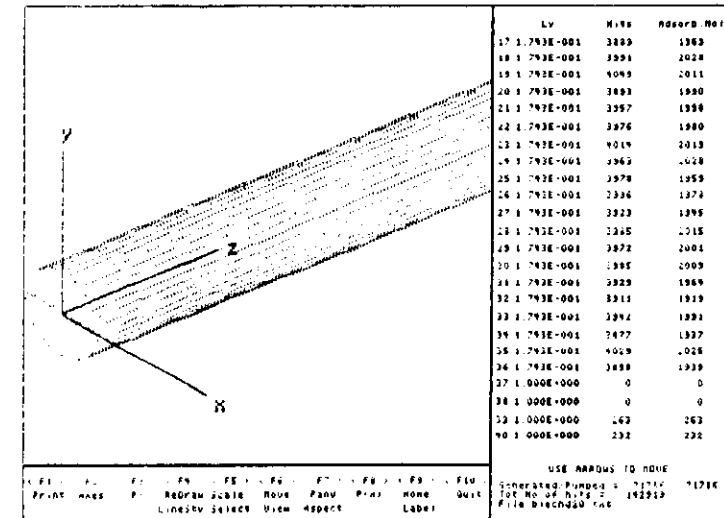
Fig.5.2.1 Transmission of light with cosine initial distribution. L/D=20, r=0.5

Referring to fig.5 of ref.[6], here a transmission probability of (263+232)/71786=6.895E-3 is obtained compared to about 7.0E-3.

5.2.2 Radiation Transmissivity of a Chevron Type Baffle

In the following, please refer to 5.1.5. The data file is BENVEP1.TXT: the geometry is the same as in the molecular case, but the reflection properties of all of the facets in the structure have been taken as 'mirror' (i.e. the components no.22 are set=1.0). The reflectivity of the facets is taken as r=0.21, the other parameters, d and h, being the same as in the molecular case. The radiation enters the baffle diffusely, i.e. a $\cos\theta$ emission from facet no.19 is assumed.

The obtained radiation transmissivity is given by 89/8000=1.125E-2, compared to about 1.0E-2 as reported in fig.2 of ref. [9].

The given transmissivity Tp has a standard deviation of

$$\sigma_T = [T_P (1 - T_P) / 8000]^{1/2} = 1.179E-3$$
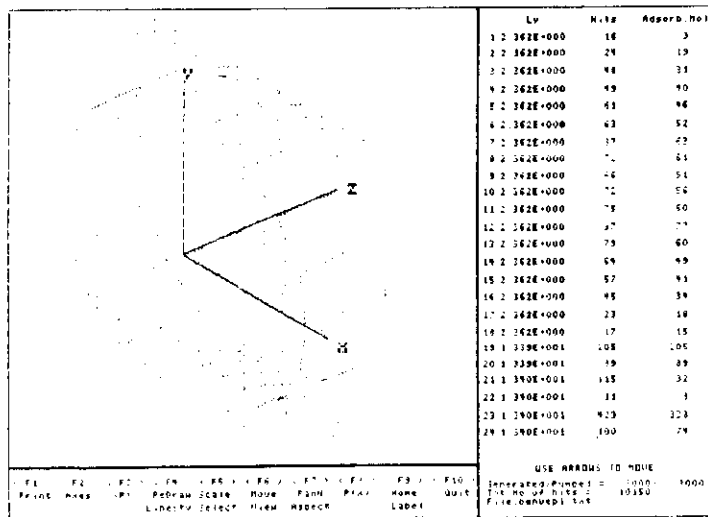
Fig.5.2.2.a) Radiation transmissivity for a chevron-type baffle [9]
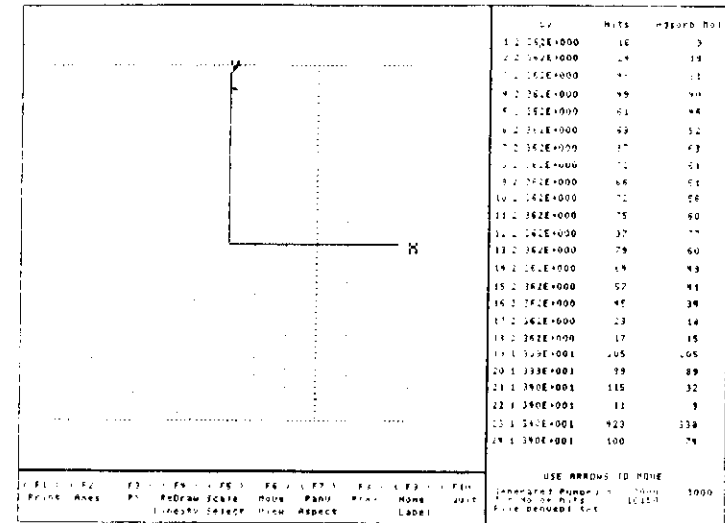
Fig.5.2.2.b).Front view, XY projection, of the chevron-type baffle

If one sets the reflectivity of the flange facets equal to one, i.e. only the chevrons absorb the incident radiation, then the optical transmissivity is almost doubled, its value becoming 2.2297E-2 (see data file BENVEP.TXT on the diskette).

5.2.3 Radiation Transmissivity of 3-D Cryopumping Structures

The possibility of 'packing' some cryopumping surfaces, thus forming so called *cryopumping arrays* has been studied in the past [8] in order to increase the pumping speed in fusion research machines.

The following data file refers to a so called 'well consisting of louve-blind elements', fig.5 of ref.[8]. Again the concept of mirror facet has been applied, in order to analyse a structure which is not limited in the Y-direction and is mirror-symmetric with respect to the two planes X=0 and X=(s+a).

The file name is HEMMP12.TXT
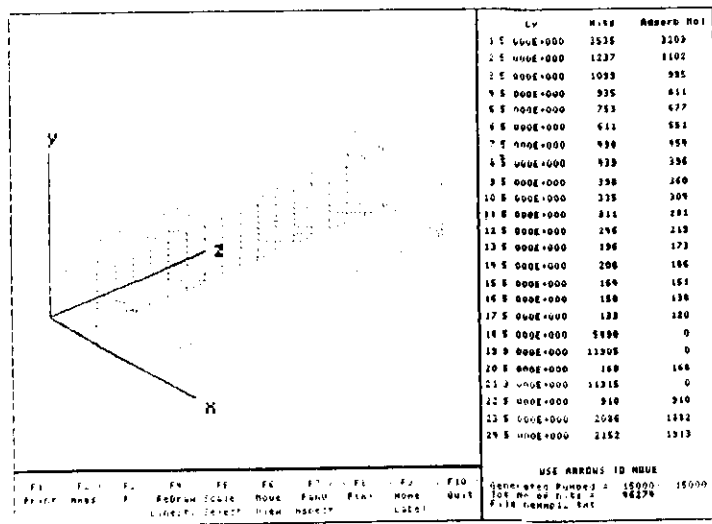
Fig.5.2.3 Well consisting of louvre-blind elements. Louvre angle is 45°, d=30 cm, s=6 cm, a=12.

Refer to section 5.1.8 for additional informations. The cryosurface is represented by facet no.20, and the reflectivity of all of the facets is 0.1. The obtained radiation transmissivity is 168/15000=1.120E-2. This value, not reported in ref.[8], gives an estimate of the total power to be removed from the LHe cryo-surface, an important parameter for a cryogenic system.

5.3 Miscellanea

Two more examples of the possibilities of MOLFLOW will be described.

5.3.1 Pressure Profiles in Accelerator Vacuum Chambers

MOLFLOW may be useful for finding the pressure profiles in accelerator vacuum chambers. For example, let's consider the U5.0 undulator vacuum chamber proposed for the Advanced Light Source at LBL [31].

The data file is ALSID4.TXT. Facets no.26 through 31 included represent the six 600 l/s/60 l/s TSP/SIP pump combinations, with a net pumping speed at the chamber connection of 173 l/s, while facet no.19 is the 1450 l/s absorber pump.

The obtained pressure profiles in the beam chamber (facet no.32) and ante-chamber (facet no.41), are shown in the following figure. These profiles are quite different compared to those shown in [31], which have been obtained using a so-called 'flow model'. Note that MOLFLOWR had to be slightly modified in the P_start procedure, in order to obtain both the thermal desorption and SR-induced desorption as given in ref.[31].
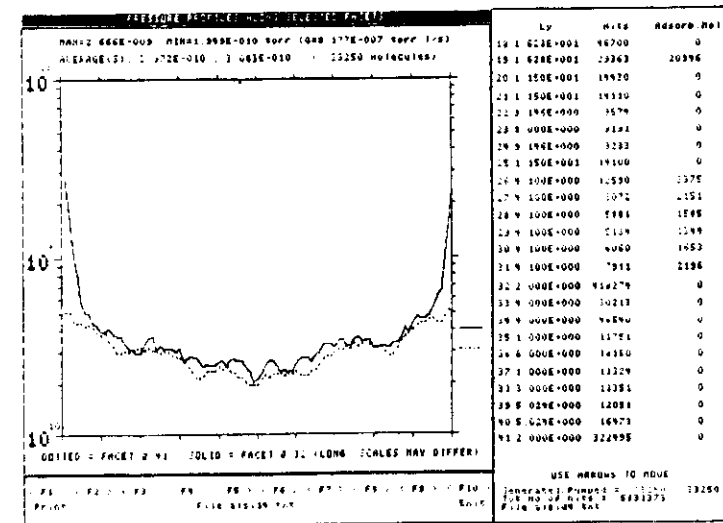
Fig.5.3.1 ALS U5.0 undulator vacuum chamber. The obtained average pressure is 32% higher than reported in [31]

5.3.2 Pumping Speed Test Dome

The procedure of pumping speed measurement for a lumped NEG pump (LNP) proposed for the ELETTRA sorage ring [41], following the 'known conductance method' is shown [42].

There is a CF 150 dome with a 1 cm² conductance, 2 tubulated gauges, the LNP body with the NEG module inside it.

This study has been performed using a superstructure with 2 structures, DOME04.TXT (the dome), and MODULO04.TXT (the NEG module).

The dome wall is described by facets no.1 through 23, the tubulated gauges by facets 25 through 35 (upper) and 36 through 47 (lower). Facet no.51 is the source facet in the upper dome. The LNP body is represented by facets no.52 through 64, and the connections to the other structure (the NEG module) is made via facets no.65 through 70 (sticking coeff.=2.0, transparency=0.0).

Facets no.71 and 72 (transparency=0.0) are used to define the pumping probability at LNP flange, while facets no.48 and 73 are the two pressure profile facets (transparency=-1.0).

The installed pumping speed, S_{inst}, is given by the NEG strip surface (obtained from data file MODULO04.TXT running option 3.1.5.4 (Listing of Database (Running Sum of Selected Components))), that is twice the surface area of facets no.1 through 74 (double-sided facets), times 11.77 l/s/cm² times the sticking coefficient:

$$S_{inst} = 11.77*2.0*549.5*0.04 = 517.41 \text{ l/s}$$

The effective pumping speed, S_{eff}, at the pump's throat is given by the ratio between the hits on the transparent facets no.71 and 72, times 11.77 l/s/cm² times their surface area (85 cm²):

$$S_{eff} = 11.77*85.0*(2584-1967)/2584 = 238.88 \text{ l/s}$$

The measured pumping speed, S_{meas}, measured by the two tubulated gauges (as in the real dome geometry), is given by the formula used in the 'known conductance method' procedure, that is

$$S_{meas} = 11.77*(P2-P1)/P1 = 11.77*(7278-363)/363 = 224.21 \text{ l/s}$$

where P2 ans P1 are the number of hits on facets no.33 and 45, the tubulated gauges.
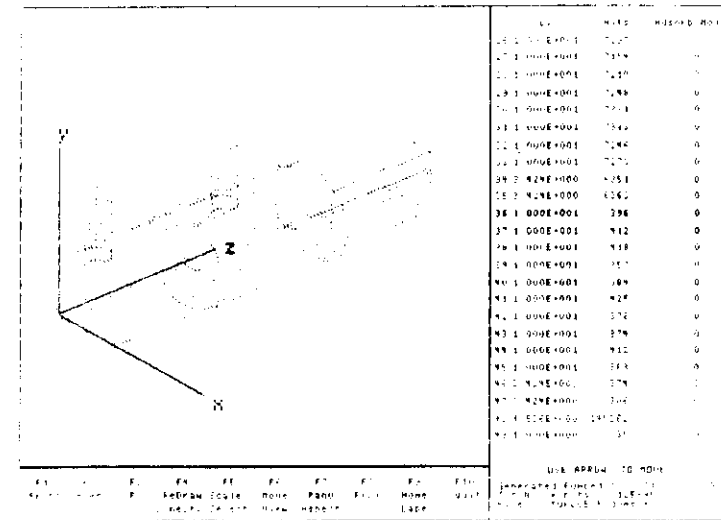
Fig.5.3.2 LNP pumping speed measurement setup

5.3.2 A 180° Circular Elbow

The three data files CELBOW1.TXT, CELBOW2.TXT and CELBOW3.TXT define a superstructure representing a 180° circular elbow, with inner radius r=2 cm and bending radius R=10 cm.

The inlet area A is 11.76 cm², the transmission probability has been found to be Tr=(85009-74724)/85009=1.210E-1, and therefore the conductance C of the elbow is

$$C = 11.77*11.76*1.210E-1 = 16.746 \text{ l/s}$$

The following figure shows the geometry of the elbow:

Fig.5.3.3 180° circular elbow. A total of 3x62 facets defines the superstructure

7. References

The following literature partly covers the subject of Monte-Carlo simulations applied to the calculation of molecular flows and photon trajectories:

[1] *Monte Carlo Calculation of Molecular Flow Rates through a Cylindrical Elbow and Pipes of Other Shapes*, D. H. Davis, J. Appl. Phys. **31**, 1169 (1960).

[2] *Free Molecular Conductance of a Cylindrical Tube with Wall Sorption*, C. G. Smith, G. Lewin, J. Vac. Sci. Technol. 3, **92** (1965).

[3] *A review of the molecular flow conductance for systems of tubes and components and the measurement of pumping speed*, W. Steckelmacher, Vacuum **16**, 561 (1966).

[4] *Monte Carlo analysis of pumping speed test dome performance for several vapour diffusion pump geometries*, J. N. Chubb, Vacuum **16**, 591 (1966).

[5] *Monte Carlo computations on molecular flow in pumping speed test domes*, E. Fischer, H. Mommsen, Vacuum **17**, 309.

[6] *Monte Carlo study of light transmission through a cylindrical tube*, D. Blechschmidt, J. Vac. Sci. Technol. **11**, 570 (1974).

[7] *The use of the resistance concept in transmission probability calculations*, L. Fustoss, Vacuum **22**, 111.

[8] *Pumping efficiencies of three-dimensional cryopumping structures*, J. L. Hemmerich, E. B. Deksnis, J. Vac. Sci. Technol. **19**, 96 (1981).

[9] *Molecular and radiation transmissivities of chevron type baffles for cryopumping*, C. Benvenuti, D. Blechschmidt, G. Passardi, J. Vac. Sci. Technol. **19**, 100 (1981).

[10] *Monte Carlo analysis in a refrigerator cryopump*, L. Bingkun, Q. Jin, Proc. 11-th Int. Vac. Congress IVC-11, Cologne 1989.

[11] *A dynamic flow calibration system with four-sphere construction*, L. Wangkui, L. Qiang, L. Shiliang, Proc. 11-th Int. Vac. Congress IVC-11, Cologne 1989.

[12] *A Macintosh Computer Program for Monte Carlo Simulation of Molecular Gas Flow*, A. Pace, CERN PS/ML/NOTE 87-3 (1987).

[13] *Monte Carlo Simulations of Molecular Gas Flow: Some Applications in Accelerator Vacuum Technology Using a Versatile Personal Computer Program*, A. Pace, A. Poncet, CERN PS/89-49 (ML) (1989); Proc. 11-th Int. Vac. Congress IVC-11, Cologne 1989.

[14] *Measurement of conductances of models in the molecular and viscous flow regime*, W. Buschbeck, U. Hoechner, W. Schwarz, Vacuum **41**, 2050 (1990).

[15] *Calculated and measured flow conductance for butterfly valves*, G. Hummer, G. Halter, M. Grossl, Vacuum **41**, 2126 (1990).

[16] *Optimizing the conductance of right-angle valves*, M. H. Hablanian, F. J. Nuzzi, T. L. Pflanz, J. Vac. Sci. Technol. A **9**, 2062 (1991).

[17] *Monte Carlo calculations for free molecular and near-free molecular flow through axially symmetric tubes*, L. Fustoss, Vacuum **31**, 243 (1981).

[18] *The resistance concept and the dynamical characterization of molecular gas flow*, L. Fustoss, G. Toth, Vacuum **40**, 43 (1990).

[19] *Monte Carlo analysis for the gauge location for an American Vacuum Society standard high vacuum pump speed measurement dome*, M. D. Boeckmann, J. Vac. Sci. Technol. A **4**, 353, (1986).

[20] *The angular distribution of thermal molecular beams formed by single capillaries in the molecular flow regime*, S. Adamson, C. O'Carroll, J. F. McGilp, Vacuum **38**, 463 (1988).

[21] *Wall Collisions, angular flux, and pumping requirements in molecular flow through tubes and microchannel arrays*, D. M. Murphy, J. Vac. Sci. Technol. A **7**, 3075 (1989).

[22] *A further discussion about gas flow patterns at the entrance and exit of vacuum channels*, T. Ji-Yuan, Vacuum **38**, 555 (1988).

[23] *A further exploration of an important factor affecting the pumping performance of turbomolecular pumps*, J. Y. Tu, N. H. Yang, S. J. Pang, Y. Zu, J. Vac. Sci. Technol. A **6**, 2535 (1988).

[24] *The problem of the approximate calculation for molecular conductance*, F. Yu-Guo, Vacuum **31**, 319 (1981).

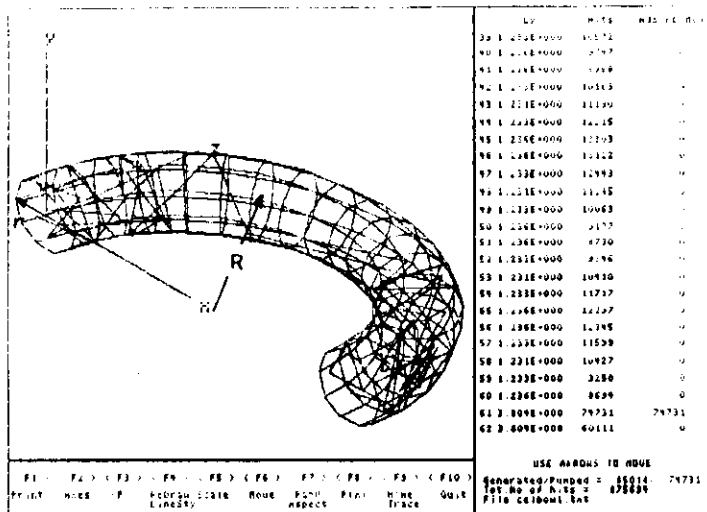[25] *New concepts in molecular gas flow*, D. J. Santeler, J. Vac. Sci. Technol. A **4**, 338 (1986).

[26] *Measurement of the effective pressure distribution in axial direction in a dynamic vacuum system*, J. K. N. Sharma, D. R. Sharma, J. Vac. Sci. Technol. A **6**, 2508 (1988).

[27] *Theory of getter pump evaluation. Sticking coefficients of common gases on continuously deposited getter films*, G. I. Grigorov, K. K. Tzatzov, Vacuum **33**, 139 (1983).

[28] *Apparent and real values of common gas sticking coefficients on titanium films and application to getter pump devices with periodic active film renovation*, G. I. Grigorov, Vacuum **34**, 513 (1984).

[29] *Monte Carlo simulation of the pressure and of the effective pumping speed in the Large Electron Positron collider (LEP)*, T. Xu, J-M. Laurent, O. Groebner, CERN-LEP-VA/86-02.

[30] *Performance Characteristic of Lumped NEG Pump*, S. R. In, S. Yokouchi, S. H. Be, T. Maruyama, Proc. Workshop on SR Light Sources, Argonne APS, Nov 1990.

[31] *Vacuum Chamber Pressure Distribution*, E. Hoyer, LBL Eng. Note M6844, 1989.

[32] *Matrix calculation of pressures in high-vacuum systems*, H. Hirano, Y. Kondo, N. Yoshimura, J. Vac. Sci. Technol. A 6, 2865, 1988.

[33] D. C. Chen et al., Jour. Vac. Soc. R.O.C. 1 (1) 24, 1989 (in chinese).

[34] *Synchrotron Radiation Outgassing Curves and Pressure Profiles in the ELETTRA Vacuum Chamber*, M. Bernardini, R. Kersevan, Proc. 2nd European Vac. Conf. EVC-2, Trieste (I), 1990.

[35] *7 GeV Advanced Photon Source Conceptual Design Report*, ANL-87-15, Argonne Nat.l Lab., 1987.

[36] *Vacuum System for KEK B-Factory*, K. Kanazawa, Y. Suetsugu, Y. Hori, KEK Internal Note Preprint.

[37] *CESR-B Conceptual Design for a B-Factory Based on CESR*, CLNS 91-1050, Cornell Univ., Ithaca, 1990.

[38] *Precise Satellite Skin-Force Modelling by Means of Monte-Carlo Ray Tracing*, H. Klinkrad, Ch. Koeck, P. Renard, ESA Jour. **14**, 409, 1990.

[39] *SPring-8 PROJECT (FACILITY DESIGN 1990)*, JAERI-RIKEN SPring-8 Project Team, 1991.

[40] *Performance of the Vacuum System fro SORTEC 1 GeV Electron Storage Ring*, Proc. of the 2nd European Part. Acc. Conf., Nice, 1990.

[41] *Pumping Speed of a NEG Module for Gases H_2, N_2, CO, CO_2 at Different Temperature Conditions*, M. Bernardini, R. Kersevan, J. Miertusova, paper presented at the 3-rd European Vacuum Congress, Vienna Sept 1991.

[42] *Vacuum Technology*, A. Roth, Elsevier Science Publ., p.279, 1982.

[43] *Numerical Recipes, the Art of Scientific Computing*, W. H. Press et al., Cambridge Univ. Press, Cambridge 1986.

A1 Hardware and Software

This first appendix deals with the hardware and software requirements. Let's start with software.

The MOLFLOW package, both the editor program (MOLFLOWE) and the MC simulation program (MOLFLOWR), has been originally written in Turbo Pascal, version 3.02A, since a real-time graphic output was available using this compiler while existing FORTRAN compilers had not the graphic capabilities of the Graphix Toolbox routines (at least to our knowledge). Therefore the programs suffer in terms of computational speed and memory capacity due to the very old version of the Turbo Pascal compiler used, dated 1986.

The drawbacks are mainly:

1) only *.COM files can be obtained, i.e. there is the limitation of 64 Kbytes for the maximum size of the compiled code. The possibility of defining so called overlays partly removes this limitation;

2) The maximum size of the sum code plus data bytes is 640 Kbytes, as imposed by the MS-DOS operating system. This is the main reason why the maximum numbers of points, facets and points/facet of each structure are, respectively 200, 80 and 19 (refer to 3.2.1 (Database Structure)).

The MC simulation program has been adapted in order to be compiled by ver.5.5 of the Turbo Pascal compiler also, but in this case only the calculations are performed, i.e. there is no graphic output. This version of the compiler, which has code optimised for the 80387 coprocessor, is about 3 times faster than the 3.02A version. The file MOLFLOWR.EXE can be found on the accompanying diskette.

A complete upgrade to the latest version of the Turbo Pascal compiler and the Graphix Toolbox library is one of the tasks to be fulfilled in the future, together with a FORTRAN version compatible with both MS-DOS FORTRAN compilers and VAX VMS FORTRAN.

Hardware requirements:

You need a PC with at least a 640 Kbytes RAM, a 3.5" floppy and a numeric coprocessor 80x87. A hard-disk is recommended, since both the editor program MOLFLOWE and the MC simulation program MOLFLOWR use the overlay files which are stored on disk. Therefore, if you run the programs on a floppy disk, then every time you invoke one of the options which are written as overlay files it happens that you have to wait until the programs load these options in the RAM of the computer.

An EGA graphic card and an EGA monitor are required.

About the PC microprocessor and clock speed requirements, it can be said that an 80386 is recommended, even if a fast 80286 can be satisfactory. If you have a slow 80286 or an 8086, then running the programs may result very tedious, since the graphic windows, the structure and trajectory drawings, and the MC calculations become very slow (at least with the 3.01 version of the compiler).

Every time you invoke the < F1 > command, *Print*, then you must be sure that the output file is of the correct type compared to the printer connected to your PC. The following compatibility table is taken from the Graphix Toolbox User's Manual:

MODE	RESOLUTION (points/line)	COMPATIBILITY
0, 4, 5	640	(Epson mode 4)
1	960	(Epson mode 1)
2	960	(Epson mode 2)
3	1920	(Epson mode 3)
6	720	(Epson mode 6)

Installation of the programs:

In order to install the programs and data files on your PC, you simply have to copy the content of the accompanying diskette on your hard-disk.

(*) Turbo Pascal, Graphix Toolbox are tradenames of BORLAND.

(*) MS-DOS is a tradename of Microsoft.

(*) All the referenced microprocessors and coprocessors are INTEL products.

(*) VAX is a tradename of Digital.

A2 Analytical Formulation of the Transmission Probability of a Tube

It will now be recalled an alternative approach to Monte Carlo simulations which is interesting from the historical point of view, and shows the reason why MC simulations are very useful.

The following equations have been taken by ref.[3]. They give the transmission probability W for a tube of circular cross-section, as obtained by Clausing:

$$W = \int_0^L W_{SR}(x)\, w(x)dx + W_{SS}(L)$$

where w(x) can be obtained solving an integral equation of the form

$$w(x) = \int_0^L W_{RR}(\xi-x)d\xi\, w(\xi) + W_{RS}(L-x)$$

In the case of a circular tube w(x) has the form

$$w(x) = \frac{1}{4R} \int_0^L \left\{ 2 + \frac{(\xi-x)^3}{\left[(\xi-x)^2 - 4R^2\right]^{3/2}} - \frac{3(\xi-x)}{\left[(\xi-x)^2 + 4R^2\right]^{1/2}} \right\}$$

$$w(\xi)\, d\xi + \frac{1}{4R} \left\{ \left[(L-x)^2 + 4R^2\right]^{1/2} + \frac{(L-x)^2}{\left[(L-x)^2 + 4R^2\right]^{1/2}} - 2(L-x) \right\}$$

where W_{SR}, W_{SS}, W_{RR} and W_{RS} are appropriate functions of R related to the probabilities of molecular passage and emittance of molecules (assuming a cosine law of emission) from the different parts of the tube wall.

In order to solve these equations, Clausing had to made some assumptions about the form of w(x). He based these assumptions on the necessity of obtaining W=8R/3L for long tubes, a result previously obtained by Knudsen.

A more recent analysis of this procedure can be found in ref.[21].

It is easily understood that solving the integral equations is not a trivial task. The functions W_{SR}, W_{SS}, W_{RR} and W_{RS} can be calculated analytically only when a 'simple' geometry is concerned, a cylindrical tube as shown before. In addition to this, it can be said that the integral equation method is usually lengthy.

Running MOLFLOWE.EXE on a 33 MHz 80386/80387 PC takes about 22 minutes to obtain the transmission probability of a cylindrical round tube with a length to radius ratio of 40 (see section 5 (Examples and Applications)).

axis, to obtain the X'Y'Z' frame of reference, while α is a rotation about the X' axis giving the X"Y"Z" frame of reference:

$$\begin{pmatrix} X'' \\ Y'' \\ Z'' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & \sin\alpha \\ 0 & -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} X' \\ Y' \\ Z' \end{pmatrix}$$

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} X'' \\ Y'' \\ Z'' \end{pmatrix}$$

Therefore, if a molecule (or photon) is desorbed by this facet, call it the *source* facet, in a direction identified by the two azimuthal and polar angles ϕ and θ, then
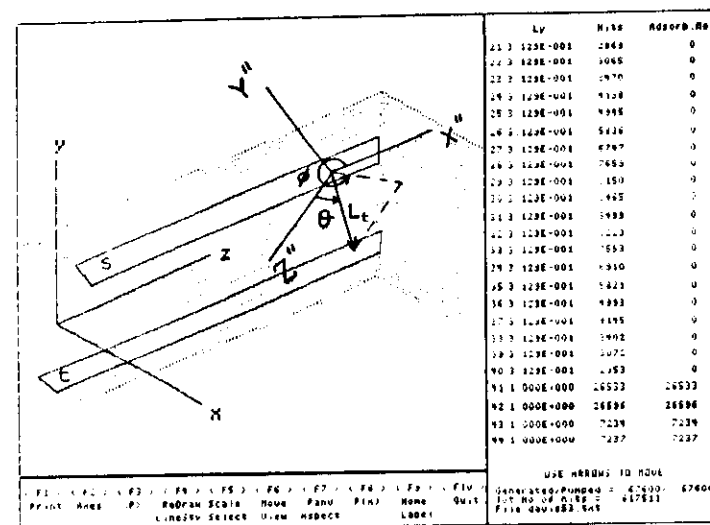
Fig.A3.2 Source facet, s, emission angles θ and ϕ, and target facet, t

$$\begin{cases} x'' = L\sin\theta\cos\phi \\ y'' = L\sin\theta\sin\phi \\ z'' = L\cos\theta \end{cases}$$

Combining the above relations, if we call (x_t, y_t, z_t) the coordinates of the *target* point and (x_s, y_s, z_s) those of the source point on the facet, then after some algebra we get:

$$\begin{cases} x_t = x_s + L_t\,(\sin\theta\,\cos\phi\,\cos\beta_s - \sin\theta\,\sin\phi\,\sin\alpha_s\,\sin\beta_s - \cos\theta\,\cos\alpha_s\,\sin\beta_s) \\ y_t = y_s + L_t\,(\sin\theta\,\sin\phi\,\cos\alpha_s - \cos\theta\,\sin\alpha_s) \\ z_t = z_s + L_t\,(\sin\theta\,\cos\phi\,\sin\beta_s + \sin\theta\,\sin\phi\,\sin\alpha_s\,\cos\beta_s + \cos\theta\,\cos\alpha_s\,\cos\beta_s) \end{cases}$$

Therefore, if there are N facets (i.e. planes) and the molecule (photon) is desorbed by the i-th facet, then the last equations are solved (N-1) times for all facets except the i-th, i.e. $t = 1, 2, ..., (i-1), (i+1), ..., N;\ s = i$, with

$$\begin{cases} L_t = - (A_t x_s + B_t y_s + C_t z_s + D_t)/U \\ U = (A_t(\sin\theta\,\cos\phi\,\cos\beta_s - \sin\theta\,\sin\phi\,\sin\alpha_s\,\sin\beta_s - \cos\theta\,\cos\alpha_s\,\sin\beta_s) + \\ \quad + B_t(\sin\theta\,\sin\phi\,\cos\alpha_s - \cos\theta\,\sin\alpha_s) + \\ \quad + C_t(\sin\theta\,\cos\phi\,\sin\beta_s + \sin\theta\,\sin\phi\,\sin\alpha_s\,\cos\beta_s + \cos\theta\,\cos\alpha_s\,\cos\beta_s)) \end{cases}$$

Each L_t is substituted into the previous equation and another check is made: in fact, each point (x_t, y_t, z_t) always belongs to a plane $(A_t x + B_t y + C_t z + D_t = 0)$, but doesn't belong necessarily to the target facet: in fact, a facet is only a part of a plane. A boolean function in the MC program checks whether the point is inside the facet contour or not, and accepts or rejects the target point and its L_t.

The boolean function works as follows. Let's consider the target point in the X"Y"Z" frame of reference: then the target facet is defined as a polygon in the X"Y" plane.

In order to check if the target point is inside or outside this polygon, it is sufficient to calculate the sum of all angles formed by the vectors connecting the target point and the vertices of the polygon [12]: if this sum is equal to $\pm 2\pi$ radians then the point is inside the polygon, i.e. belongs to the target facet, while if the sum is equal to zero then the point is outside.
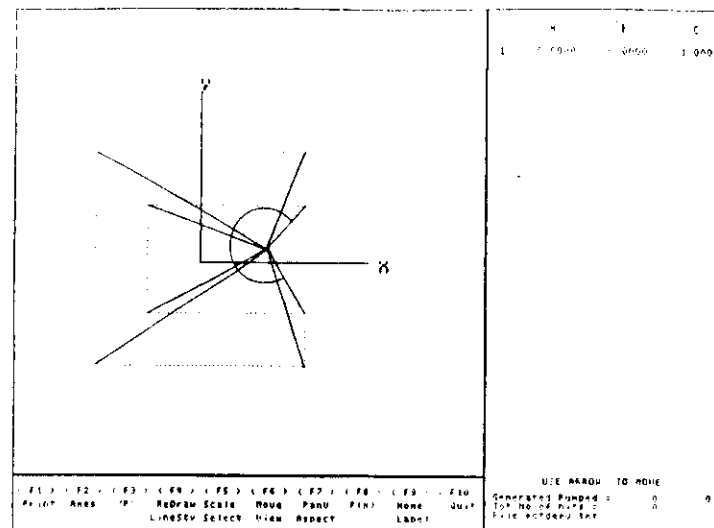
Fig.A3.3 A possible algorithm for finding if point $P(x_t, y_t)$ is inside a polygon or not [12]. In this case it is outside

This procedure works well but is very time consuming, since it involves a lot of arctan(x) calculations. That's the reason why it has been looked for a different algorithm. A description of it follows.

Let's consider the segments making up a polygon. If we call n_found the number of segments whose X" coordinates contain x_t, and n_updown is a variable which is increased by one if the point lies above a segment and is decreased by one if it lies below the segment, then it has been found that the boolean function

Inside(n_found,n_updown) ::= (odd(n_found div 2)=not odd(n_updown div 2))

which is the same as

Inside(n_found,n_updown) ::= (odd(n_found div 2) xor odd(n_updown div 2))

is true if and only if the point is inside the polygon (i.e. the facet).

These calculations do not involve any transcendental function but only sums, multiplications and boolean evaluations which are faster. We have called odd(n) the boolean function which is true if and only if the integer n is an odd number; (m div n) is the integer division; not and xor are the logical negation and the logical exclusive disjunction respectively. They are standard Turbo Pascal functions. The symbol '::=' means 'defined as'.

Now an indication about the precision of the MC calculation is given in terms of statistics:

If $P_{i,j}$ denotes the probability for N_i particles of entering from the i-th facet to reach the j-th, then the standard deviation [1,13] is given by

$$\sigma_{P_{i,j}} = [\, P_{i,j}\,(1 - P_{i,j})\,/\,N_i\,]^{1/2}$$

For a $P_{i,j}$ of 0.2 and $N_i = 10,000$ one gets a standard deviation σ of 4.0E-3.

A4 Comments about Functions and Procedures; Diskette Contents

Some of the functions and procedures implemented in the Monte-Carlo simulation program, MOLFLOWR, will be commented in order to allow the user to understand better the program and to modify it if required.

In fact, in author's opinion, it proved to be very useful to introduce some minor modifications in the program in order to analyse the behaviour of several structures which have not been discussed in section 5 (Examples and Applications) and its sub-sections: MOLFLOWR had been successfully modified and then applied to the analysis of molecular-beam epitaxy experiments [20], the optimization of titanium sublimation pumps [27,28], the saturation of NEG modules in high-energy electron synchrotrons [34,37] and to the calculation of satellite skin-force modelling [38].

A list a some functions and procedures of MOLFLOWR.PAS follows. Refer to section 2.1 (Database Organisation) for additional informations:

procedure typedef.sys:	Graphix Toolbox routines;
procedure graphix.sys:	" ";
procedure kernel.sys:	" ";
procedure windows.sys:	" ";
procedure Draw_Ref_Frame:	draws in the first graphic window the XYZ frame of reference;
procedure Draw_Solid:	draws the structure(s);
procedure write_P:	writes the parameters and attributes of the structure currently selected in the second graphic window;
procedure graphic_windows:	calls Draw_Solid and Draw_Ref_Frame;
function ran3:	random number generator, taken from ref.[43];
function acos:	inverse cosine: this is not a Turbo Pascal built-in function;
function asin:	inverse sine, same as above;
procedure teta_fi:	random number generator for polar, θ, and azimuthal, ϕ, angles of desorption; diffuse ($\cos\theta$) and uniform desorption are implemented here: mirror reflection is implemented in the program: Calls ran3;

procedure Find_Plane_eq:	finds the equation $Ax + BY + Cz + D = 0$ of the plane describing a facet in the database, and sets parameters no.1, 2, 3 and 4 (see section 2.1 (Database Structure));
procedure Find_alfa_beta:	finds the two angles of rotation α and β of a facet, and sets its parameters no.5, 6, 7, 8, 19 and 20;
procedure Find_Q:	finds the polygon describing a facet in the X"Y" frame of reference (Z"=0): sets facet parameters no.13, 14, 15 and 16; each bi-dimensional polygon is stored in the array Q_in[i,j,k] (i=1, ..., nmf; j=1, ..., nmp_fc; k=1, 2) at the beginning of the program, just after reading the data files. Q_in needs to be re-calculated throughout the program only when double-sided facets are encountered (transparency coefficient Tr>1.0).
procedure Find_Surface:	calculates the geometrical surface of a facet, without taking into account its transparency coefficient; needs Find_Q to be called first;
function min:	gives the smaller between its two real arguments;
function max:	" greater " " ";
procedure Inside:	finds whether the intersection between particle's trajectory and the plane representing a facet is inside the facet's contour or not: needs Find_Q to be called first (see Appendix A3(The Monte-Carlo Algorithm) for details);
procedure Inverse_transf:	takes the coordinates (x_2,y_2,z_2) in the XYZ frame of reference to $(x_p,y_p,z_p=0)$ in X"Y"Z";
procedure Direct_transf:	takes $(x_p,y_p,z_p=0)$ in X"Y"Z" to (x_1,y_1,z_1) in XYZ;
procedure Find_structure_des:	finds which structure generates a particle; the probability for a structure of being selected for particle generation is proportional to the ratio of its desorbing surface divided by the total desorbing surfaces of all of the structures. The array Tot_Des_Sum[j] (j=1, .., No_of_struct), is the running sum of these surfaces;

111

procedure Find_n1_n2:	finds the indeces of the (max two) pressure test facets (i.e. those facets with transparency coefficient=-1.0). Calls calculate_des_surf;
procedure Find_n_des:	finds, for the structure selected by Find_structure_des, which facet generates a particle: the probability for a facet of being selected for particle generation is proportional to the ratio of its desorbing surface divided by the total desorbing surface of all facets in the structure. The array Des_Sum[i] (i=1, .., n_fc), is the running sum of these surfaces;
procedure P_start:	generates a particle by calling Find_structure_des and Find_n_des. Then it generates a random point (x_p,y_p) in the rectangle defined by xmin and (xmin+Lx) for x_p, and ymin and (ymin+Ly) for y_p in the X"Y"Z" frame of reference (the selected facet's frame): this rectangle contains the facet. Calls the boolean function Inside in order to find if (x_p,y_p) belongs to the facet or lies outside of it. If Inside is true then calls Direct_transf to convert $(x_p,y_p,z_p=0)$ in X"Y"Z" to (x_1,y_1,z_1) in XYZ, otherwise generates another random (x_p,y_p) and calls Inside again. The speed of this procedure is proportional to the ratio of facet's area divided by the area of the mentioned rectangle;
procedure x2y2z2:	takes the source point (x_1,y_1,z_1) to the target point (x_2,y_2,z_2) after finding the actual trajectory intersection, see next procedure;
procedure Find_Length:	this is the most important part of the MC simulation program, where the actual trajectory calculations are made taking into account the structure's geometry and the parameters and attributes of all facets. i_prec is an integer variable pointing to the source facet, while i_struct points to the current structure and i_struct_prec points to the structure where the particle was before being on the current source facet (useful only for superstructures, otherwise i_struct_prec is always set equal to i_struct). This procedure scans all facets in the current structure, except i_prec, and calculates the length, L, of the intersection (if any) of the trajectory

112

from the source facet to all other facets: every time a geometrical intersection is found, i.e. the particle's trajectory intersects a facet (function Inside is called to this purpose), then a check for a *physical* intersection is made: this is accomplished by looking at the facet's attributes (it's transparency and sticking coefficients). When a physical intersection is found, Find_Length sets the integer variable imin to the facet's number (index i in the for i:=1 to n_fc loop...), and the real variable Lmin to L (the length of the geometrical trajectory) *only if L is smaller than Lmin*. It is as if the procedure would calculate the trajectory intersections and lengths with all facets and then find the smaller L among them. After completion of the for-loop on all facets two things may happen: either a physical intersection has been found (imin>0) or not (imin=0): in the first case a final comparison of Lmin with the array Lmintreq0 is made: this unidimensional array contains the lengths of the geometrical intersections between particle's trajectory and all facets with transparency coefficient equal to zero (i.e. those facets used only as test facets). Same comparison is made with Lmin_Pr, i.e. with the pressure profile test facets (transparency coefficient=-1.0). The target facet is taken as the source facet for the next intersection. Before exiting Find_Length, the polar and azimuthal angles of incidence of the physical intersection (target facet) are calculated and the number of hits of the target facet is increased by one. If imin=0, i.e no physical intersection has been found, then the number of 'bad hits' is increased by one and an error message is sent either to the screen or to the line printer: procedure Find_Length is left and a new particle is generated. Find_Length calls x2y2z2, Inverse_transf, Inside, ran3, Find_alfa_beta, Find_Q and acos. The number of these function and procedure calls is variable, depending on the geometry of the structure and its facets' attributes.

procedure write_data: writes a data file to the specified drive/directory;

procedure read_data: reads a data file from the specified drive/directory;

procedure Draw_Ref_Frame; draws the XYZ axis in the first graphic window;

procedure Draw_Trajectory: draws the trajectory of the particles being generated;

procedure Draw_Solid: draws the structure(s);

procedure ReDraw_Window: this procedure simply refreshes the first graphic window: it calls Draw_Solid and Draw_Ref_Frame;

procedure write_P: writes in the second graphic window the parameters and the attributes of the structure currently analysed;

procedure F3:   shows the average pressures on the facets of the structure currently analysed;

procedure F8:   shows the pressure profiles on the (maximum) two test facets (i.e. those facets with transparency coeff.=-1.0); if no facet is selected then a message is displayed and you must press <ENTER> to continue;

procedure key_pressed: 'reads' the keyboard and accepts the function-key codes so as to perform proper actions;

procedure calculate_des_surf: calculates the desorption array Des_Sum[i], used by procedure Find_n_des, and calls Find_Q and Find_alfa_beta;

procedure Find_n1_n2:   finds the two indexes pointing to the (max) two pressure test surfaces: calls calculate_des_surf;

procedure templatr: writes program's template on the PC screen;

procedure boundary_conditions: it should be called for analysing superstructures with periodic boundary conditions (as for instance in a periodic particle accelerator). This last procedure deserves some detailed discussion, due to its importance.

Refer to the superstructure made up of the four structures LEPQ.TXT, LEPB1.TXT, LEPB2.TXT and LEPB3.TXT, describing a 39.5 m long section of the LEP accelerator [29]. In this case the sticking coefficient of facet no.26, a *boundary facet*, in

LEPQ.TXT has been set equal to 4.1. This tells the program to load data corresponding to the fourth structure and to look for a boundary facet with a fractional part of its sticking coefficient equal to 0.1. In LEPB3.TXT, facet no.40 has a sticking coefficient of 1.1, its fractional part being exactly 0.1, therefore the molecular trajectory is started from this facet at the proper position and orientation (these values have been stored in (x_p, y_p) for the position and (polar_angle, angle of incidence) for ϕ and θ, the direction. The same happens when the molecular trajectory hits facet no.40 in LEPB3.TXT, the only difference being that the traced molecule 'exits' from the right of the superstructure to 'enter' from the left. Some comments:

i) if you need another boundary facet for each structure, then you should set the fractional part of them equal to 0.2, therefore you would have a facet with sticking coefficient 4.2 in the first structure and 1.2 in the fourth structure. You can therefore have a maximum of 9 rectangular boundary facets connecting two structures in a superstructure, corresponding to fractional parts of the sticking coefficient equal to 0.1, 0.2, ..., 0.9.

ii) each couple of boundary facets used for the boundary conditions should have the same rectangular shape and dimensions, otherwise the position (x_p, y_p) on the corresponding facet of the other structure could not possibly be set exactly, leading to a 'bad hit' condition. If you need boundary facets with arbitrary shapes then you should set their sticking coefficients equal to integer values, but in this case you cannot manage periodic boundary conditions. Data files LEPQ1.TXT, LEPB11.TXT, LEPB21.TXT and LEPB31.TXT correspond to the other four mentioned files, but procedure boudary_conditions is used to allow molecules to 'travel' in the four structures: as you can see these last four structures are not positioned following the real geometry of the vacuum system they represent but, nevertheless, a correct MC simulation is done. Its up to you to create a *real geometry model* or not: if not then you should invoke procedure boundary_conditions in the program just suitably setting the sticking coefficient of the boundary facet.

For example, figure A4.1 shows the longitudinal pressure profile obtained for the LEP machine: the agreement with the curve reported in ref.[29] is pretty good, even if a higher average pressure is obtained. The superstructure is made up of data files LEPQ.TXT, LEPB1.TXT, LEPB2.TXT and LEPB3.TXT. Only two rectangular boundary facets ('entrance' and 'exit' of the periodic cell) have been used.

Figure A4.2 shows the same *physical* structure represented in a different way, just using 8 boundary facets instead of 2. Data files are LEPQ1.TXT, LEPB11.TXT LEPB21.TXT and LEPB31.TXT.
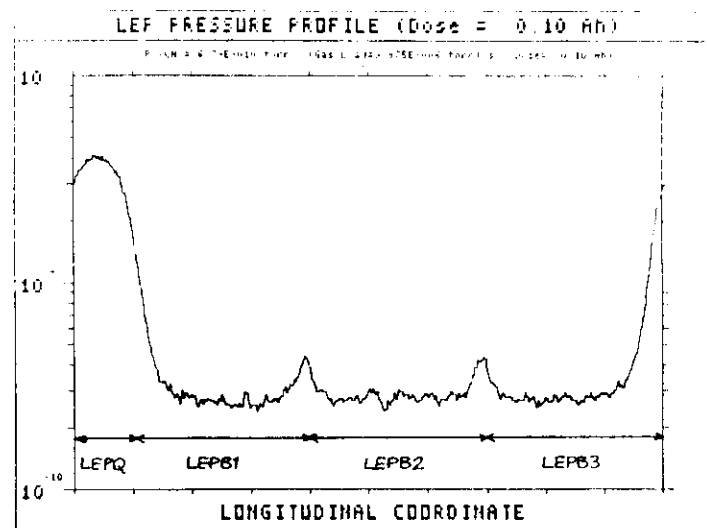

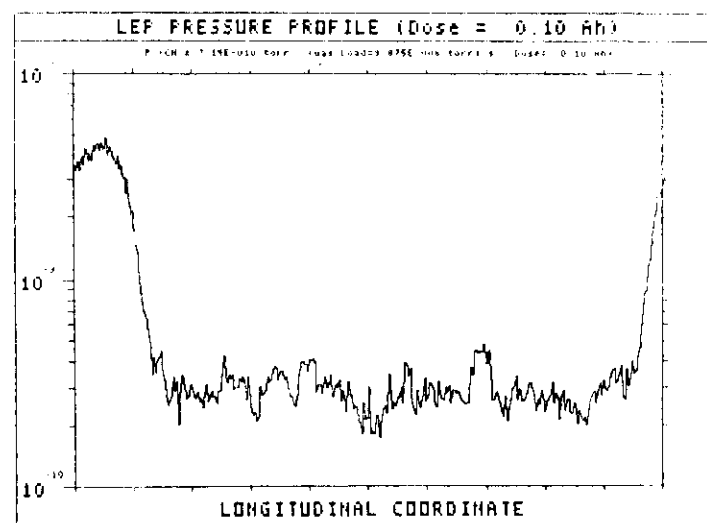Fig.A4.1 Longitudinal pressure profile for LEP geometry [29]. A grand total of 42498 molecules have been generated

Fig.A4.2 Same as in A4.1, but using 8 boundary facets calling **procedure boundary_conditions**. You can even translate independently the four structures and the MC simulation still runs properly. Only 2999 molecules have been generated

The accompanying diskette is arranged has a root directory and two sub-directories.

In the root directory B:\ there are the following files:

- the two programs written in Turbo Pascal ver.3.02A, both MOLFLOWE.PAS (the editor program) and MOLFLOWR.PAS (the MC simulation program);

- four *.FON files, the font files for the Graphix Toolbox routines, and an error message file, ERROR.MSG;

- the two executable files MOLFLOWE.COM and MOLFLOWR.COM, together with their overlay files *.000, *.001, etc... . You run the two programs simply invoking these two files;

- the data files *.TXT corresponding to the examples shown and discussed in the User's Guide;

The sub-directory B:\TURBO5.5 contains the following files:

- MOLFLOWR.PAS, the ver.5.5 Turbo Pascal MC simulation program (without graphics). If you have a Turbo Pascal compiler then you can modify and re-compile this program;

- MOLFLOWR.EXE, the executable file for running the MC simulation: it is much faster than MOLFLOWR.COM;

The sub-directory B:\ATT contains the following files, for OLIVETTI and ATT personal computers which have different EGA graphic boards:

- MOLFLOWE.COM, and the three overlays MOLFLOWE.000, MOLFLOWE.001 and MOLFLOWE.002;

- MOLFLOWR.COM, and the four overlays MOLFLOWR.000, MOLFLOWR.001, MOLFLOWR.002 and MOLFLOWR.003.

Should your PC not be compatible with any of these configurations, please contact the author for additional informations.