CLM-R 54

CULHAM LIBRARY
REFERENCE ONLY

CULHAM LABORATORY
LIBRARY
- 6 APR 1966
b

CLM-R 54

United Kingdom Atomic Energy Authority

RESEARCH GROUP

Report

A MONTE CARLO COMPUTER PROGRAMME FOR ANALYSIS OF MOLECULAR GAS FLOW

J. N. CHUBB

Culham Laboratory,

Culham, Abingdon, Berkshire

1966

Available from H. M. Stationery Office

SIX SHILLINGS NET

© - UNITED KINGDOM ATOMIC ENERGY AUTHORITY - 1966
Enquiries about copyright and reproduction should be addressed to the Librarian, Culham Laboratory, Culham, Abingdon, Berkshire, England.

U.D.C.
533.6.011
681.3.06 : 519.285

UNCLASSIFIED
(Approved for Sale)

CLM - R 54

A MONTE CARLO COMPUTER PROGRAMME FOR ANALYSIS OF MOLECULAR GAS FLOW

by

J.N. CHUBB

A B S T R A C T

Molecular gas flows cannot be studied analytically within vacuum systems in which a pumping orifice or surface forms an appreciable fraction of the total internal surface area of the system. Such systems may be studied successfully by the Monte Carlo method in which an average picture of the molecular flow is by mathematical simulation of the course of a large number of individual molecular histories within a mathematical representation of the vacuum system.

A description is given of a Monte Carlo computer programme which has been developed for analysis of molecular gas flow, with emphasis placed on the ease of use and on the practical application of the information which may be extracted. The application of this programme is illustrated by examples of calculations which have been performed on experimental apparatus for the measurement of sticking coefficients, and on test domes for measuring the performance of diffusion pumps.

U.K.A.E.A. Research Group,
Culham Laboratory,
Nr. Abingdon,
Berks.

December, 1965

CONTENTS

		Page
1.	INTRODUCTION	1
2.	DESCRIPTION OF PROGRAMME	1
	General Features of Programme	1
	Presentation for Calculation	3
	Print Out of Results	6
	Programme Testing	8
3.	EXAMPLES	8
	Measurement of Sticking Coefficients	8
	Angular Distribution of Molecules From the Ends of Tubes	9
	Pumping Speed Test Dome Design	10
	Conclusions	11
	Acknowledgement	11
	References	12

1. INTRODUCTION

1. The free molecular flow of gas through simple cylindrical and rectangular tubes may be calculated analytically using the equations derived by Knudsen, [1] Clausing [2,3] and others. This direct analytic approach cannot be applied, however, to more complex duct structures or to vacuum chambers in which the speed of pumping causes the gas density to vary appreciably across a duct cross-section, and the gas pressure to depend upon the direction of observation. Space simulation chambers and the magnetic trap type of plasma physics experiment are examples of this situation. For this type of situation the free molecular flow of gas may be successfully analysed by the Monte Carlo method. In this method of calculation the trajectories of a large number of molecules are analysed within a mathematical representation of the vacuum chamber to build up a picture of average molecular behaviour. Since a very large number of accurate calculations is involved, it is only practical to apply this technique using a high speed digital computer.

2. Previous Monte Carlo computer programmes, for example those used by Levenson, Milleron and Davies [4-9], have concentrated on the molecular flow of gas through non-adsorbing vacuum duct units. The programme described in the present paper deals with axisymmetric vacuum structures, and makes provision for the independent specification of adsorption coefficients, in the range 0.0 to 1.0, on any of the structure surfaces.

3. The aim of the present report is to give a brief description of the Monte Carlo computer programme which has been developed for molecular gas flow analysis, and then to describe the method of presentation for calculation and give some examples illustrating some practical applications. A Fortran listing, in S2 dialect, of the programme is given in Appendix 1 for those readers requiring more detailed information on programme operation. The calculations used to illustrate the application of the programme were performed on the IBM 7030 (Stretch) computer at A.W.R.E., Aldermaston or the English Electric KDF 9 computer at Culham.

2. DESCRIPTION OF PROGRAMME

GENERAL FEATURES OF PROGRAMME

4. For vacuum systems in the molecular flow regime, interactions between molecules in the gas phase may be entirely neglected in comparison to interactions between molecules and surfaces of the containing vacuum chamber. In this regime it is therefore reasonable to consider the history of an individual molecule from the time of its introduction into a vacuum system to the time it leaves, or is adsorbed, in isolation from all other molecules which may be present in the system. Application of the Monte Carlo technique to this situation involves setting up a mathematical representation of the vacuum chamber structure and of using a fast digital computer to simulate the trajectories of a large number of molecules through the various interactions which may occur within the structure. For this simulation to be accurate it is necessary for these molecules to have, on average, the same angular distribution on entry into the system as real molecules, and the same angular distribution after scattering from a surface.

These two distributions are achieved by calculating the direction cosines of the molecular trajectories, in either case, on the basis of a choice of random numbers within appropriate constraining distributions. While it is desirable to choose the input distribution to suit the structure being studied (for example; cosine, isotropic or beamed) the distribution to trajectories after scattering interactions with surfaces has been chosen to follow a cosine distribution law. According to this law, the numbers of molecules scattered at an angle θ with respect to the perpendicular from the surface varies in proportion to $\cos \theta$. If the scattering from a surface was known to be non-cosine or partially specular then these alternative scattering distributions could easily be substituted for the present cosine law.

5. The general type of structure which may be handled with the present programme is illustrated schematically in Fig. 1. The structure is considered as a number of coaxial elements of conical surfaces, and these may vary in form from diaphragms of nominally zero axial length to fully cylindrical elements. Each length element may also include a second surface within the outer surface. Provision may be made for molecules to enter the region within the inner surfaces by specifying a neighbouring inner surface element to be transparent.

6. To allow the molecular flow of gas to be analysed in complete vacuum systems, including pumping facilities, provision has been made for a sticking coefficient, in the range 0.0 to 1.0, to be assigned to each length element of conical surface. At any interaction of a molecular trajectory with a surface, a test is made for adsorption by comparing a random number in the range 0.0 to 1.0 with the specified sticking coefficient - if it is smaller the molecular history is terminated at this point, and a new molecule is generated at the gas input.

7. This feature of the programme allows all forms of vacuum pumping included in the structure being studied to be represented by suitable values of sticking coefficients at appropriate locations along the structure. The pumping provided for example by a diffusion pump may be considered as equivalent to the pumping provided by a partially adsorbing surface over the orifice of the pump. A diffusion pump mounted in the wall of a vacuum chamber may then be represented by further reducing this equivalent sticking coefficient in the ratio of the actual area of the pump orifice to the total surface area of the length element of wall representing it. The possible errors introduced by gas streaming and gas flow asymmetry need to be considered if the pumping port area is appreciable in comparison to the cross section of the main vacuum structure, or if the speed of the pump is appreciably dependent on the gas inflow distribution.

8. The input surface for the gas molecules may be placed at any point within the structure. The molecules may be introduced with either cosine or isotropic distributions, and these distributions may be directed forwards or backwards along either the X, Y, or Z axes, where the Z axis corresponds to the main axis of the vacuum structure. Each molecular trajectory is traced from the input surface through the various length elements of the structure until the molecule either leaves the structure or a scattering interaction occurs with a surface. If the molecule is scattered at a surface then a new trajectory is generated within a cosine distribution relative to the local surface. The

tracing process is continued until each molecule either leaves the structure through either end, or is adsorbed on one of the internal surfaces. A new molecule is then generated at the input point and its history is traced through in a similar manner.

9. From the records kept of the numbers of interactions with each surface during trajectory tracing, the computer programme is able to build up, for example, a picture of the distribution of numbers of interactions per unit area of each surface of the structure (impact density) per unit quantity of gas input to the structure.

10. An ionisation gauge is usually used for the measurement of vacuum, and the output of this device is dependent on the gas density within the sensitive volume of the gauge structure. Some care, however, needs to be exercised in using an ion gauge to measure gas density or molecular impingement rate at a surface, because without special precautions a tubulated ion gauge is susceptible to gas streaming effects in the vicinity of the tubulation orifice. Only if the distribution of molecules at the gauge tubulation opening is fairly close to cosine will the gas density within the gauge correspond to the local gas density at the tubulation orifice and correlate with the local impingement rate. Although the present programme cannot allow a tubulated ion gauge geometry to be included in the structure being studied (unless the gauge happens to be on the system axis) it is hoped to allow this possibility in future developments of the programme. For the present therefore it is necessary either to assume a cosine incidence distribution upon a tubulated gauge orifice, or to design the tubulation to be insensitive to the incident angular distribution. (10)

PRESENTATION FOR CALCULATION

11. The calculation of molecular flow of gas within any structure using the Monte Carlo programme (listed in Appendix 1) requires the description of the structure by a set of data cards, and the presentation of this set of data cards together with the Monte Carlo programme and appropriate control cards to the computer. To minimise handling of the programme card deck it is most convenient at Culham to use the version of the programme stored on the computer disc file. For this presentation the card deck is made up as follows:-

```
*   (Job card - including time for calculation)
*   X E Q
*   DISC PROGRAM MONTE CARLO 3
*   DATA
    (Data Cards)
*   END JOB
```

12. A single card, in I7 format, must come at the beginning of the data card deck, but before any data cards describing structures, to allocate storage space in the computer for the data describing each structure to be studied. This first card defines a parameter MAXNCS, and this must be at least one greater than the maximum number of elements in any of the structures defined in the subsequent data cards.

13. The set of data cards describing any structure begins with two preliminary cards defining the method of introducing the molecules and the number of molecules to be studied. The first of these two cards defines the following parameters, in 3I7, 3F14.7, 7x,I2 format:-

ICASE IREF INCONE RINNR ROUTR RCENTR INAXIS. The meaning of these parameters is explained below.

ICASE The number of the case being studied. Since this number also defines the starting point of the random number sequence in the programme it is necessary to change ICASE for a second run on a particular structure if any improvement in accuracy is hoped for by the addition of the two sets of results.

ICASE > 1000 will cause the necessary instructions to be produced for drawing a full section of the structure being studied on the Benson-Lehrner Model J graph plotter. If ICASE is so specified an extra card *10D TAPE 100/IBM-BL/SAVE must be inserted after the *XEQ card and an extra data card must follow the set of data cards describing this structure. This extra data card may be used to allow the date (columns 2-9) and a brief title (columns 11-30) of the structure to be printed on the drawing of the structure. ICASE <0 stops the programme.

IREF Determines the angular distribution of molecules entering the structure from the surface specified by INCONE RINNR ROUTR and RCENTR.

IREF = 0 gives a cosine input distribution

$0 <$ IREF $<$ 180,000 gives an isotropic distribution into a cone of half angle IREF/1000.

IREF > 0 gives the input along the positive axis direction, and IREF < 0 in the reverse direction.

IREF $>$ 180,000 gives a $(\cos)^2$ input distribution.

INCONE Number of the length element at whose entrance plane the molecules are introduced.

RINNR, ROUTR } The radii of the annular surface from which the molecular histories start, with random choice of position over the annulus.

RCENTR The displacement of the centre of the annular surface, defined by RINNR and ROUTR, from the system axis along the x direction.

INAXIS Chooses the direction of the axis along which the molecules are introduced within IREF choice of distribution.

INAXIS = 0 along Z axis
INAXIS = 1 along X axis
INAXIS = 2 along Y axis
INAXIS < 0 along -Z axis

The programme will set the latter five parameters to the following values, if they are left unspecified:-

INCONE = 1
RINNR = RI (INCONE)
ROUTR = RO (INCONE)
RCENTR = 0.0
INAXIS = 0

14. The second preliminary data card defines the following parameters in 3I7 format:-

NCS NP IPRINT

NCS	the number of length elements in the structure.
NP	the number of molecular histories to be studied.
IPRINT	the number of molecular histories studied per interval between printing our results.

All three of these numbers are obligatory and it is necessary to ensure that NCS corresponds to the number of elements described in the subsequent set of data cards.

15. The general form of the structure handled by the programme is illustrated in Fig. 1. Each length element of the structure is defined by the radii of the inner and outer surfaces at each end of the element and by the element length. Since the output-side radii of one element are the input-side radii of the next element, each element may be specified using only the input end radii and the element length. The output side radii of the final element of the structure, however, must be specified. Each element is described on a single data card by the following parameters in 5 F14.7, I2 format:-

RI RO A PI PO MREF

RI	radius of the inner surface at input end
RO	radius of the outer surface at the input end
A	axial length of element
PI	sticking coefficient of inner surface. PI positive applies to outside of inner surface, and negative to inside of inner surface.
PO	sticking coefficient of outer surface
MREF	MREF > 0 makes the inner surface transparent so that molecular trajectories pass through undeflected.
	MREF = 0, or unspecified, allows scattering from either inside or outside of inner surface.

MREF = ± 2 causes printout of the distribution of path lengths for molecules from introduction into the structure up to first interaction with the inner surface of this element.

MREF = ± 3 causes printout of the distribution of path lengths to first interaction with the outer surface of this element.

After the card sequence describing the above parameters for all the elements in the structure, there must be a card giving in 2F14.7 format the output-side radii of the last element, RI (NCS + 1), RO (NCS + 1).

16. The above method of describing a structure may be illustrated by considering the vacuum structure which was used for the experimental cryopumping studies discussed in para. 26 et seq. The physical form of the vacuum apparatus used for these studies is shown in Fig. 6. The set of cards used to describe this structure and present it to the computer for calculation is shown in Fig. 2. Fig. 3 shows the print out produced by the computer from this input data. The correct specification of the structure studied by the programme may readily be checked by setting the parameter ICASE > 1000 to cause a drawing of the structure to be produced by the Benson-Lehrner graph plotter. Such a drawing of the cryopumping apparatus is illustrated in Fig. 5.

PRINT OUT OF RESULTS

17. The results of the Monte Carlo calculations are printed out by the computer in five sections - as shown in the example presented in Fig. 4. The first section gives the total numbers of molecules adsorbed in the structure, transmitted through the output end orifice and reflected back through the input end orifice. In the example of the cryopumping experiment illustrated, the structure was closed at both ends so that all the molecules introduced ended up by being adsorbed. The dispersion, probability and percentage error factors relate to the statistics of the adsorption, transmission or reflection events.

18. The second section of the print out gives the distribution along the structure of adsorptions, interactions and interaction probabilities per unit area for the inner and outer surfaces. Element numbers and adsorption probabilities are included in this table to help correlation of this information with the form of the structure described in the input table (see Fig. 3). The "Adsorptions" and "Interactions" columns give the total numbers of these events which have occurred on each element for the total number of molecules examined up to the time of print out in the present example. The surface interaction probabilities listed in columns 5 and 10 of the table are calculated as the number of interactions per unit area of the element per molecule introduced into the structure. This surface interaction probability may be quantitatively related to the physical behaviour of molecules in a vacuum system through Avogadro's number (the number of molecules per unit volume at unit pressure) and the rate of incidence of molecules on unit area at unit pressure. The pressure may be related to the surface interaction probability and the gas inflow with the following expression:-

$$\text{Pressure(torr)} = \frac{(\text{surface interaction probability}) \times (\text{gas inflow } (\text{torr.litre.sec}^{-1}))}{F}$$

For a system at ambient temperature (20°C) and system dimensions in inches F = 285.0 for hydrogen, 76.5 for nitrogen and 64.0 for argon.

19. Distinction between events on the inside and the outside of the inner surface elements is made by printing out the adsorptions, interactions and surface interaction probabilities in two lines, the first of which refers to the inner surface and the second to the outer surface of the inner elements.

20. The probability of a molecule being ionised within a volume, for example by an electron beam, is related to the time spent by the molecule in that volume. For gas molecules of a given velocity distribution the ionisation is hence related to the molecular path length within the volume - without regard to the angular distribution of the molecular paths. The present programme provides the facility for calculating molecular path lengths within defined volumes, and uses the transparent surface of inner elements to define the volume. This calculation is performed whenever an inner surface is specified to be transparent (MREF(I) > 0) and the result, which is termed the volume interaction probability, is printed out in column 6 of the output table. The volume interaction probability calculated is the average path length per molecule per unit volume within the volume bounded by the cylindrical surface of the inner element and its input and output apertures. For structural dimensions in inches this may be related to an equivalent gas pressure at ambient temperature by the following expression:-

$$\text{Pressure(torr)} = \frac{(\text{volume interaction probability}) \times (\text{gas inflow } (\text{torr.litre.sec}^{-1}))}{G}$$

where G = 1140 for hydrogen, 306 for nitrogen, and 256 for argon.

21. This volume interaction probability can be used directly for interpreting the readings of either nude or tubulated ion gauges mounted on the axis of the vacuum structure since the results automatically take account of any gas streaming effects present.

22. The accuracy of calculated values of surface or volume interaction probability is determined by the number of relevant interactions with the surface in question. Since the simulation of individual molecular histories is based upon the use of random numbers, there will be the normal 0.68 probability that the calculated number N will be within $\pm (N)^{\frac{1}{2}}$ of the true value of N. Thus, for example, a calculation based on 1000 events will have an expected error of $\pm$ 3%.

23. The third section gives the distribution of molecular impact density around the outer surface of each element so that the degree of symmetry of gas flow in the structure may be assessed. This is calculated by dividing each outer surface into twenty equal segments and comparing the impact density in each of these with the average impact density for the whole surface given in the preceding table. Since the number of interactions for each of these calculations has been reduced by a factor of 20, in comparison to the number of interactions for the whole element, the statistical errors of these calculations will be correspondingly large.

24. The fourth section of the print out gives a table of the numbers of molecules with total path lengths, from the point of entry into the structure to their point of leaving or adsorption, in 10% intervals of the total length of the structure. If any element has been specified with MREF $\pm$ 2 or $\pm$ 3, a similar table is produced giving the

distribution of path lengths up to first interaction of molecules with this element. This facility can be used, for example, to calculate the initial stage of transient molecular gas flow in a system at uniform temperature.

The fifth section of print out gives the numbers of molecules undergoing M interactions, from M=1 to 30, between entry into the structure and leaving the structure, or being adsorbed.

PROGRAMME TESTING

25. Correct operation of the computer programme has been checked during development in two ways - first, by using fully closed structures for most applications so that any leakage of molecules from the structure can be observed and traced. Second, by using special test examples for which the results could be readily predicted. An instance of this is the use of a fully adsorbing sphere with small non-adsorbing targets at each pole to test the various input law distributions and the cosine scattering distribution law.

3. EXAMPLES

MEASUREMENT OF STICKING COEFFICIENTS

26. The conventional way to measure the sticking coefficient of a surface capable of adsorbing molecules is to measure the pumping speed exhibited by a defined area of the surface. Some observations of this type were made [11] to measure the sticking coefficient of hydrogen condensing on liquid helium cooled surfaces using the apparatus shown in Fig. 6. As it was anticipated that a high pumping speed at the condensing surface might produce a significant pressure gradient along the apparatus, some Monte Carlo studies were made of the relationship between the apparent pumping speed at the ion gauge position and the sticking coefficient at the condensing surface. The presentation of this problem to the computer has already been described in para. 11 et seq., and an example of the results printed out by the computer for a sticking coefficient of 0.9 is shown in Fig. 4. The variation of molecular impact density along the length of the apparatus can be clearly seen in these results in the tenth column of the table of adsorptions and interactions surface interaction probability. The pumping speed exhibited in the structure at any point is expressed by:-

$$\text{Speed (litre/sec)} = \frac{F}{\text{(Surface interaction prob.)}}$$

where F has the same values as in para. 18 for different gases. Curves can therefore be drawn, as shown in Fig. 7, relating the pumping speed which may be observed at any point to the sticking coefficient at the adsorbing surface.

27. It can be seen that unity sticking coefficient on this relatively small surface would cause a sufficient pressure gradient along the apparatus to reduce the observed pumping speed to only 70% of the true speed available at the condensing surface. The assumption was made in the experimental work with this apparatus that the angular distribution of molecules at the tubulated ion gauge orifice was close enough to cosine

for the ion gauge measurements to be used directly for calculating apparent pumping speeds at the orifice position.

28. The above method of measuring sticking coefficients is at best only as accurate as the calibration of the ion gauge, which is not very great for hydrogen. As initial studies [11] showed that the sticking coefficient of hydrogen condensing on to liquid helium cooled surfaces was fairly near to unity, it was realised that much more accurate measurements of sticking coefficients could be made through observation of reflection coefficients.

29. For some of his studies of titanium getter film pumping, Clausing [12] made measurements of sticking coefficients by reflection type observations. A large scale apparatus was required for these studies to minimise errors from shadowing of the gas input by the ion gauge used to observe the reflection from the surface. As a similar scale of apparatus was not practical for cryopumping studies, the Monte Carlo programme was used to help the design, and subsequent interpretation, of a smaller scale experiment.

30. Fig. 8 shows small sketches of the four basic geometries studied, together with sketches of the variations of the pressure at the ion gauge detector with sticking coefficient for constant gas inflow rates. These studies showed that there was no significant difference in performance between the first three designs, as judged by the sensitivity of the observed pressure to variations in the sticking coefficient. Design number 4 was much inferior, as was expected, and interpreted values of sticking coefficients close to unity would still be very susceptible to the accuracy of calibration of the ion gauge detector.

31. Design No. 3 was therefore chosen for the second stage of the cryopumping work, as this design gave the greatest structural simplicity and ease of adjustment of observation facilities. The interpretation of the actual experimental observations has been based on Monte Carlo calculations on a detailed representation of the actual experimental apparatus. This representation included the short length of tube through which the gas was introduced, so that the gas input distribution to the condensing surface was accurately simulated.

ANGULAR DISTRIBUTION OF MOLECULES FROM THE ENDS OF TUBES

32. The Monte Carlo programme has been used to study the angular distribution of molecules leaving tubes of various length to diameter ratios. The vacuum structure for these studies consisted of the tube with its exit orifice mounted in the centre of a fully adsorbing hemisphere. The radius of the hemisphere was made very large in comparison to the tube radius, by a factor of 2000. With this arrangement, the distribution of adsorbed molecules on the hemisphere is determined only by the angular distribution with which molecules leave the tube, and is unaffected by the radial position at which they leave the tube. For our programme the hemisphere was generated from 16 fully adsorbing conical surfaces. Molecules were introduced at the entrance of the tube with a cosine distribution. The entry orifice of the tube was closed with a non-adsorbing plane surface to scatter back into the tube, with a cosine distribution, any molecules which would leave the tube through the entry orifice.

33. The results of these studies are presented as polar diagrams in Fig. 9 for L/R values of 0, 1, 2, 5 and 10. The distance from the origin in any direction is proportional to the probability of a molecule leaving the tube into unit solid angle in that direction. All the diagrams are to the same scale. Although it may seem that the changes in the forward component of the distribution are not balanced by changes in the more lateral components it should be noted that the forward changes take place with a relatively small solid angle, within about 20° of the axis. Not too much account should be taken of the exact form of the lobe tip of the polar diagrams because of the relatively poor statistical accuracy of the near axis results. The results presented show that an appreciable degree of collimation is produced by flow through tubes with L/R ratios as small as 2, and agree fairly well with the analytic results calculated by Dayton [13].

PUMPING SPEED TEST DOME DESIGN.

34. The pumping speed of diffusion and other unit types of vacuum pump are usually tested by introducing a measured gas flow rate into a test dome mounted on the pump orifice, and observing the pressure developed within the test dome. Although an apparent speed may be calculated for the pump directly from these measurements, it is unlikely that this will correspond to the actual speed exhibited at the entrance to the pump. The discrepancy between the two speeds is due to the pressure gradient associated with the nett flow of gas molecules from the gas inlet into the pump and will vary in size and sign with the design of the test dome and the location of the pressure gauge.

35. The problems of the design of a test dome for reliable pumping speed measurements may readily be tackled with the present Monte Carlo computer programme. Two particular designs of test dome were included in the draft ISO proposals (ISO/TC112 (Secretariat-8) 8) for methods of measuring the performance characteristics of vacuum pumps. The Monte Carlo analysis of these two designs presented below was also incorporated in the above document as an annexe.

36. The forms of the two test domes studied are shown in Fig. 10. To take account of possible streaming effects between the pumping orifice and the top jet of the diffusion pump, the structures studied by the Monte Carlo programme included the portion of the diffusion pump down to the level of the top jet. The pumping effect of the diffusion pump was represented by using the plane annular surface between the lip of the top jet and the pump wall as an adsorbing surface, with a sticking coefficient chosen in the range 0.0 to 1.0.

37. The performance of the two test domes was examined by comparing the "effective sticking coefficient" exhibited by the pump orifice, in terms of the computed fraction of molecules incident upon the orifice which are adsorbed, with the "apparent sticking coefficient" or (Ho coefficient). The "apparent sticking coefficients" were calculated as the ratio of "apparent speed" to the maximum theoretical speed of the pump orifice. The "apparent speed" is obtained in practice from test dome measurements from the pressure at the gauge per unit gas inflow.

38. For the results quoted, the gas was introduced from the specified input position with a cosine distribution. A single test run was, however, also made for each test dome with the gas introduced through a narrow tube. These tests gave the same results, within the limits of statistical errors, as with the cosine input distributions.

39. Monte Carlo calculations were performed with both test dome structures for several values of sticking coefficient for the surface across the top jet gap of the diffusion pump

40. In the case of test dome type A, two sets of results are shown in Fig. 11 for the two positions of the ion gauge orifice. The usual values of "apparent sticking coefficients" (or the Ho coefficients) for diffusion pumps lie in the range 0.3 to 0.45.

41. The ion gauge in position (a) will give values of pumping speed between $8\frac{1}{2}\%$ and $16\frac{1}{2}\%$ too high. Analysis of the pressure gradient along the wall of this test dome showed, however, that direct indication of the true speed of the pump could be obtained within about 1% in the usual operating range if the centre of the ion gauge orifice were located 0.6 D above the top of the lip of the top jet - that is, 0.35 D from the pump orifice for this particular pump geometry. This graph is shown as curve (b).

42. The graph shown in Fig. 12 indicates that the test dome type B, with the particular configuration shown, will give measurements of pumping speed about $6\frac{1}{2}\%$ too low.

43. There are two points to note in connection with the application of the above results, first if, as noted in para. 8 the flux of molecules incident on the orifice of a tubulated ionisation gauge were appreciably different from cosine, the gauge observations would not correspond to the molecular impact density calculated by the computer programme for the local test dome surface. (The susceptibility of a tubulated gauge to such gas streaming effects might conveniently be avoided in practice either by using large bore tubulation to the gauge connected to the test dome through a relatively small area thin walled orifice, or by using a fully immersed nude gauge.) Second, the above results only apply for the paricular diffusion pump geometry illustrated in Fig. 9. Different results may be expected for vacuum pumps of different internal geometries.

CONCLUSIONS

44. The above examples have demonstrated just a few of the capabilities of the Monte Carlo method of calculation and of the particular computer programme which has been developed. A great advantage of the Monte Carlo method is the ease with which more detailed information may be obtained by modifications to the programme.

45. Although the programme which has been developed may not be a model of computing elegance or economy, it is very easy to apply and it has proved very useful in the analysis of a wide range of vacuum physics problems.

ACKNOWLEDGEMENT

46. The present programme has been developed from a Monte Carlo computer programme written in the summer of 1963 by K.Heron, a Vacation Student at Culham, under the

supervision of M. Larkin of the Theory Division at Culham. The writer wishes to express his gratitude for this work, and for subsequent discussions with Mr. Larkin.

REFERENCES

1. KNUDSEN, M., Ann. Physik, Vol. 28, 1909. p.75.

2. CLAUSING, P., Physica, vol. 9, 1929. p.65.

3. CLAUSING, P. On the molecular flow with Langmuirian adsorption of the molecules on the wall of the tube; a correction, Physica, vol. 28, 1962 p.298.

4. DAVIS, D.H., Monte Carlo calculation of molecular flow rates through a cylindrical elbow and pipes of other shapes, J. App. Phys., vol. 31, no. 7, 1960 p.1169.

5. DAVIS D. H., LEVENSON, L. L. and MILLERON, N., Effect of "rougher than rough" surfaces on molecular flow through short ducts. (UCRL-6787, July 1963.) J. App. Phys. vol 35, no. 3, 1964. p. 259.

6. MILLERON, N., LEVENSON, L.L. and DAVIS, D.H., Effect of rougher than rough surfaces on molecular flow through short ducts, Bull. Am. Phys. Cos., vol. 7, 1962, p.260.

7. LEVENSON, L.L., MILLERON, N. and DAVIS, D.H., Molecular flow conductance, Le Vide, vol. 103, January 1963. p.42.

8. LEVENSON, L. L., MILLERON, N. and DAVIS, D. H. Optimisation of molecular flow conductance, Proc. 7th Nat. Symp. on Vacuum Technology, 1960. Oxford Pergamon Press, 1961. (UCRL Report 6014, August 1960).

9. LEVENSON, L. L., MILLERON, N., and DAVIS, D. H., Molecular flow conductance. UCRL Report 6253, August 1961.

10. BUHL, R. and TRENDELENBURG, E. A. Avoiding systematic errors in measuring the speed of high vacuum pumps. Vacuum, vol. 15, No. 5, 1965. p.231.

11. CHUBB, J. N. and POLLARD, I. E., Experimental studies of hydrogen condensation on to liquid helium cooled surfaces. Vacuum vol.15, no.10, 1965. p.491.

12. CLAUSING, R.E. Sorption of gases by vapour deposited titanium films. ORNL-3481, March 1964.

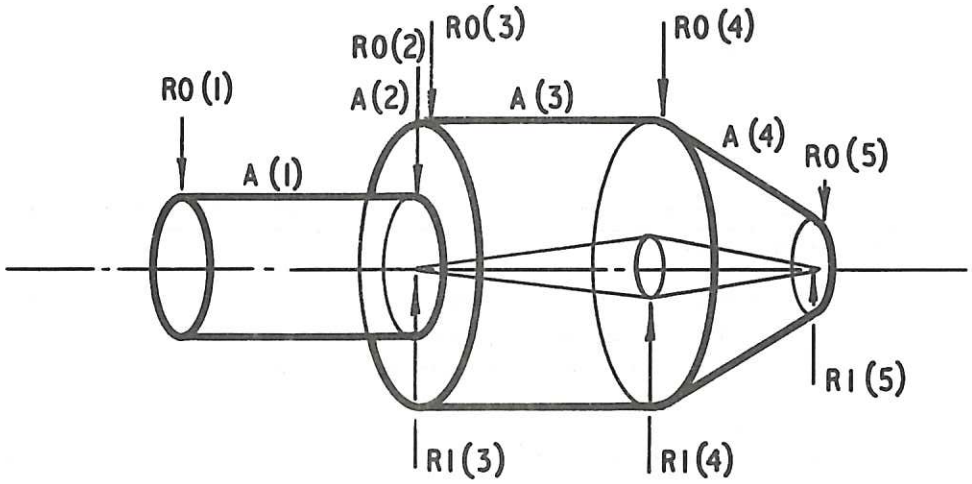

Fig. 1 Example of vacuum structure (CLM-R54)

```
#      JOB054200/JCMCRG/MONTE-CARLO /CHUBB        /              *PRODUCTION
#      XEQ
#      IOD TAPE 100/IBM/SAVE
#      DISC PROGRAM MONTE CARLO 3
#      DATA
     100
    1106       0       2
      15    1000     100
      0.0              0.00001          0.00001          0.0              0.0
      0.0              0.25             0.00001          0.0              0.0
      0.0              2.925            0.8              0.0              0.0
      0.0              2.925            1.5              0.0              0.0
      0.0              2.925            1.1              0.0              0.0
      0.0              2.925            0.00001          0.0              0.0
      0.0              3.0              2.5              0.0              0.0
      0.0              3.0              5.0              0.0              0.0
      0.0              3.0              5.0              0.0              0.0
      0.0              3.0              0.00001          0.9              0.0
      1.75             3.0              0.00001          0.0              0.0
      1.875            3.0              6.75             0.0              0.0
      1.875            3.0              0.00001          0.0              0.0
      0.75             3.0              4.55             0.0              0.0
      0.75             3.0              0.00001          0.0              0.0
      0.75             0.75
  5   8 65 MODEL B CRYOPUMP
#      ENDJOB
```

Fig. 2 (CLM-R54)
Example of make-up of card deck for computation

MONTE CARLO PROGRAM NUMBER 3 FOR FLOW OF PARTICLES THROUGH SEQUENCE OF CONICAL ANNULI

CASE NUMBER 1106

MOLECULAR HISTORIES INITIATED AT ENTRANCE PLANE OF NUMBER 2 CONE

FROM ANNULAR SURFACE BETWEEN RADII 0.0000000AND

0.2500000 CENTERED 0.0000000 FROM THE SYSTEM AXIS ALONG X AXIS

COSINE INPUT LAW

ALONG THE DIRECTION OF THE Z AXIS.

COSINE REFLECTION LAW

INPUT TABLE

COMPONENT NO.	INNER RADIUS	OUTER RADIUS	LENGTH	INNER ADS PROB	OUTER ADS PROB	MREF
1	0.0000000	0.0000100	0.0000100	0.0000000	0.0000000	0
2	0.0000000	0.2500000	0.0000100	0.0000000	0.0000000	0
3	0.0000000	2.9250000	0.8000000	0.0000000	0.0000000	0
4	0.0000000	2.9250000	1.5000000	0.0000000	0.0000000	0
5	0.0000000	2.9250000	1.1000000	0.0000000	0.0000000	0
6	0.0000000	2.9250000	0.0000100	0.0000000	0.0000000	0
7	0.0000000	3.0000000	2.5000000	0.0000000	0.0000000	0
8	0.0000000	3.0000000	5.0000000	0.0000000	0.0000000	0
9	0.0000000	3.0000000	5.0000000	0.0000000	0.0000000	0
10	0.0000000	3.0000000	0.0000100	0.9000000	0.0000000	0
11	1.7500000	3.0000000	0.0000100	0.0000000	0.0000000	0
12	1.8750000	3.0000000	6.7500000	0.0000000	0.0000000	0
13	1.8750000	3.0000000	0.0000100	0.0000000	0.0000000	0
14	0.7500000	3.0000000	4.5500000	0.0000000	0.0000000	0
15	0.7500000	3.0000000	0.0000100	0.0000000	0.0000000	0
	0.7500000	0.7500000				

TOTAL LENGTH OF STRUCTURE IS 27.2063200 UNITS

MODEL B CRYOPUMP

NEW PAGE NO 1106 ON GRAPH PLOTTER

GRAPH SCALE IS 0.367935

TOTAL SURFACE AREA OF OUTER ELEMENTS IS 565.9443630 LENGTH UNITS SQUARED

Fig. 3 (CLM-R 54)

Example of print out of input data by computer programme resulting from card deck shown in Fig. 2

OUTPUT TABLES CASE NUMBER 1106

	PARTICLES	DISPERSION	PROBABILITY	P/C ERROR
ADSORPTIONS	300	0.0000000	1.0000000	0.0000000
TRANSMISSIONS	0	0.0000000	0.0000000	0.0000000
REFLECTIONS	0	0.0000000	0.0000000	0.0000000

AVERAGE MOLECULAR PATH LENGTH IS 337.4431235 LENGTH UNITS

DISTRIBUTION OF ADSORPTIONS AND INTERACTIONS

	INNER CONES					OUTER CONES			
ELEMENT NO. (I)	ADSORPTION PROB. (PI(I))	ADSORPTIONS (LNAI(I))	INTERACTIONS (MNAI(I))	SURFACE INTERACTION PROB. (DMNAI(I))	VOLUME INTERACTION PROB. (DMNAI(I))	ADSORPTION PROB. (PO(I))	ADSORPTIONS (LNAO(I))	INTERACTIONS (MNAO(I))	SURFACE INTERACTION PROB. (DMNAO(I))
1	0.00000	0	0	0.0000000		0.00000	0	9	0.1527887
		0	0	0.0000000					
2	0.00000	0	0	0.0000000		0.00000	0	1269	0.1610327
		0	0	0.0000000					
3	0.00000	0	0	0.0000000		0.00000	0	720	0.1632356
		0	0	0.0000000					
4	0.00000	0	0	0.0000000		0.00000	0	1422	0.1719418
		0	0	0.0000000					
5	0.00000	0	0	0.0000000		0.00000	0	1052	0.1734587
		0	0	0.0000000					
6	0.00000	0	0	0.0000000		0.00000	0	59	0.1406740
		0	0	0.0000000					
7	0.00000	0	0	0.0000000		0.00000	0	2248	0.1590135
		0	0	0.0000000					
8	0.00000	0	0	0.0000000		0.00000	0	3847	0.1360898
		0	0	0.0000000					
9	0.00000	0	0	0.0000000		0.00000	0	2956	0.1065471
		0	0	0.0000000					
10	0.90000	0	0	0.0000000		0.00000	0	1	0.1004766
		300	331	0.1146781					
11	0.00000	0	0	0.0000000		0.00000	0	0	0.0000000
		0	41	0.0960091					
12	0.00000	0	0	0.0000000		0.00000	0	4093	0.1072298
		0	2554	0.1070569					
13	0.00000	0	0	0.0000000		0.00000	0	0	0.0000000
		0	260	0.0934188					
14	0.00000	0	0	0.0000000		0.00000	0	2377	0.0923837
		0	592	0.0920339					
15	0.00000	0	0	0.0000000		0.00000	0	777	0.0977093
		0	0	0.0000000					

ANGULAR DISTRIBUTION OF RELATIVE MOLECULAR IMPACT DENSITY AROUND OUTER CONICAL SURFACE OF ELEMENTS

-X			-Y					X					Y					-X
0.00	2.22	0.00	0.00	2.22	4.44	2.22	0.00	0.00	4.44	0.00	0.00	0.00	0.00	0.00	2.22	0.00	2.22	0.00	0.00
1.04	0.95	0.79	1.04	0.81	1.04	0.73	0.82	1.02	0.92	0.98	1.18	0.99	0.95	0.84	1.26	1.26	1.29	1.19	0.92
1.08	0.92	0.69	1.14	0.86	0.78	0.56	0.97	0.94	1.14	1.06	1.06	1.03	1.03	1.06	1.33	1.06	1.31	0.97	1.03
1.11	0.97	0.87	0.98	0.93	0.75	1.13	0.76	1.08	1.03	1.17	1.07	0.91	1.00	0.90	1.20	1.03	1.03	1.21	0.91
1.14	1.18	0.97	1.03	1.10	1.16	0.82	1.06	0.82	1.08	1.20	1.01	0.70	0.89	0.78	0.87	1.01	1.14	0.99	1.05
0.68	2.03	1.36	0.68	0.68	0.68	1.69	0.68	1.36	0.34	0.68	0.34	1.69	1.02	1.36	0.68	1.36	1.02	0.34	1.36
0.93	1.09	1.10	0.93	0.93	0.96	1.09	0.80	1.00	1.08	0.96	1.05	1.03	1.03	0.91	1.03	1.08	1.09	0.93	0.99
1.08	1.05	0.87	1.02	0.97	1.07	1.03	1.06	1.07	1.00	1.02	1.00	0.97	0.99	0.95	1.04	1.01	0.87	0.97	0.97
1.10	1.07	1.01	0.99	0.87	1.17	0.87	0.93	1.09	0.89	0.92	1.04	1.05	0.97	0.96	0.99	1.02	1.15	1.01	0.89
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	20.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.75	0.90	0.93	1.08	0.84	1.02	1.02	0.94	0.91	0.82	1.06	1.04	1.09	1.17	1.03	1.04	1.21	1.04	1.02	1.11
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.82	1.02	0.92	1.02	1.10	1.09	0.94	1.09	1.09	0.95	1.28	0.96	1.06	0.93	0.99	0.98	0.94	1.03	0.99	0.84
0.64	1.06	0.98	0.80	1.16	0.98	1.11	0.93	1.26	1.34	1.00	1.03	1.03	1.16	0.80	0.90	0.85	1.00	1.06	0.93

TABLE OF NUMBERS OF MOLECULES WITH PATH LENGTHS WITHIN DECIMAL INTERVALS OF THE TOTAL LENGTH OF THE STRUCTURE IN THE RANGE 0.0 TO 10.0 BY 0.1 STEPS

0	0	0	0	0	1	0	2	3	3
2	4	8	3	4	3	4	3	0	2
3	5	0	4	3	0	3	2	2	3
3	3	4	3	1	5	1	3	3	2
2	3	4	2	1	2	0	3	0	1
1	0	2	5	1	0	3	0	4	0
0	2	3	0	1	0	1	1	0	2
0	3	1	0	1	2	1	0	2	3
3	2	2	0	0	1	1	2	0	1
0	1	2	2	0	0	0	2	0	0

129 PATHS GREATER THAN 10.0 TIMES THE LENGTH OF THE STRUCTURE

TABLE OF NUMBERS OF MOLECULES UNDERGOING N INTERACTIONS

1 0 4 3 8 7 6 3 3 5 4 8 4 1 5 4 10 3 3 8 2 3 0 4 4 2 1 4 5 3

TIME USED BY LAST CALCULATION 163.156 SECONDS

Fig. 4 (CLM-R 54)

Example of print out of output results by computer programme resulting from work on card deck shown in Fig. 2

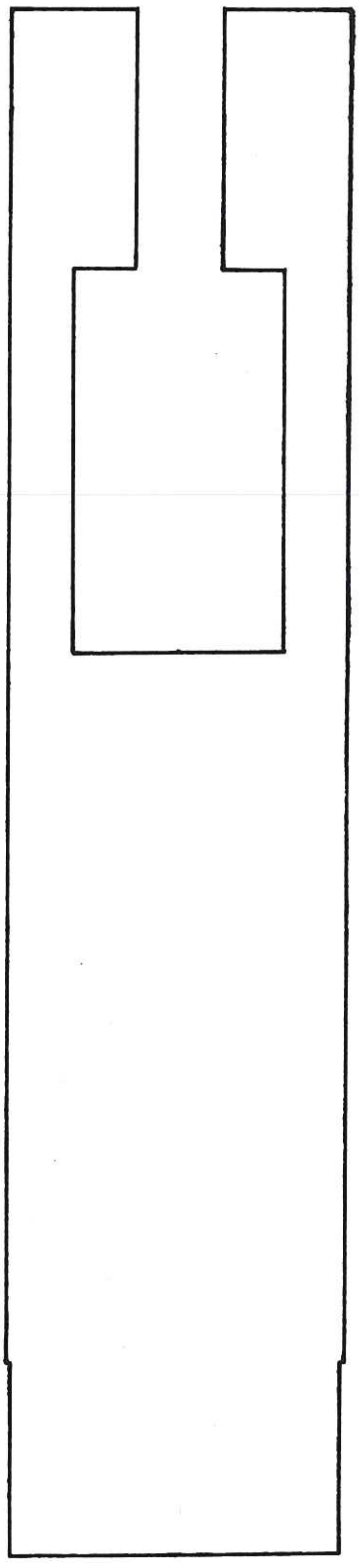

Fig. 5 (CLM-R54)
Vacuum structure produced by Benson-Lehner
Model 'J' Graph Plotter

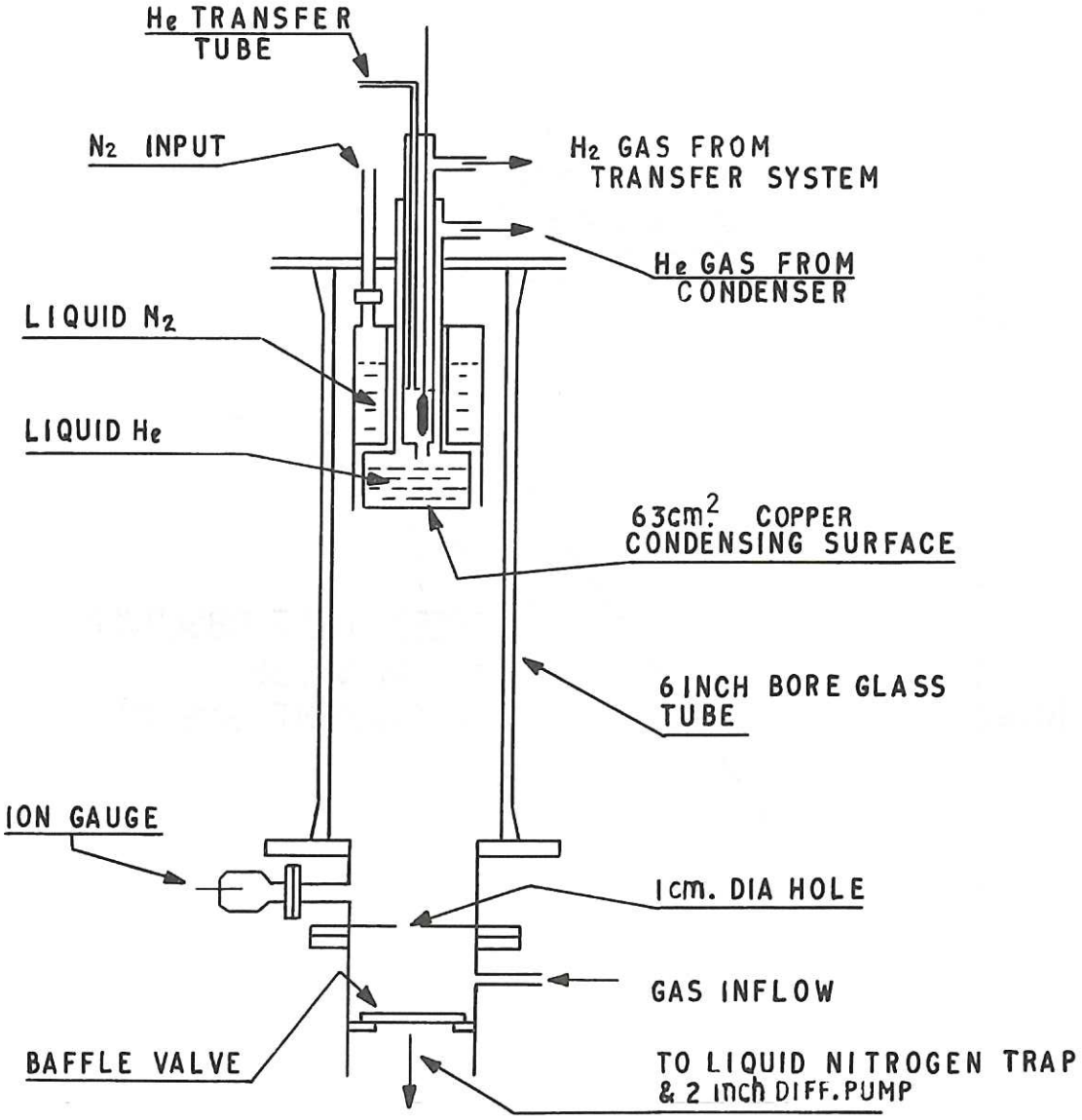

Fig. 6 Apparatus for initial cryo-pump studies (CLM-R54)

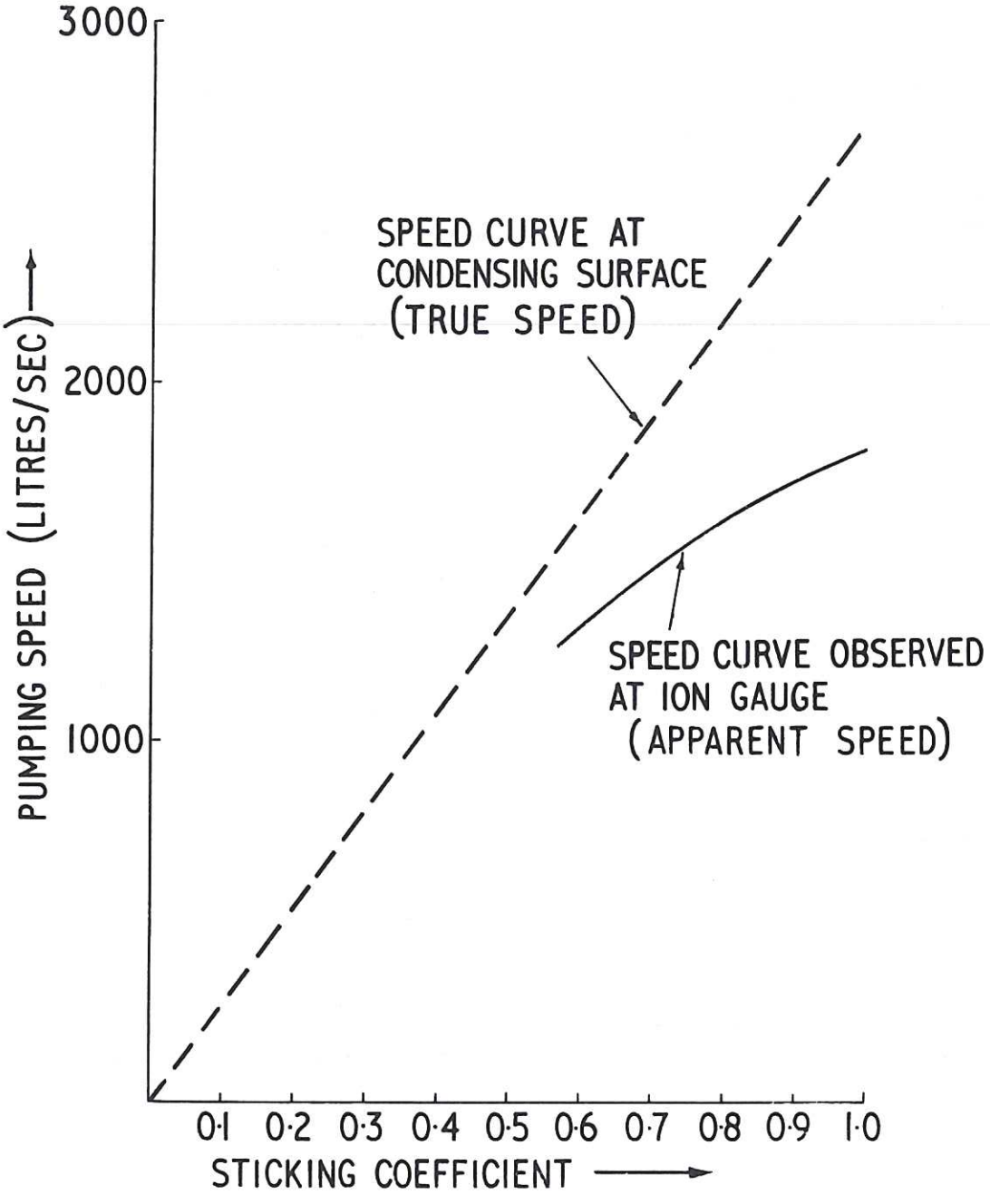

Fig. 7 (CLM-R 54)

Pumping speed v Sticking coefficient for hydrogen in model B cryo-pump based on Monte Carlo calculations

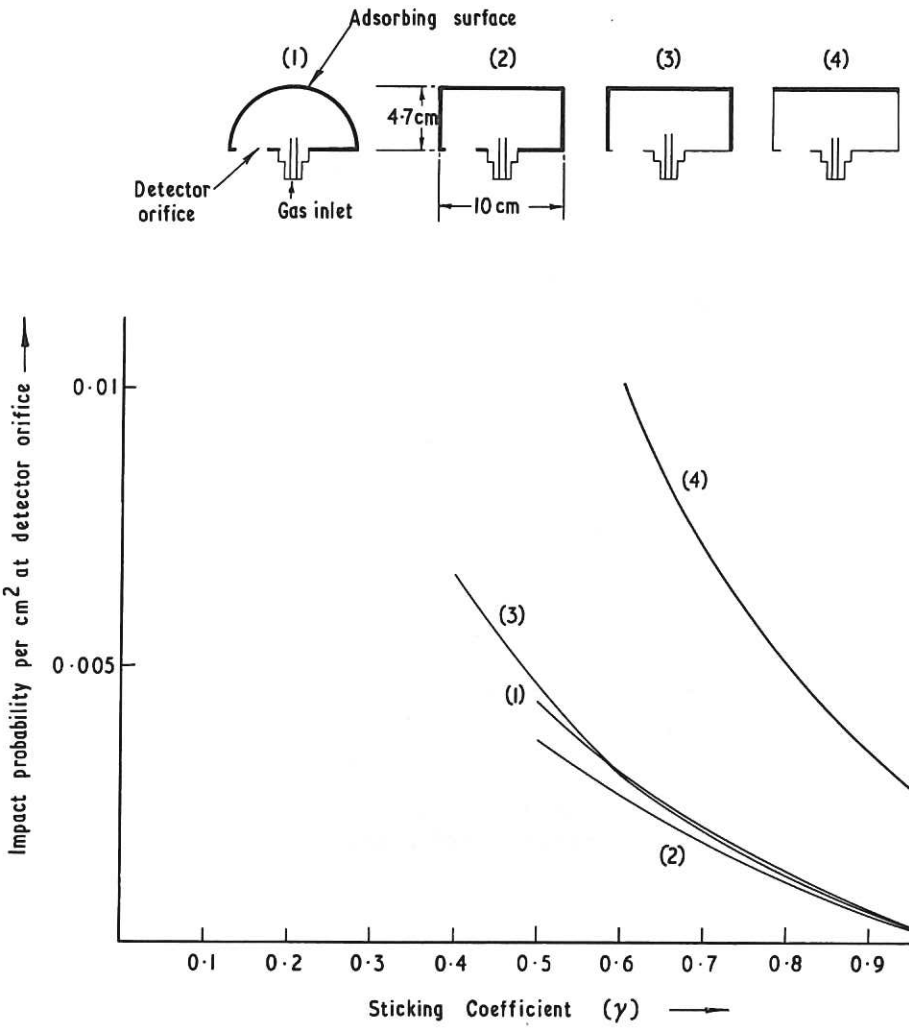

Fig. 8 (CLM-R 54)

Comparison of geometrics for the accurate experimental measurements of sticking coefficients

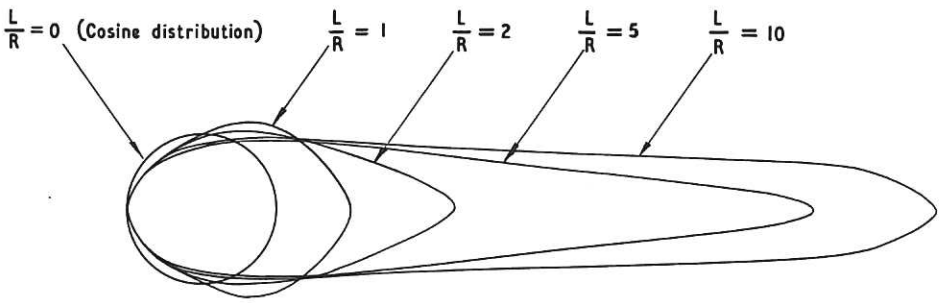

Fig. 9 (CLM-R 54)

Angular distribution of molecules leaving tubes

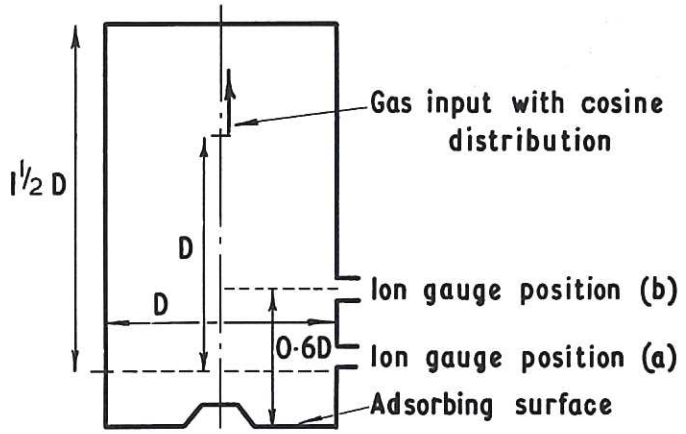

Fig. 10a Type A pumping speed-test dome (CLM-R 54)

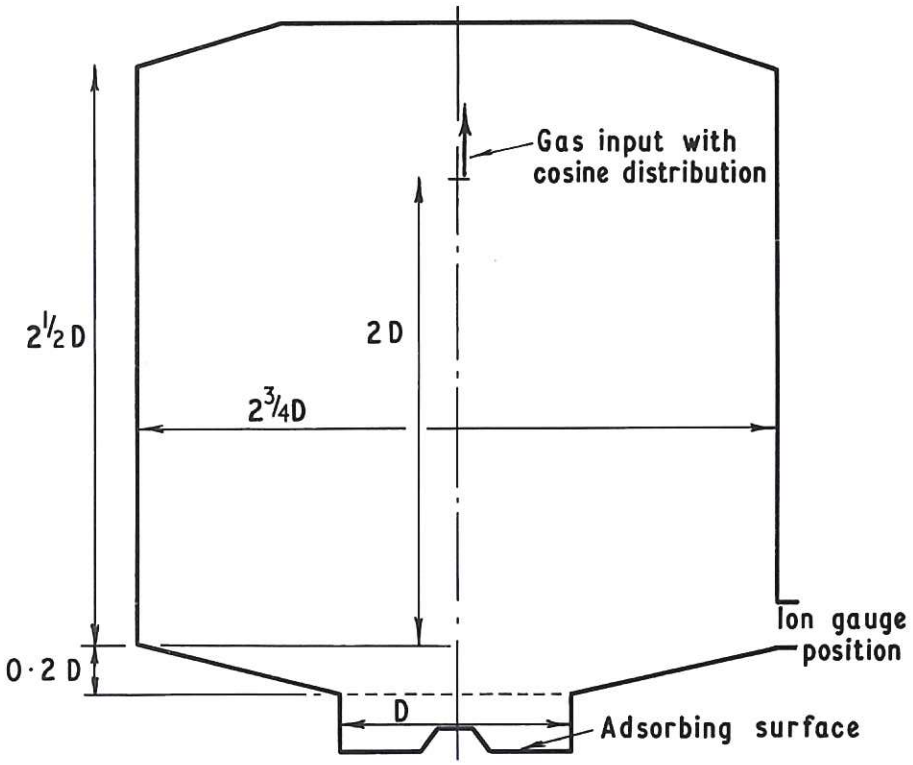

Fig. 10b Type B pumping speed-test dome (CLM-R 54)

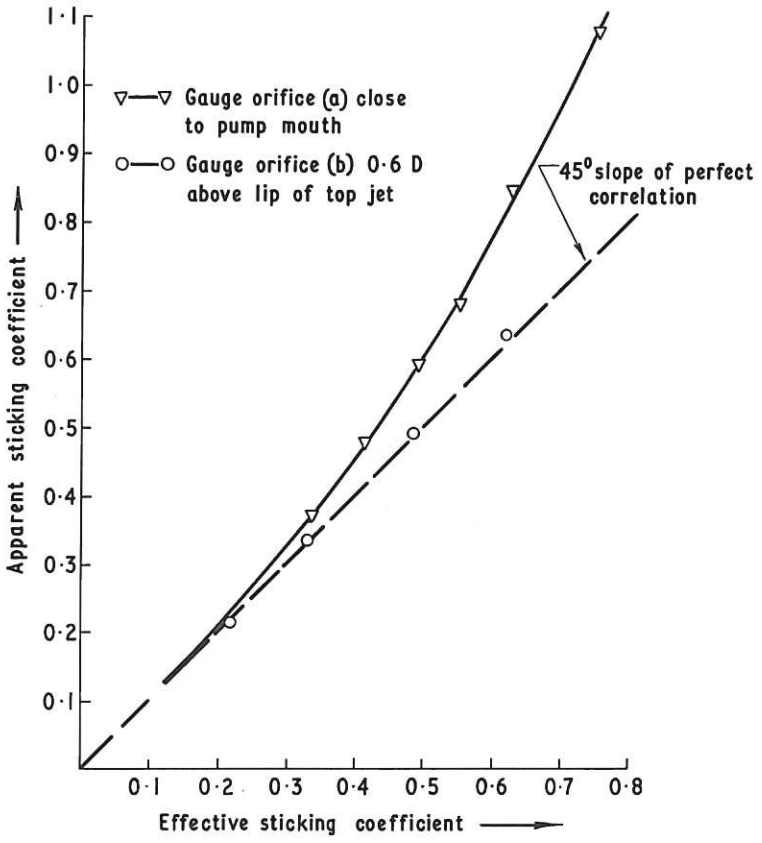

Fig. 11 (CLM-R 54)
Calculations for test dome type A for the two ion gauge orifice positions

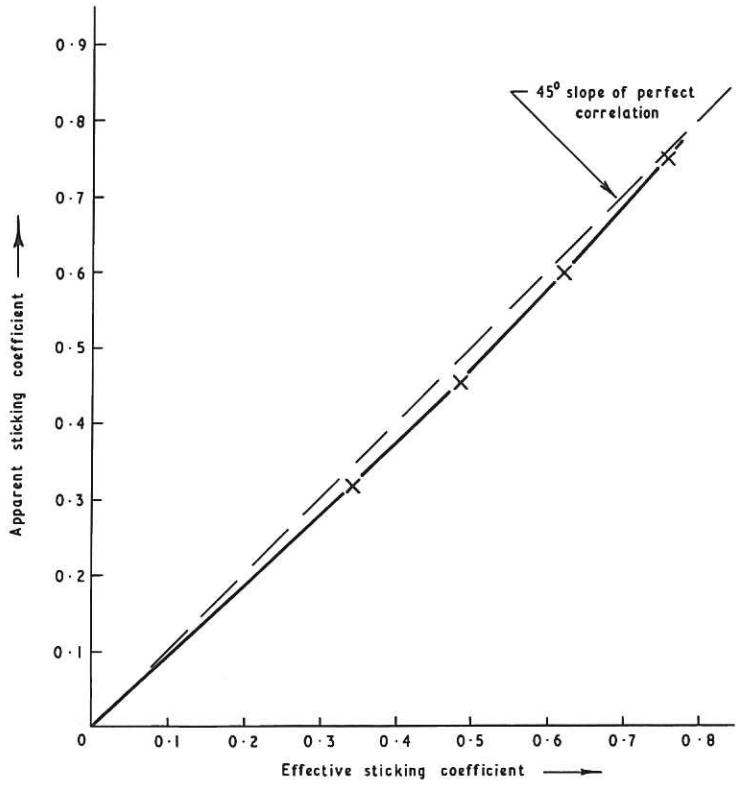

Fig. 12 (CLM-R 54)
Calculations for test dome type B for ion gauge orifice position indicated

APPENDIX I

LISTING OF MONTE CARLO PROGRAMME 3

```
C    THIS PROGRAMME IS FOR USE ON KDF9
      COMMON A,BI,BO,RI,RO,SINALI,SINALO,COSALI,COSALO,PI,PO,LNII,LNOI,
     1LNAO,MNII,MNOI,MNAO,DMNII,DMNOI,DMNAO,MAXNCS,NCS,MREF,DIST,DATA,
     2KP,NTOTAL,KQ,HIT
C
      DIMENSION A(MAXNCS),BI(MAXNCS),BO(MAXNCS),RI(MAXNCS),RO(MAXNCS),
     1SINALI(MAXNCS),SINALO(MAXNCS),COSALI(MAXNCS),COSALO(MAXNCS),
     2PI(MAXNCS),PO(MAXNCS),LNII(MAXNCS),LNOI(MAXNCS),LNAO(MAXNCS),
     3MNII(MAXNCS),MNOI(MAXNCS),MNAO(MAXNCS,21),
     4DMNII(MAXNCS),DMNOI(MAXNCS),DMNAO(MAXNCS,21),MREF(MAXNCS),
     5DIST(MAXNCS),DATA(17),KP(100),NTOTAL(100),KQ(100),HIT(20)
      READ 100,MAXNCS
  100 FORMAT(I7)
      CALL BOCAF(LOCN)
      A=LOCN-MAXNCS
      BI=A-MAXNCS
      BO=BI-MAXNCS
      RI=BO-MAXNCS
      RO=RI-MAXNCS
      SINALI=RO-MAXNCS
      SINALO=SINALI-MAXNCS
      COSALI=SINALO-MAXNCS
      COSALO=COSALI-MAXNCS
      PI=COSALO-MAXNCS
      PO=PI-MAXNCS
      LNII=PO-MAXNCS
      LNOI=LNII-MAXNCS
      LNAO=LNOI-MAXNCS
      MNII=LNAO-MAXNCS
      MNOI=MNII-MAXNCS
      MNAO=MNOI-MAXNCS*21
      DMNII=MNAO-MAXNCS
      DMNOI=DMNII-MAXNCS
      DMNAO=DMNOI-MAXNCS*21
      MREF=DMNAO-MAXNCS
      DIST=MREF-MAXNCS
      DATA=DIST-17
      KP=DATA-100
      NTOTAL=KP-100
      KQ=NTOTAL-100
      HIT=KQ-20
      CALL BOCAS(HIT)
      CALL PREOUT(1)
      END
```

```
C         ****** MONTE CARLO PROGRAM NO 3    ********
C
C              MODIFIED LAST 15-9-65
C
C
C
      COMMON A,BI,BO,RI,RO,SINALI,SINALO,COSALI,COSALO,PI,PO,LNII,LNOI,
     1LNAO,MNII,MNOI,MNAO,DMNII,DMNOI,DMNAO,MAXNCS,NCS,MREF,DIST,DATA,
     2KP,NTOTAL,KQ,HIT
C
C
      DIMENSION A(MAXNCS),BI(MAXNCS),BO(MAXNCS),RI(MAXNCS),RO(MAXNCS),
     1SINALI(MAXNCS),SINALO(MAXNCS),COSALI(MAXNCS),COSALO(MAXNCS),
     2PI(MAXNCS),PO(MAXNCS),LNII(MAXNCS),LNOI(MAXNCS),LNAO(MAXNCS),
     3MNII(MAXNCS),MNOI(MAXNCS),MNAO(MAXNCS,21),
     4DMNII(MAXNCS),DMNOI(MAXNCS),DMNAO(MAXNCS,21),MREF(MAXNCS),
     5DIST(MAXNCS),DATA(17),KP(100),NTOTAL(100),KQ(100),HIT(20)
C
      TIME=ZA01AS(T)
      PRINT 771
  771 FORMAT(1H1//15X,107HIN THE TABLE LISTING THE DISTRIBUTION OF ADSOR
     1PTIONS AND INTERACTIONS THE SURFACE INTERACTION PROBABILITIES/
     25X,122H(DMNAI(I)) AND (DMNAO(I)) ARE CALCULATED AS THE NUMBER OF I
     3NTERACTIONS OCCURING IN THE (I)TH ELEMENT PER UNIT SURFACE AREA/
     44X,55H OF THE ELEMENT PER PARTICLE INTRODUCED INTO THE SYSTEM//
     6 5X,122HIF THE STRUCTURAL DIMENSIONS ARE IN INCHES THEN (DMNAI(I))
     7OR (DMNAO(I)) MULTIPLIED BY THE NETT GAS FLOW INTO THE STRUCTURE/4
     8X,106H IN LITRE.TORR PER SEC. AND DIVIDED BY 264.0 GIVES THE PRESS
     9URE AT THE (I)TH ELEMENT IN TORR. FOR HYDROGEN//)
C
      PRINT 772
  772 FORMAT(12X,111HTHE VOLUME INTERACTION PROBABILITY IS THE AVERAGE P
     1ATH LENGTH PER UNIT VOLUME OF THE INNER ELEMENT PER MOLECULE/
     34X,118HENTERING THE SYSTEM. ASSUMING AMBIENT TEMPERATURE MOLECULAR
     4 ENERGIES THE EFFECTIVE PRESSURE IN TORR WILL BE THE VOLUME/
     54X,117HINTERACTION PROBABILITY MULTIPLIED BY THE GAS INFLOW IN LIT
     6RE.TORR PER SEC. AND BY 0.000876 FOR DIMENSIONS IN INCHES.)
C
      INAXIS=0
      IREF=0
C
   99 READ 201,ICASE,IREF,INCONE,RINNR,ROUTR,RCENTR,INAXIS


C
C          ICASE=NUMBER OF THE CASE BEING STUDIED
C
C          IREF= NUMBER ALLOWING CHOICE OF PARTICLE INPUT
C            AND REFLECTION CONDITIONS
C
C              IF IREF EQUAL ZERO COSINE INPUT AND REFLECTION LAW
C
C         IF (IREF) ABOVE OR BELOW ZERO ISOTROPIC INPUT LAW AND COSINE
C            REFLECTION LAW
C
```

```
C           (INCONE) IS AN INTEGER BETWEEN 1 AND NCS WHICH ALLOWS THE
C             MOLECULAR HISTORIES TO BE STARTED AT THE ENTRY PLANE OF
C             THE (INCONE)TH ELEMENT.
C
C           (RINNR) AND (ROUTR) ARE THE RADII OF THE ANNULAR SURFACE FROM
C             WHICH THE MOLECULAR HISTORIES ARE INITIATED .
C
C           (RCENTR) IS THE X DISPLACEMENT OF THE CENTER OF THE ANNULUS
C             FROM THE SYSTEM AXIS .
C
C          (INAXIS) DETERMINES THE DIRECTION OF THE INPUT DISTRIBUTION
C               ZERO - FOR ALONG THE Z AXIS
C               NEGATIVE FOR ALONG THE -Z AXIS
C          +1   ALONG THE X AXIS
C          +2   ALONG THE Y AXIS
C
C
C
  201 FORMAT(3I7,3F14.7,7X,I2)
      IF (ICASE)51,52,52
   51 STOP
   52 PRINT 105,ICASE
  105 FORMAT(1H1//15X,99HMONTE  CARLO  PROGRAM  NUMBER  3   FOR  FLOW  O
     1F  PARTICLES  THROUGH  SEQUENCE  OF  CONICAL  ANNULI/15X,99H------
     2-----------------------------------------------------------------
     3-------------------------/22X,12HCASE  NUMBER,I7//)
  700 READ 102,NCS,NP,IPRINT
C
C           NCS= NUMBER OF CONES AND CYLINDERS IN SYSTEM
C
C           NP= TOTAL NUMBER OF PARTICL ENTRIES TO BE EXAMINED
C
C           IPRINT= NUMBER OF PARTICLE ENTERIES PER PRINT OUT INTERVAL
C



  102 FORMAT(3I7)
      CALL FAQIDS(12345,ICASE)
C           THIS SETS THE RANDOM NUMBER GENERATING ROUTINE AT DIFFERENT
C             STARTING POINTS FOR DIFFERENT CASE NUMBERS
      LRAF=0
      KREF=0
      STOT=0.0
      SAV=0.0
      HTOT=0.0
      KREST=0
      L1=0
      L2=0
      MREST=0
C
      DO 764 I=1,NCS
      RI(I)=0.00000
      PI(I)=0.00000
      MREF(I)=0
      DIST(I)=0.0000
  764 CONTINUE
      DO 765 I=1,100
      NTOTAL(I)=0
      KP(I)=0
      KQ(I)=0
  765 CONTINUE
```

```
C
  504 READ 103,(RI(I),RO(I),A(I),PI(I),PO(I),MREF(I),I=1,NCS),RI(NCS+1),
     1RO(NCS+1)
  103 FORMAT(5F14.7,I2)
C
C          (MREF(I)) ABOVE ZERO INDICATES THAT THE INNER SURFACE IS TO BE
C         TRANSPARENT - AND THIS WILL CAUSE THE TRAJECTORY LENGTH PER UNIT
C         VOLUME OF THE INNER ELEMENT TO BE CALCULATED
C
C          (MREF(I)) =2 OR -2 WILL CAUSE THE DISTRIBUTION OF PATH LENGTHS FOR
C         FIRST INTERACTION WITH INNER SURFACE OF (I)TH ELEMENT TO BE CALCULATED
C
C          (MREF(I)) =3 OR -3 WILL CAUSE THE DISTRIBUTION OF PATH LENGTHS FOR
C         FIRST INTERACTION WITH OUTER SURFACE OF (I)TH ELEMENT TO BE CALCULATED
      IF(INCONE)838,839,838
  839 INCONE=1
  838 PRINT 840,INCONE
  840 FORMAT(22X,57HMOLECULAR HISTORIES INITIATED AT ENTRANCE PLANE OF N
     1UMBER,I7,2X,4HCONE/)



C
      RIMAX=RI(1)
      ROMAX=RO(1)
        EA=0.0
C
  884 IF(ROUTR)861,885,861
  885 ROUTR=RO(INCONE)
      RCENTR=0.0
  861 PRINT 868,RINNR,ROUTR,RCENTR
  868 FORMAT(22X,34HFROM ANNULAR SURFACE BETWEEN RADII,F14.7,3HAND//22X,
     1F14.7,2X,8HCENTERED,F14.7,2X,33HFROM THE SYSTEM AXIS ALONG X AXIS)
      IF(IREF)507,506,507
  507 ANGLE=(FLOATF(IREF))/1000.0
      PRINT 508,ANGLE
  508 FORMAT(//22X,28HISOTROPIC INPUT DISTRIBUTION/22X,13HBETWEEN 0 AND
     1,F14.7,2X,7HDEGREES)
      GO TO 502
  506 PRINT 509
  509 FORMAT(//22X,16HCOSINE INPUT LAW)
  502 IF(INAXIS)515,511,510
  511 PRINT 512
  512 FORMAT(/22X,34HALONG THE DIRECTION OF THE Z AXIS.)
      GO TO 514
  515 PRINT 516
  516 FORMAT(/22X,35HALONG THE DIRECTION OF THE -Z AXIS.)
      GO TO 514
  510 IF(INAXIS-1)517,517,518
  517 PRINT 513
  513 FORMAT(/22X,34HALONG THE DIRECTION OF THE X AXIS.)
      GO TO 514
  518 PRINT 519
  519 FORMAT(/22X,34HALONG THE DIRECTION OF THE Y AXIS.)
  514 PRINT 505
  505 FORMAT(//22X,21HCOSINE REFLECTION LAW)
```

```
  761 PRINT 200,(I,RI(I),RO(I),A(I),PI(I),PO(I),MREF(I),I=1,NCS)
  200 FORMAT(//5X,11HINPUT TABLE/5X,11H----- -----/5X,13HCOMPONENT NO.,8
     1X,12HINNER RADIUS,5X,12HOUTER RADIUS,10X,6HLENGTH,5X,14HINNER ADS
     2PROB,5X,14HOUTER ADS PROB,4X,4HMREF,//(5X,I7,12X,F14.7,3X,F14.7,2X
     3,F14.7,5X,F14.7,5X,F14.7,5X,I2))
      PRINT 763,RI(NCS+1),RO(NCS+1)
  763 FORMAT(24X,F14.7,3X,F14.7)
C
C          PROTECT PROGRAMME FROM DATA ERRORS .
C
  940 DO 796 I=1,NCS


      IF(RO(I)-RI(I))794,786,786
  794 PRINT 795,I
  795 FORMAT(22X,33HINNER RADIUS EXCEEDS OUTER RADIUS,I7,1X,20HCONE - CA
     1SE REJECTED)
      KREF=-1
  786 IF(INCONE-I)796,797,796
  797 IF(RO(I)-ROUTR-RCENTR)798,796,796
  798 PRINT 799,I
  799 FORMAT(22X,28HINPUT ANNULUS PARTLY OUTSIDE,I7,1X,4HCONE)
      KREF=-1
  796 CONTINUE
      IF(NCS-INCONE)810,811,811
  810 PRINT 812
  812 FORMAT(22X,44HINPUT CONE OUTSIDE STRUCTURE - CASE REJECTED)
      KREF=-1
  811 IF(KREF)99,770,770
C
C
C
C          COMPUTE B-THE DISTANCE TO THE CONE APEX-AND THE SINE AND
C          COSINE OF ALPHA-THE CONE HALF ANGLE-FOR INNER CONES .
C
  770 DO 128 I=1,NCS
      IF(MREF(I))780,768,769
  769 PI(I)=0.0
      LRAF=1
  780 IF(XABSF(MREF(I))-1)768,768,781
  781 L1=I
      L2=MREF(I)
C
  768 LNII(I)=0
      LNOI(I)=0
C
C        LNII(I) IS THE NUMBER OF MOLECULES ADSORBED ON INSIDE OF INNER CONE
C
C        LNOI(I) IS THE NUMBER OF MOLECULES ADSORBED ON OUTSIDE OF INNER CONE
C
      MNII(I)=0
      MNOI(I)=0
C
C        MNII IS THE NUMBER OF INTERACTIONS ON THE INSIDE OF INNER CONE
C
C        MNOI IS THE NUMBER OF INTERACTIONS ON THE OUTSIDE OF INNER CONE
C
```

```
      A(I)=A(I)+0.001*MAXIF(ABSF(RO(I)-RO(I+1)),ABSF(RI(I)-RI(I+1)))



      EA=EA+A(I)
      RIMAX=MAXIF(RIMAX,RI(I))
C
      IF(ABSF(RI(I)-RI(I+1))-(A(I)*1.0E-6))2,2,3
    2 BI(I)=RI(I)
C          IF CYLINDER PUT BI(I)=RI(I)
      SINALI(I)=0.0
      COSALI(I)=1.0
      GO TO 128
    3 HI=SQRTF(A(I)*A(I)+(RI(I+1)-RI(I))*(RI(I+1)-RI(I)))
      SINALI(I)=(RI(I+1)-RI(I))/HI
      COSALI(I)=SQRTF(1.0-SINALI(I)*SINALI(I))
      BI(I)=RI(I)*A(I)/(RI(I+1)-RI(I))
  128 CONTINUE
C
C          COMPUTE B=THE DISTANCE TO THE CONE APEX-AND THE SINE AND
C          COSINE OF ALPHA-THE CONE HALF ANGLE-FOR OUTER CONES .
C
      DO 1 I=1,NCS
      LNAO(I)=0
C        LNAO(I) IS THE NUMBER OF MOLECULES ADSORBED ON INSIDE OF OUTER CONE
C
      ROMAX=MAXIF(ROMAX,RO(I))
      DOMAX=2.0*ROMAX
C
      IF(ABSF(RO(I)-RO(I+1))-(A(I)*1.0E-6))78,78,79
   78 BO(I)=RO(I)
C          IF CYLINDER PUT BO(I)=RO(I)
      SINALO(I)=0.0
      COSALO(I)=1.0
      GO TO 1
   79 HO=SQRTF(A(I)*A(I)+(RO(I+1)-RO(I))*(RO(I+1)-RO(I)))
      SINALO(I)=(RO(I+1)-RO(I))/HO
      COSALO(I)=SQRTF(1.0-SINALO(I)*SINALO(I))
      BO(I)=RO(I)*A(I)/(RO(I+1)-RO(I))
    1 CONTINUE
C
C
C               NA= NUMBER OF PARTICLES ABSORBED BY SYSTEM
C               NPE2= NUMBER OF PARTICLES TRANSMITTED BY SYSTEM
C               NPE1= NUMBER OF PARTICLES REFLECTED BY SYSTEM
      NI=0
      NO=0
      NP100=0
      NREF=0



      NA=0
      NPE1=0
      NPE2=0
      NREST=0
```

```
   75 DO 77 I=1,NCS
      DO 76 K=1,21
      MNAO(I,K)=0
      DMNAO(I,K)=0.0
   76 CONTINUE
   77 CONTINUE
C
      GAPOUT=RO(NCS+1)-RI(NCS+1)
      GAPIN=RO(1)-RI(1)
C
      PRINT 370,EA
  370 FORMAT(///1X,28HTOTAL LENGTH OF STRUCTURE IS,F14.7,2X,5HUNITS)
C
C          GRAPH PLOTTING FACILITY IF (ICASE) ABOVE 1000
C
      IF(ICASE-1000)62,960,960
  960 SCALE=1.0
      CALL INSTBQ(DATA,0)
      CALL PAGEBQ(DATA,ICASE)
      IF(ICASE-10000)135,135,136
  135 DMAX=MAX1F(DOMAX,EA)
      SCALE=10.0/DMAX
  136 PRINT 137,SCALE
  137 FORMAT(//22X,14HGRAPH SCALE IS,F9.6)
      DATA(1)=6.5
      DATA(2)=0.0
      DATA(3)=0.0
      DATA(4)=0.0
      DATA(5)=1.0/SCALE
      DATA(6)=1.0/SCALE
      DATA(7)=0.0
      DATA(8)=13.0
      DATA(9)=0.0
      DATA(10)=13.0
      DATA(11)=13.0
      DATA(12)=13.0
      CA=1.0
      NC=NCS+1
C
C



      CALL PLOTBQ(RO(1),1.0,DATA,1,-2)
C
      DO 970 I=1,NCS
      CA=CA+A(I)
      CALL PLOTBQ(RO(I+1),CA,DATA,0,-2)
  970 CONTINUE
      RONEG=-RO(1)
      CALL PLOTBQ(RONEG,1.0,DATA,1,-2)
      CA=1.0
      DO 138 I=1,NCS
      CA=CA+A(I)
      RONEG=-RO(I+1)
      CALL PLOTBQ(RONEG,CA,DATA,0,-2)
  138 CONTINUE
```

```
      IF(RIMAX-0.00001)62,62,974
C
  974 CA=1.0
      NLP=0
      CALL PLOTBQ(RI(1),1.0,DATA,1,-2)
C
      DO 971 I=1,NCS
      CA=CA+A(I)
      IF(RI(I)+RI(I+1)-0.0001)972,977,977
  977 IF(MREF(I))973,973,972
  972 NLP=1
      GO TO 976
  973 NLP=0
  976 CALL PLOTBQ(RI(I+1),CA,DATA,NLP,-2)
  971 CONTINUE
C
      NLP=0
      CA=1.0
      RINEG=-RI(1)
      CALL PLOTBQ(RINEG,1.0,DATA,1,-2)
C
      DO 141 I=1,NCS
      CA=CA+A(I)
      IF(RI(I)+RI(I+1)-0.0001)142,147,147
  147 IF(MREF(I))143,143,142
  142 NLP=1
      GO TO 146
  143 NLP=0
  146 RINEG=-RI(I+1)
      CALL PLOTBQ(RINEG,CA,DATA,NLP,-2)



  141 CONTINUE
      CALL GPFIN
C
   62 IF(NP-NP100)99,99,80
C
C
C
C           THE NEXT DO LOOP GENERATES AND ANALYSES THE MOLECULAR HISTORIES
C             IN THE SPECIFIED STRUCTURE
C
   80 DO 400 M=1,IPRINT
      X=RCENTR
      Y=0.0
      Z=0.0
      SNP=0.0
      STOI=0.0
      MP=0
      NTOT=0
      KT=10
C
      DO 189 N=1,20
      HIT(N)=0
  189 CONTINUE
```

```
C                CALCULATE ENTRANCE COORDS
      CALL RAND3(RINNR,ROUTR,X,Y,Z,AL,AM,AN,IREF,INAXIS)
C
      I=INCONE
      J=1
      IF(INAXIS)893,889,888
  893 AN=-AN
  889 IF(AN)5,8,8
  888 IF(Z)890,891,891
  890 I=I-1
      Z=Z+A(I)
      IF(Z)890,896,896
  896 IF(AN)897,895,895
  897 Z=A(I)-Z
      GO TO 894
  891 IF(A(I)-Z)892,896,896
  892 Z=Z-A(I)
      I=I+1
      GO TO 891
C
C                IF J=1 Z IS INCREACING


C                IF J=0  Z IS DECREACING
    8 PSINAL=SINALI(I)
      PB=BI(I)
      OSINAL=SINALO(I)
      OB=BO(I)
   14 DA=A(I)
      PCOSAL=COSALI(I)
      OCOSAL=COSALO(I)
      PP=PI(I)
      OP=ABSF(PO(I))
      NI=100
      IF(XABSF(MREF(I))+KT-12)162,161,160
  161 NI=10
C          THIS INDICATES THAT PATH LENGTH UP TO FIRST INTERACTION WITH
C            INNER SURFACE IS DESIRED
      GO TO 162
  160 IF(XABSF(MREF(I))+KT-13)162,163,162
  163 NI=20
C          THIS INDICATES THAT PATH LENGTH UP TO FIRST INTERACTION WITH
C            OUTER SURFACE IS DESIRED
  162 L=I+1-J
      RADIN=SQRTF((X*X)+(Y*Y))
      IF(RADIN-RO(L))917,917,12
  917 IF(LRAF)915,915,916
  915 NREF=0
      GO TO 453
C
C          (NREF) ABOVE ZERO, INTERACTION OF TRAJECTORY WITH INNER CONE
C            RECORDED BUT TRAJECTORY UNDEFLECTED.
C
C          (NREF) EQUAL TO ZERO, INTERACTION ONLY WITH OUTSIDE SURFACE
C              OF INNER CONE .
C
C          (NREF) BELOW ZERO, INTERACTION WIH INSIDE SURFACE OF INNER CONE.
```

```
  916 IF(MREF(I))909,909,911
  909 IF(RADIN-RI(L))910,912,912
  910 NREF=-1
      GO TO 453
  912 NREF=0
      GO TO 453
  911 IF(RADIN-RI(L))913,914,914
  913 NREF=3
      GO TO 453
  914 NREF=1


C
C           TEST FOR INTERACTION IN (I)TH ELEMENT .
  453 CALL RING1(DA,PB,OB,PSINAL,OSINAL,PCOSAL,OCOSAL,PP,OP,X,Y,Z,AL,AM,
     1AN,NREF,NI,NO,MP,HIT)
C
      IF(NREF)170,171,171
  170 MNII(I)=MNII(I)+XABSF(NI)
      GO TO 172
  171 MNOI(I)=MNOI(I)+XABSF(NI)
  172 MNAO(I,21)=MNAO(I,21)+XABSF(NO)
C
C         MNAO(I,21) IS THE TOTAL NUMBER OF INTERACTIONS ON THE OUTER CONE
C
C              (OP) OUT OF RINGO GIVES THE PATH LENGTH WITHIN THE ELEMENT
C            (PB) OUT OF RINGO GIVES THE PATH LENGTH TO FIRST INTERACTION
C                 IN THIS ELEMENT
      IF(ABSF(PB)-1.0E-6)164,164,165
  165 STOI=SNP+PB
      KT=0
  164 SNP=SNP+OP
      STOT=STOT+OP
      Z=0.0
      DO 188 N=1,20
      MNAO(I,N)=MNAO(I,N)+HIT(N)
      HIT(N)=0
  188 CONTINUE
      IF(NREF)450,450,471
  471 DIST(I)=DIST(I)-PP
      GO TO 454
  450 NTOT=NTOT+XABSF(NI)
  454 NTOT=NTOT+XABSF(NO)
      IF(NI)449,465,465
  449 IF(NREF)173,174,174
  173 LNII(I)=LNII(I)+1
      NA=NA+1
      GO TO 4
  174 LNOI(I)=LNOI(I)+1
C           COUNT ONE PARTICLE ADSORBED ON INNER CONE IF (NI) LESS THAN ZERO
      NA=NA+1
      GO TO 4
  465 IF(NO)466,467,467
  466 LNAO(I)=LNAO(I)+1
C           COUNT ONE PARTICLE ADSORBED ON OUTER (I)TH CONE.
    6 NA=NA+1
      GO TO 4
```

```
C
C           IF (J)=0  REFLECT THE CONE THE MOLECULE NOW ENTERS AND CONTINUE
  467 IF(J)11,11,10
   11 AN=-AN
   10 IF(AN)5,4,7
    7 I=I+1
  895 J=1
C                 REPEAT USING THE INDEX J UNTIL THE PARTICLE EXITS
      IF(NCS-I)12,8,8
    5 I=I-1
  894 J=0
      IF(I)12,12,9
    9 AN=-AN
      IF(SINALI(I))13,455,13
  455 PSINAL=SINALI(I)
      PB=BI(I)
      GO TO 456
   13 PSINAL=-SINALI(I)
      PB=-BI(I)-A(I)
  456 IF(SINALO(I))458,457,458
  457 OSINAL=SINALO(I)
      OB=BO(I)
      GO TO 14
  458 OSINAL=-SINALO(I)
      OB=-BO(I)-A(I)
      GO TO 14
   12 IF(AN)15,15,16
   15 NPE1=NPE1+1
      IF(GAPIN-1.0E-3)42,42,4
   42 PRINT 41,X,Y,Z,AL,AM,AN,NA,NTOT,MP,NREF,LRAF,I,J,RO(L),RADIN,SNP
      GO TO 400
   16 NPE2=NPE2+1
      IF(GAPOUT-1.0E-3)40,40,4
   40 PRINT 41,X,Y,Z,AL,AM,AN,NA,NTOT,MP,NREF,LRAF,I,J,RADIN,RO(L),SNP
   41 FORMAT(2X,3F14.7,3F10.7,2I4,5I3,2X,3F10.7)
      GO TO 400
    4 SAV=STOT/FLOATF(NA+NPE1+NPE2)
C             COMPARE CURRENT MOLECULE PATH WITH TOTAL LENGTH OF STRUCTURE
      NST=XINTF(10.0*SNP/EA)+1
      IF(NST-99)350,350,351
  350 KP(NST)=KP(NST)+1
      GO TO 354
  351 KREST=KREST+1
  354 IF(STOI-1.0E-6)357,358,358
  358 MST=XINTF(10.0*STOI/EA)+1



      IF(MST-99)355,355,356
  355 KQ(MST)=KQ(MST)+1
      GO TO 357
  356 MREST=MREST+1
  357 IF(NTOT-100)180,180,181
  180 NTOTAL(NTOT)=NTOTAL(NTOT)+1
       GO TO 400
  181 NREST=NREST+1
C
C                 REPEAT FOR ALL PARTICLES
C
  400 CONTINUE
```

```
C
C              CALCULATE IMPACT DENSITY IN (I)TH SECTION IN TERMS
C           OF NETT PARTICLE FLOW INTO SYSTEM AND DATA DIMENSION UNITS.
      DO 800 I=1,NCS
      IF(ABSF(RI(I)+RI(I+1))-1.0E-6)460,461,461
  461 IF(MREF(I))463,463,464
  464 IF(ABSF(RI(I)-RI(I+1))-1.0E-10)468,468,469
  468 G=3.14159265*RI(I)*RI(I)*A(I)*FLOATF(NA+NPE2+NPE1)
      GO TO 472
  469 G=1.04719755*(RI(I+1)*RI(I+1)*(BI(I)+A(I))-RI(I)*RI(I)*BI(I))*FLOA
     1TF(NA+NPE2+NPE1)
  472 DMNOI(I)=DIST(I)/G
      GO TO 462
  463 G=(3.1415926*(RI(I)+RI(I+1))*SQRTF((RI(I)-RI(I+1))*(RI(I)-RI(I+1))
     1+A(I)*A(I))*FLOATF(NA+NPE2+NPE1))
  470 DMNII(I)=(FLOATF(MNII(I)))/G
      DMNOI(I)=(FLOATF(MNOI(I)))/G
      GO TO 462
  460 DMNII(I)=0.0
      DMNOI(I)=0.0
  462 H=(3.1415926*(RO(I)+RO(I+1))*SQRTF((RO(I)-RO(I+1))*(RO(I)-RO(I+1))
     1+A(I)*A(I)))
      DMNAO(I,21)=(FLOATF(MNAO(I,21)))/(H*FLOATF(NA+NPE1+NPE2))
C
      DO 182 M=1,20
      DMNAO(I,M)=(FLOATF(MNAO(I,M)))*20.0/(H*FLOATF(NA+NPE1+NPE2)*DMNAO(
     1I,21))
  182 CONTINUE
C
      HTOT=HTOT+H
  800 CONTINUE
C



      IF(NP100)374,374,376
  374 PRINT 375,HTOT
  375 FORMAT(/39HTOTAL SURFACE AREA OF OUTER ELEMENTS IS,F18.7,2X,20HLEN
     1GTH UNITS SQUARED)
C
  376 IF(NP100-NP)743,60,60
  743 NP100=NP100+IPRINT
   60 NZ=NP100
      DPAB=SQRTF(FLOATF(NA)*FLOATF(NZ-NA)/FLOATF(NZ))
      DPTR=SQRTF(FLOATF(NPE2)*FLOATF(NZ-NPE2)/FLOATF(NZ))
      DPRE=SQRTF(FLOATF(NPE1)*FLOATF(NZ-NPE1)/FLOATF(NZ))
      PRAB=FLOATF(NA)/FLOATF(NZ)
      PRTR=FLOATF(NPE2)/FLOATF(NZ)
      PRRE=FLOATF(NPE1)/FLOATF(NZ)
      ERAB=DPAB*100.0/FLOATF(NA)
      ERTR=DPTR*100.0/FLOATF(NPE2)
      ERRE=DPRE*100.0/FLOATF(NPE1)
C
      PRINT 100,ICASE,NA,DPAB,PRAB,ERAB,NPE2,DPTR,PRTR,ERTR,NPE1,DPRE,
     1PRRE,ERRE,SAV
  100 FORMAT(1H1//1X,28HOUTPUT TABLES    CASE NUMBER,I7/1X,28H----------
     1--      ----------/25X,9HPARTICLES,5X,10HDISPERSION,5X,11HPROBABIL
     2ITY,5X,9HP/C ERROR//5X,11HADSORPTIONS,9X,I7,3X,F14.7,2X,2F14.7/5X,
     313HTRANSMISSIONS,7X,I7,3X,F14.7,2X,2F14.7/5X,11HREFLECTIONS,9X,I7,
     43X,F14.7,2X,2F14.7/5X,32HAVERAGE MOLECULAR PATH LENGTH IS,F14.7,2X
     5,12HLENGTH UNITS)
```

```
      PRINT 129
  129 FORMAT(/2X,44HDISTRIBUTION OF ADSORPTIONS AND INTERACTIONS/2X,44H=
     1----------------------------------------/29X,12HINNER  CONES,
     253X,12HOUTER  CONES)
      PRINT 130
  130 FORMAT(              9X,62H----------------------------------------
     3----------,4X,50H----------------------------------------
     4----------/48X,7HSURFACE,6X,6HVOLUME,49X,7HSURFACE/
     51X,7HELEMENT,1X,10HADSORPTION,28X,11HINTERACTION,2X,11HINTERACTION
     6,4X,10HADSORPTION,29X,11HINTERACTION/3X,3HNO.,4X,5HPROB.,5X,
     711HADSORPTIONS,2X,12HINTERACTIONS,3X,5HPROB.,8X,5HPROB.,10X,
     85HPROB.,6X,11HADSORPTIONS,2X,12HINTERACTIONS,3X,5HPROB./
     94X,3H(I),3X,7H(PI(I)),4X,9H(LNAI(I)),4X,9H(MNAI(I)),5X,
     910H(DMNAI(I)),2X,10H(DMNAI(I)),6X,7H(PO(I)),5X,9H(LNAO(I)),4X,
     99H(MNAO(I)),5X,10H(DMNAO(I)))
      DO 474 I=1,NCS
      IF(MREF(I))475,475,476
  475 PRINT 477,I,PI(I),LNII(I),MNII(I),DMNII(I),PO(I),LNAO(I),MNAO(I,21
     1),DMNAO(I,21),LNOI(I),MNOI(I),DMNOI(I)
  477 FORMAT(I7,F10.5,5X,I7,6X,I7,2X,F14.7,14X,3X,F10.5,5X,I7,4X,I7,3X,
     1F14.7/22X,I7,6X,I7,2X,F14.7/)
      GO TO 474
  476 PRINT 488,I,PI(I),LNOI(I),MNOI(I),DMNOI(I),PO(I),LNAO(I),MNAO(I,21
     1),DMNAO(I,21)
  488 FORMAT(I7,F10.5,5X,I7,6X,I7,2X,14X,F14.7,3X,F10.5,5X,I7,4X,I7,3X,
     1F14.7/)
  474 CONTINUE
C
      PRINT 187
  187 FORMAT(//3X,98HANGULAR DISTRIBUTION OF RELATIVE MOLECULAR IMPACT D
     1ENSITY AROUND OUTER CONICAL SURFACE OF ELEMENTS/1X,2H-X,28X,2H-Y,
     228X,2H X,28X,2H Y,28X,2H-X/)
      DO 185 I=1,NCS
      PRINT 186,(DMNAO(I,K),K=1,20)
  186 FORMAT(2X,20F6.2)
  185 CONTINUE
C
C
      PRINT 371
  371 FORMAT(///109HTABLE OF NUMBERS OF MOLECULES WITH PATH LENGTHS WITH
     1IN DECIMAL INTERVALS OF THE TOTAL LENGTH OF THE STRUCTURE/30X,37HI
     2N THE RANGE 0.0 TO 10.0 BY 0.1 STEPS//)
      KSM=1
      KSN=10
      DO 360 KS=1,10
      PRINT 361,(KP(I),I=KSM,KSN)
  361 FORMAT(5X,10I9)
      KSM=KSM+10
      KSN=KSN+10
  360 CONTINUE
C
      PRINT 372,KREST
  372 FORMAT(/I9,2X,57HPATHS GREATER THAN 10.0 TIMES THE LENGTH OF THE S
     1TRUCTURE//)
```

```
      IF(XABSF(L2)-2)382,381,380
  380 PRINT 383,L1
  383 FORMAT(/119HDISTRIBUTION OF PATH LENGTHS IN DECIMAL FRACTIONS OF T
     1HE TOTAL LENGTH OF THE STRUCTURE FOR FIRST INTERACTION WITH OUTER/
     25X,10HSURFACE OF,I4,2X,7HELEMENT/)
      GO TO 385
  381 PRINT 384,L1
  384 FORMAT(/119HDISTRIBUTION OF PATH LENGTHS IN DECIMAL FRACTIONS OF T


     1HE TOTAL LENGTH OF THE STRUCTURE FOR FIRST INTERACTION WITH INNER/
     25X,10HSURFACE OF,I4,2X,7HELEMENT/)
  385 KSM=1
      KSN=10
      DO 390 KA=1,10
      PRINT 391,(KQ(I),I=KSM,KSN)
  391 FORMAT(5X,10I9)
      KSM=KSM+10
      KSN=KSN+10
  390 CONTINUE
      PRINT 372,MREST
C
  382 PRINT 152
  152 FORMAT(/5X,55HTABLE OF NUMBERS OF MOLECULES UNDERGOING N INTERACTI
     1ONS)
      PRINT 151,(NTOTAL(I),I=1,30)
  151 FORMAT(5X,30I4)
C
      TIME=ZA01AS(T)-TIME
      IF(TIME-0.1)131,131,132
  132 PRINT 300,TIME
  300 FORMAT(///,25X,31HTIME USED BY LAST CALCULATION  ,F6.3,8H SECONDS)
  131 TIME=ZA01AS(T)
      GO TO 62
      END
```

```
      SUBROUTINE RINGI(A,PB,OB,PSINAL,OSINAL,PCOSAL,OCOSAL,PP,OP,X,Y,Z,
     1AL,AM,AN,NREF,NI,NO,MP,HIT)
      DIMENSION HIT(21)
C
C           SUBROUTINE RINGO  - TO BE USED IN A MONTE CARLO CALCULATION
C           INVOLVING FLOW IN ANNULAR SPACE BETWEEN TRUNCATED CONES OR CYLINDERS
C           WITH FLOW POSSIBLE INSIDE AS WELL AS OUTSIDE THE INNER CONE
C
      KT=NI
C  NI=10    THIS INDICATES THAT PATH LENGTH UP TO FIRST INTERACTION WITH
C             INNER SURFACE IS DESIRED
C  NI=20    THIS INDICATES THAT PATH LENGTH UP TO FIRST INTERACTION WITH
C             OUTER SURFACE IS DESIRED
      K=0
      D=1.0E+32
      S=0.0
      SO=0.0
      NI=0
      NO=0
      SUMS=0.0
      STOI=0.0
C
    1 APCOS=1.0/PCOSAL
      AOCOS=1.0/OCOSAL
C
C
C           TEST FOR INTERSECTION WITH INNER CONE OR CYLINDER FIRST.
C
   51 IF(PSINAL)2,3,2
    3 WI1=1.0-AN*AN
      WI2=AL*X+AM*Y
      WI3=X*X+Y*Y-PB*PB
      IF(K)73,73,90
    2 WI1=1.0-(AN*APCOS)*(AN*APCOS)
      WI2=AL*X+AM*Y-AN*(PB+Z)*PSINAL*PSINAL*APCOS*APCOS
      WI3=X*X+Y*Y-((PB+Z)*PSINAL*APCOS)*((PB+Z)*PSINAL*APCOS)
C
      IF(K)73,73,90
C
C      (K) ABOVE ZERO INDICATES TRAJECTORY STARTED FROM SURFACE OF INNER CONE
C
   90 IF(WI1)113,113,94
   94 S=-2.0*WI2/WI1
      IF(S*AN+Z-A)95,113,113



   95 IF(S*AN+Z)113,113,12
C
   73 XI=WI2*WI2-WI1*WI3
      IF(XI)20,75,74
C
C           IF XI GREATER OR EQUAL TO ZERO THEN PARTICLE TRAJECTORY
C              INTERSECTS INNER CONE
C
C           IF (XI) BELOW ZERO THEN PARTICLE TRAJECTORY INTERSECTS
C              OUTER CONE OR EXITS
```

```
   75 S=-2.0*WI2/WI1
      GO TO 16
   74 IF(WI1)4,11,4
   11 S=-WI3/(2.0*WI2)
      GO TO 16
C
    4 S1=(SQRTF(XI)-WI2)/WI1
      S2=(-WI2-SQRTF(XI))/WI1
      IF(S1)56,56,52
   56 IF(S2)20,20,55
   52 IF(S2)53,53,54
   53 S=S1
      GO TO 6
   55 S=S2
      GO TO 6
   54 S=MIN1F(S1,S2)
C     (S) IS THE TRAJECTORY DISTANCE TO INTERACTION WITH INNER
C     CONE FROM A STARTING POINT WITHIN CONE ELEMENT.
      D=MAX1F(S1,S2)
C
C     CHECK FOR INTERACTION WITHIN LENGTH OF (I)TH CONE
C
   16 IF(S)7,7,6
    6 IF(S*AN+Z-A)8,7,7
    8 IF(S*AN+Z)7,7,12
    7 IF(NREF)106,20,20
   12 NI=NI+1
      IF(NI+KT-11)158,159,158
  159 STOI=SUMS+S
      KT=1000
  158 IF(NREF)71,71,84
   71 X=S*AL+X
      Y=S*AM+Y
      Z=S*AN+Z



      K=1
      IF(NREF)83,72,84
C
C          (NREF) ABOVE ZERO, INTERACTION OF TRAJECTORY WITH INNER CONE
C            RECORDED BUT TRAJECTORY UNDEFLECTED
C
C          (NREF) EQUALS ZERO, INTERACTION ONLY WITH OUTSIDE SURFACE
C            OF INNER CONE
C
C          (NREF) BELOW ZERO, INTERACTION WITH INSIDE
C             SURFACES OF INNER CONE
C
   83 JREF=0
C     JREF=0 FOR INTERACTION ON INSIDE OF INNER CONE
      IF(PP)13,13,85
   85 PP=0.0
C          ADSORPTION ON INSIDE OF INNER SURFACE OF INNER ELEMENT
C            IF PP BELOW ZERO
      GO TO 13
   72 JREF=1
C     JREF=1 FOR INTERACTION ON OUTSIDE OF INNER CONE
      IF(PP)86,13,13
   86 PP=0.0
   13 IF(ABSF(PP)-1.0001)150,151,151
  151 IF(MP)152,152,153
  152 PP=PP-10.0*INTF(PP/10.0)
      MP=1
      GO TO 157
```

```
  153 PP=INTF(PP/10.0)/100.0
      MP=1
      GO TO 157
  150 MP=0
  157 SUMS=SUMS+S
      CALL RAND(PB,PSINAL,PCOSAL,PP,X,Y,Z,AL,AM,AN,JREF)
      IF(AN-2.0)57,57,15
C           AN=3.0 IF ADSORPTION OCCURS
   15 NI=-NI
      AN=0.0
      PB=STOI
      OP=SUMS
      RETURN
C
   57 IF(JREF)51,51,20
C
C           MEASURE TRAJECTORY DISTANCE WITHIN INNER CONE ELEMENT .



   84 IF(NREF-2)201,202,202
  202 S3=S
      S4=ABSF(A/AN)
      SINI=MINIF(S3,S4)
      NREF=1
      PP=PP-SINI
      GO TO 20
C
  201 S5=D-S
      S6=ABSF((A-Z)/AN-S)
      SINI=MINIF(S5,S6)
      PP=PP-SINI
C
C
C           EXAMINE INTERACTION WITH OUTER CONE
C
   20 IF(OSINAL)21,22,21
   22 WO1=1.0-AN*AN
      WO2=AL*X+AM*Y
      WO3=X*X+Y*Y-OB*OB
      IF(K)101,40,40
   21 WO1=1.0-AN*AN*AOCOS*AOCOS
      WO2=AL*X+AM*Y-AN*(OB+Z)*(OSINAL*AOCOS)*(OSINAL*AOCOS)
      WO3=X*X+Y*Y-(OB+Z)*(OB+Z)*OSINAL*OSINAL*AOCOS*AOCOS
      IF(K)101,46,46
  101 IF(WO1)23,23,104
   23 IF(AN)119,120,120
  104 SO=-2.0*WO2/WO1
C       (SO)IS THE TRAJECTORY DISTANCE TO INTERACTION WITH
C      OUTER CONE FROM STARTING POINT IN CONE ELEMENT.
      GO TO 107
   46 IF(OSINAL)47,40,40
   47 IF(WO1)24,42,24
   42 SO=-WO3/(2.0*WO2)
      GO TO 107
   40 IF(WO1)113,113,24
   24 XO=WO2*WO2-WO1*WO3
      IF(XO)113,32,32
   32 SO=(-WO2+SQRTF(XO))/WO1
```

```
  107 IF(SO*AN+Z-A)108,113,113
  108 IF(SO*AN+Z)113,113,31
  113 GO TO 106
  106 IF(AN)119,120,120
  119 X=-Z*AL/AN+X
      Y=-Z*AM/AN+Y


      SUMS=SUMS+Z*SQRTF(1.0+(AL*AL)/(AN*AN)+(AM*AM)/(AN*AN))
      PB=STOI
      OP=SUMS
      RETURN
  120 X=(A-Z)*AL/AN+X
      Y=(A-Z)*AM/AN+Y
      SUMS=SUMS+(A-Z)*SQRTF(1.0+(AL*AL)/(AN*AN)+(AM*AM)/(AN*AN))
      PB=STOI
      OP=SUMS
      RETURN
   31 X=SO*AL+X
      Y=SO*AM+Y
      Z=SO*AN+Z
C
C           COUNT ONE INTERACTION ON INSIDE OF OUTER CONE
      NO=NO+1
      JREF=0
      K=-1
      IF(OP-1.001)160,161,161
  161 IF(MP)162,162,163
  162 OP=OP-10.0*INTF(OP/10.0)
      MP=1
      GO TO 167
  163 OP=INTF(OP/10.0)/100.0
      MP=1
      GO TO 167
  160 MP=0
  167 SUMS=SUMS+SO
      N=XINTF(10.0*ATANNQ(X,Y)/3.1415926+10.0)+1
      HIT(N)=HIT(N)+1
      IF(NO+KT-21)168,169,168
  169 STOI=SUMS
      KT=1000
  168 CALL RAND(OB,OSINAL,OCOSAL,OP,X,Y,Z,AL,AM,AN,JREF)
      IF(AN-2.0)51,33,33
C
C           COUNT ONE ADSORPTION ON INSIDE OF OUTER CONE
   33 NO=-NO
      AN=0.0
      PB=STOI
      OP=SUMS
      RETURN
      END
```

```
      SUBROUTINE RAND3(RI,RO,X,Y,Z,AL,AM,AN,IREF,INAXIS)
C                THIS SUBROUTINE CALCULATES THE COORDINATES AND DIRECTION
C           COSINES, IN A RANDOM FASHION, OF A PARTICLE ENTERING BETWEEN
C           RADII RI AND RO
      B=X
  100 RAD=RI+(RO-RI)*FA01AS(1)
C                NOTE SUBROUTINE FA01AS(1) MUST BE LOADED
    4 BETA=6.2831853071796*FA01AS(1)
      G=RAD*COSF(BETA)
      H=RAD*SINF(BETA)
      IF(INAXIS)22,22,21
C
C           (INAXIS) ZERO GIVES AN INPUT DISTRIBUTION ALONG Z AXIS
C
C            INAXIS=1 INPUT ALONG THE X AXIS
C            INAXIS=2 INPUT ALONG THE Y AXIS
C
   22 X=G+B
      Y=H
      Z=0.0
C
      IF(IREF)7,1,7
    1 VNE=FA01AS(1)
    5 AN=SQRTF(VNE)
      SRV=SQRTF(1.00000-VNE)
    3 URD=FA01AS(1)
      AURA=6.2831853071796*URD
      AL=SRV*COSF(AURA)
      AM=SRV*SINF(AURA)
      XNORM=SQRTF((1.0-AN*AN)/(AL*AL+AM*AM))
      AL=AL*XNORM
      AM=AM*XNORM
      RETURN
C            IF (IREF) NOT ZERO THEN AN CHOSEN BETWEEN 0 AND IREF/1000 DEGREES
    7 IF(IREF-180000)17,17,11
   11 WNE=FA01AS(1)
      VNE=SQRTF(WNE)
      GO TO 5
   17 AN=1.0-FA01AS(1)*(1.0-COSF(FLOATF(IREF)*0.000011111))
      SRT=SQRTF(1.0-AN*AN)
    8 PHI=6.2831853071796*FA01AS(1)
      AL=SRT*COSF(PHI)
      AM=SRT*SINF(PHI)
      XNORM=SQRTF((1.0-AN*AN)/(AL*AL+AM*AM))
      AL=AL*XNORM
      AM=AM*XNORM
      IF(IREF)9,10,10
    9 AN=-AN
   10 RETURN
   21 IF(INAXIS-1)23,23,24
   23 X=B
      Y=H
      Z=G
      GO TO 26
```

```
   24 X=G*B
      Z=H
      Y=0.0
   26 IF(IREF)37,31,37
   31 VNE=FA01AS(1)
   35 BN=SQRTF(VNE)
      SRV=SQRTF(1.00000-VNE)
   33 URD=FA01AS(1)
      AURA=6.283185307179 6*URD
      BL=SRV*COSF(AURA)
      BM=SRV*SINF(AURA)
      GO TO 25
C          IF (IREF) NOT ZERO THEN AN CHOSEN BETWEEN 0 AND IREF/1000 DEGREES
   37 BN=1.0-FA01AS(1)*(1.0-COSF(FLOATF(IREF)*0.000011111))
      SST=SQRTF(1.0-BN*BN)
   38 PHI=6.283185307179 6*FA01AS(1)
      BL=SST*COSF(PHI)
      BM=SST*SINF(PHI)
      IF(IREF)39,25,25
   39 BN=-BN
   25 IF(INAXIS-1)27,27,28
   27 AL=BN
      AM=BL
      AN=BM
      XNORM=SQRTF((1.0-AN*AN)/(AL*AL+AM*AM))
      AL=AL*XNORM
      AM=AM*XNORM
      RETURN
   28 AL=BM
      AM=BN
      AN=BL
      XNORM=SQRTF((1.0-AN*AN)/(AL*AL+AM*AM))
      AL=AL*XNORM
      AM=AM*XNORM
      RETURN
      END
```

```
      SUBROUTINE RAND(B,SINAL,COSAL,P,X,Y,Z,AL,AM,AN,JREF)
C
C                THIS SUBROUTINE CALCULATES THE DIRECTION COSINES OF
C                THE PATH OF THE REFLECTED PARTICLE AND RETURNS THESE
C                VALUES TO SUBROUTINE CONFLO OR RINGFLO
C
C                NOTE FOR A CYLINDER B = RADIUS - NOT TRUE FOR CONE
C
C                FAO1AS(1) CALLS UP A RANDOM NUMBER BETWEEN 0.0 AND 1.0
C                THIS SUBROUTINE MUST BE LOADED
C
      Q=ABSF(P)
  100 PROB=FAO1AS(1)
      IF(Q-PROB)1,2,2
C
C                IF ABSORBTION OCCURS SET AN = 3.0 AND RETURN
C
    2 AN=3.0
      RETURN
C
C
C                BL,BM,BN ARE THE DIRECTION COSINES OF THE REFLECTED
C                PARTICLE PATH W.R.T. AXES AT THE POINT OF REFLECTION
C
    1 VNE=FAO1AS(1)
   32 BN=SQRTF(VNE)
   35 SRVE=SQRTF(1.00000-VNE)
    7 URE=FAO1AS(1)
      AURE=6.2831853071796*URE
      BL=SRVE*COSF(AURE)
      BM=SRVE*SINF(AURE)
C
C                CALCULATE THE CASE OF A CYLINDER SEPARATELY
C
      IF(JREF)24,20,24
   24 BN=-BN
      BM=-BM
      BL=-BL
   20 IF(SINAL)3,4,3
    4 BX=1.0/B
      AL=BX*(BL*Y-BN*X)
      AM=-BX*(BL*X+BN*Y)
      AN=BM
   37 XNORM=SQRTF((1.0-AN*AN)/(AL*AL+AM*AM))



      AL=AL*XNORM
      AM=AM*XNORM
      RETURN
    3 BAT=COSAL/(Z+B)
      ASINAL=1.0/SINAL
C
C                AL,AM,AN ARE THE DIRECTION COSINES OF THE REFLECTED
C                PARTICLE PATH W.R.T. THE MAIN AXES
C
      AL=BAT*(ASINAL*(-BN*COSAL*X+BL*Y)+BM*X)
      AM=BAT*(ASINAL*(-BN*COSAL*Y-BL*X)+BM*Y)
      AN=BN*SINAL+BM*COSAL
   47 XNORM=SQRTF((1.0-AN*AN)/(AL*AL+AM*AM))
      AL=AL*XNORM
      AM=AM*XNORM
   22 RETURN
      END
```

Available from

HER MAJESTY'S STATIONERY OFFICE

49 High Holborn, London, W.C.1
423 Oxford Street, London W.1
13a Castle Street, Edinburgh 2
109 St. Mary Street, Cardiff
Brazennose Street, Manchester 2
50 Fairfax Street, Bristol 1
35 Smallbrook, Ringway, Birmingham 5
80 Chichester Street, Belfast

or through any bookseller.

Printed in England

S. O. Code No. 91-3-18-84