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MONTE CARLO STUDIES OF FREE MOLECULAR GAS FLOW THROUGH VARIOUS VACUUM STRUCTURES

J. N. CHUBB

Culham Laboratory
Abingdon Berkshire

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MONTE CARLO STUDIES OF FREE MOLECULAR GAS FLOW THROUGH VARIOUS VACUUM STRUCTURES

by

J.N. CHUBB

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U.K.A.E.A.
Research Group,
Culham Laboratory,
Abingdon,
Berkshire.

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CONTENTS

ABSTRACT

The rather general Monte Carlo computer program which has been developed for studying free molecular gas flow in axi-symmetric vacuum systems has been used to study the transmission characteristics of a number of structures of interest to vacuum system designers. Structures which have been studied include parallel surfaces, chevron, flat corner chevron and Z type baffles and 'macro' and 'micro' rough walled tubes. It is shown that the optimum included angles for chevron and Z type baffles are 122° and 127° respectively, which give transmission probabilities of 0·28 and 0·2. The unexpected feature of the studies of transmission through rough walled tubes is that the 'macro' rough tubes have transmission probabilities much closer to those of smooth walled tubes than do tubes with only a small scale surface roughening.

Studies of the transmission characteristics of a number of vapour diffusion pumps alone and in combination with two designs of vapour trap, and of combinations of these vapour traps and input tubes, indicate that the characteristics of these structures are not significantly affected by the design of the adjoining structure. Thus, the present Monte Carlo studies lend qualified support to the use of the Oatley equation for combining the transmission probabilities of individual components in composite vacuum structures and systems.

1. Introduction

The Monte Carlo method offers a convenient technique for studying the free molecular gas flow characteristics of basic vacuum structures as well as more complete vacuum systems. Davis (1960), and Levenson, Milleron and Davis (1960, 1964)) used this method to study a number of practical vacuum structures, and supported their calculations with experimental tests. A rather general Monte Carlo computer program has been developed by the present author (Chubb, (1965)) and this has been used to study a variety of complete vacuum systems (Chubb (1965, 1966a, 1966b)). The aim of the present paper is to give the results of some further Monte Carlo studies of vacuum structures and systems to emphasise the practical usefulness and versatility of this method of analysis.

The program used for the present studies was basically similar to that used previously (Chubb (1965)) but simplified in certain respects to speed up calculations and with improvements to the graphical output arrangements. It has also been necessary to correct an error which was present in the original program and affected the input positional distribution of molecules on entry into structures. This error was pointed out by Priestland (private communication, (1967)). The only studies affected by this error were those using relatively large input sources of molecules and recalculated results for such instances are included here.

The calculations were performed on the English Electric KDF 9 computer at Culham with graphical output obtained through the associated Benson-Lehner Model 120 microfilm plotter using a specially developed graphical output language (Larkin, (1967)).

The error values quoted with the results were calculated on the basis that the number of events of interest at any particular surface element, or aperture, would be subject to statistical errors arising from the finite number of molecules introduced into the system, N_1, and the finite number of events at the surface element, on aperture, of interest, N_2. If N_1 and N_2 are not too small, the error in N_2 will be (Chubb, (1966a))

$$\pm\ (1/N_1 + 1/N_2)^{\frac{1}{2}}$$

Although this expression indicates appreciably larger values for the errors than the expression given by (Davis (1960)) this is supported by our own calculations. In the present calculations accuracies have been aimed at which are adequate to distinguish significant practical differences in the characteristics of structures but which do not require excessive computing times. The number of molecular histories studied varied from around 2,000 up to around 10,000. Computing times ranged from 10 to 30 minutes.

2. Results of Calculations

2.1 Parallel Plates

The program allows free molecular gas flow characteristics to be studied between inner and outer surfaces of cylindrical or conical form (Chubb, (1965)). By making the separation between two cylindrical surfaces and the axial length of these surfaces very small in comparison to their mean radius a good approximation is obtained for studying the flow between semi-infinite parallel surfaces. A radial separation between the surfaces of 0·001 was used, with the axial length up to 0·01 of the mean radii between the surfaces. The variation in transmission probability of such a structure with length to spacing ratio for a cosine input distribution is shown in Fig.1.

2.2 Chevron and Z type baffles

Chevron and Z type baffle structures with essentially flat surfaces may be generated, as above, by making the radial separation between conical surfaces very small in comparison to the mean radius. Fig.2 shows the variation of the transmission probability of chevron and Z type baffles with the angle between the surfaces. This figure shows that the optimum included angle between the surfaces is about 122° for a chevron baffle and about 127° for a Z baffle.

Chevron baffle structures are used to inhibit the flow of condensable components from diffusion pumps into vacuum systems and also to inhibit the transmission of radiant heat to cryopumping surfaces. If the effective sticking coefficient or adsorption coefficient of the baffle surfaces is known the transmission probability may be calculated by the Monte Carlo program. For example, a 120° included angle chevron baffle with surfaces having sticking coefficients of 0·9 has a transmission probability of $2{\cdot}45 \times 10^{-3} \pm 0{\cdot}27 \times 10^{-3}$.

A flat corner type of chevron structure has been used in the iron oxide vapour traps developed by Pustovoit at the Kurchatov Institute in Moscow (private communication). [Some features of this type of trap have been described by (Romanoff, (1966))]. Fig.3 shows the variation of the transmission probability of this type of structure with spacing between the plates.

2.3 Rough Tubes

Davis, Levenson and Milleron (1964) showed that the free molecular flow of gas through vacuum ducts could be somewhat reduced by small scale roughening of the duct walls. A few of the structures they studied have been re-examined and the form of these is shown in Figs.4 and 5. Figs.6 and 7 show two types of 'macro-rough' tube designs. The results of studies on these tubes together with Monte Carlo results and Clausing values (Dushman (1949)) for smooth walled tubes are listed in Table 1. The main feature of these results is that the 'micro-rough' tubes have transmission probabilities much further from those of smooth tubes than do tubes with a large scale roughening - 'macro-rough' tubes.

The angular distribution of molecules transmitted through vacuum structures may be examined, as described previously (Chubb (1965)) by attaching a large fully adsorbing hemisphere to the exit aperture of the structure under examination. Distributions for some of the tube structures of Table 1 are shown in Figs.8,9 and 10. Although the accuracy of these distributions is not very high it is clear that there is some modification by surface roughness.

2.4 Vapour Diffusion Pumps and Vapour Traps

The pumping performance characteristics of five different designs of vapour diffusion pumps were examined previously (Chubb (1966a)) to see how these characteristics changed when the gas molecules entered with a cosine input distribution or from either of two designs of test dome. Results obtained after correction of the program error are presented in Table 2. These results now show that within the errors of the calculations these five pumps exhibit the same effective sticking coefficient at their pump mouths whether the molecules enter with a cosine input distribution or from either of the two designs of test dome.

Previous calculations (Chubb (1966a)) indicated that there was good correlation between the pumping performance exhibited at the entrance aperture of diffusion pumps and the performance assessed at the specified gauge locations on the test domes. Some further calculations have been made to see if this conclusion would also apply if the ISO recommended test dome (ISO/TC 112 [London 1965-6] 35 E and F) (Test dome B) was used to measure sticking coefficients at cryopumping surfaces. Fig.11 shows the variation of relative molecular incidence rate with distance up the test dome wall for two diffusion pumps and for plane cryopumping surfaces of 0·7 and 1·0 sticking coefficients. These results indicate that the optimum gauge position changes slightly with the effective sticking coefficient at the pumping aperture, but that the assessment at unity sticking coefficient would be only about 7½% too high with the recommended gauge position.

To see if the above diffusion pumps would exhibit the same effective sticking coefficients in more practical situations a few calculations were made with the pumps combined with two designs of vapour trap and with the pumps combined with a simple input tube of L/R = 10. The two designs of vapour trap are shown in Figs. 12 and 13. The transmission probabilities for a cosine input distribution of the two traps, alone, in combination with input tubes of $L/R = 5$ and in combination with a second trap of the same design, are given in Table 3. The transmission probabilities of individual sections of composite structures are calculated using transparent surfaces across the boundaries between sections to count the numbers of molecules crossing the boundaries without disturbing their trajectories.

The Oatley equation (1957) is often used for combining the transmission probabilities of a number of structures to give an overall transmission probability for a complete system. The application of the Oatley equation relies upon the assumption that the transmission probabilities of individual structures are not affected by the presence of adjoining structures. This assumption is not always valid - as Ballance (1965) showed. The results given in Tables 2 and 3 indicate that the transmission characteristics of these structures are not very much affected by the design of their adjoining structures. If Monte Carlo calculations were used to establish a number of common vacuum structures whose transmission characteristics were not significantly affected by the design of adjoining structures then the Oatley equation could be used to predict the transmission probability of complex practical vacuum systems. This approach would combine the cheapness and simplicity of Oatley equation calculations with the confidence in the performance of individual structures offered by the Monte Carlo method. Where necessary, of course, the whole system would still be studied by Monte Carlo analysis and recent program developments will enable even more complex structures to be studied than formerly - for example, systems involving multiple tee connections and cross-over links. Further work is clearly required to indicate what types of structures are suitable as basic units, to build up data sheets on commonly used vacuum components, and to estimate the magnitude of errors likely to be encountered.

3. Conclusions

The studies described in the present paper demonstrate again the usefulness of the Monte Carlo method for analysing free molecular gas flow in the types of individual components and complete structures likely to be of interest to practical vacuum system designers. Further studies of a number of vapour diffusion pumps with various gas input arrangements indicate that the characteristics of these pumps remain reasonably constant in spite of appreciable changes in the design of adjoining structures. Thus, these Monte Carlo studies provide some qualified support for the common and convenient method of combining the transmission probabilities in composite structures using the Oatley equation.

TABLE 1

TRANSMISSION PROBABILITIES OF ROUGH AND SMOOTH WALLED TUBES

L/R	Clausing Coefficient	Monte Carlo calculations				
		Smooth Tube	Rough Tubes			
			A	B	C	D
1	0·672	0·674 ± 0.008	0·631 ± 0·022	0·611 ± 0·013	0·643 ± 0·016	
1·55	0·573			0·524 ± 0·025		
2	0·5136	0·5125 ± 0·0065		0·452 ± 0·017	0·506 ± 0·009	0·497 ± 0·012
3	0·4205					0·397 ± 0·013
5	0·3146	0·3082 ± 0·0057			0·298 ± 0·022	

TABLE 2

EFFECTIVE STICKING COEFFICIENTS AT MOUTHS OF SEVERAL VAPOUR DIFFUSION PUMPS FOR VARIOUS SOURCES OF GAS INPUT

		Cosine input	Test dome A*	Test dome B⌿	Pump + Trap A	Pump + Trap B	Pump + L/10 tube
0·5 sticking coefficient at vapour jet surface	PUMP 1	0·288 ± 0·014	0·315 ± 0·019	0·307 ± 0·010			
	PUMP 2	0·358 ± 0·017	0·335 ± 0·021	0·348 ± 0·012	0·350 ± 0·017		
	PUMP 3	0·358 ± 0·008	0·372 ± 0·016	0·367 ± 0·016			
	PUMP 4	0·374 ± 0·021	0·366 ± 0·018	0·379 ± 0·013	0·344 ± 0·022		
	PUMP 5	0·395 ± 0·016	0·403 ± 0·020	0·420 ± 0·016			
0·7 sticking coefficient at vapour jet surface	PUMP 1	0·337 ± 0·026	0·329 ± 0·018	0·345 ± 0·007			
	PUMP 2	0·389 ± 0·012	0·374 ± 0·017	0·381 ± 0·012	0·369 ± 0·018		
	PUMP 3	0·450 ± 0·017	0·417 ± 0·023	0·456 ± 0·024	0·453 ± 0·023		0·448 ± 0·020
	PUMP 4	0·426 ± 0·013	0·438 ± 0·019	0·437 ± 0·011		0·444 ± 0·032	0·447 ± 0·021
	PUMP 5	0·450 ± 0·018	0·483 ± 0·020	0·524 ± 0·024		0·467 ± 0·031	0·528 ± 0·021

*Test dome A specified in ISO/TC 112 (Secretariat - 8)8 Figure 9
⌿Test dome B specified in ISO/TC 112 (London 1965-6)35 E and F

TABLE 3

TRANSMISSION PROBABILITIES OF TWO DESIGNS OF VAPOUR TRAP FOR VARIOUS SOURCES OF GAS INPUT

	Cosine input	L/R = 5 tube input	Trap A input
Trap A	0·387 ± 0·011	0·394 ± 0·016	0·356 ± 0·018
Trap B	0·324 ± 0·012	0·311 ± 0·014	

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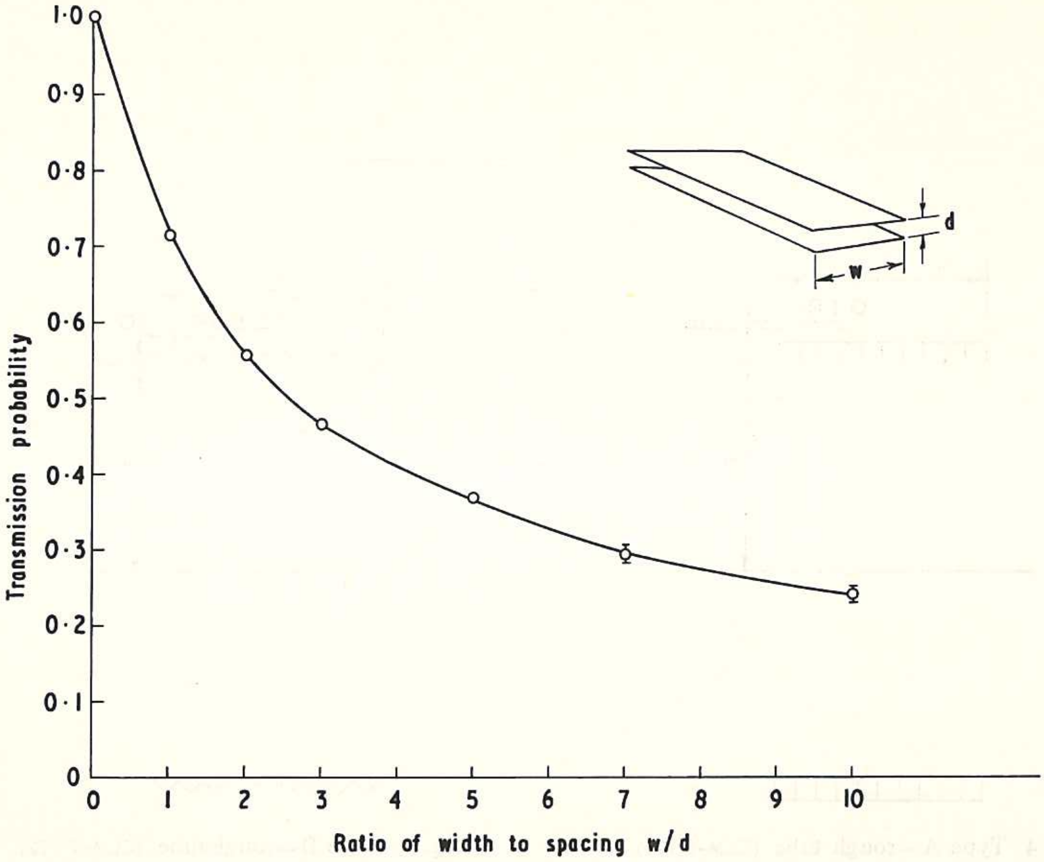

Fig. 1 (CLM-P172)
Transmission of molecules between long parallel surfaces

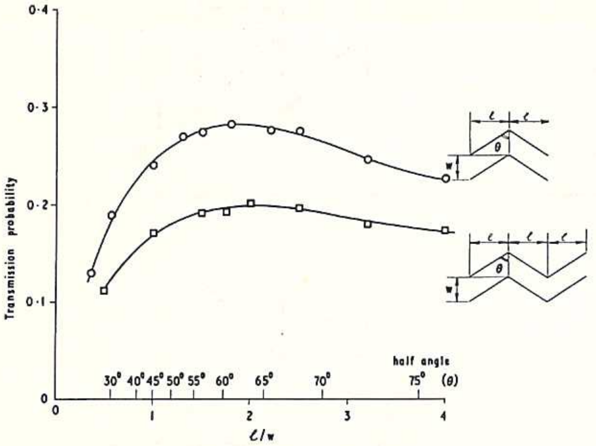

Fig. 2 (CLM-P172)
Transmission characteristics of
Chevron and Z baffle structures

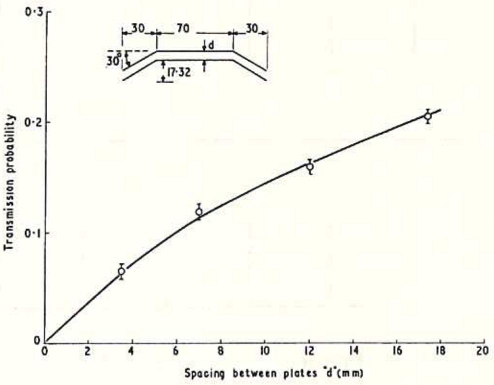

Fig. 3 (CLM-P172)
Transmission characteristics of
flat corner Chevron structure

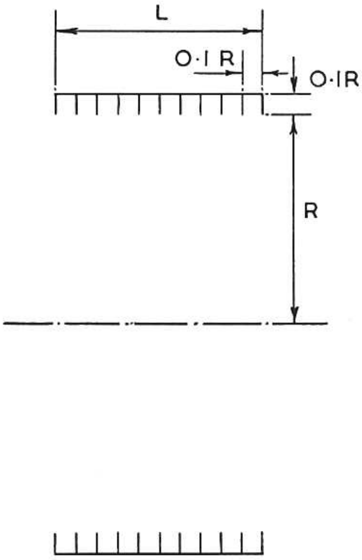

Fig. 4 Type A – rough tube (CLM-P172)

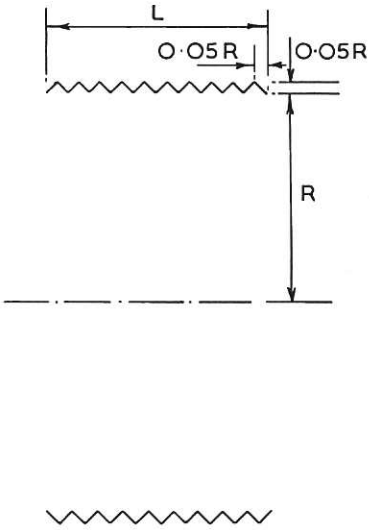

Fig. 5 Type B – rough tube (CLM-P172)

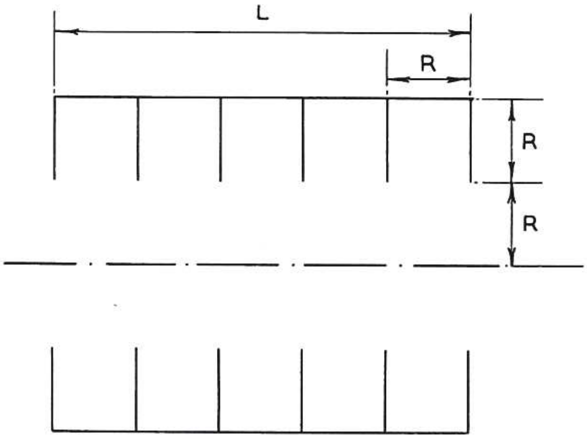

Fig. 6 (CLM-P172)
Type C – Macro-rough tube

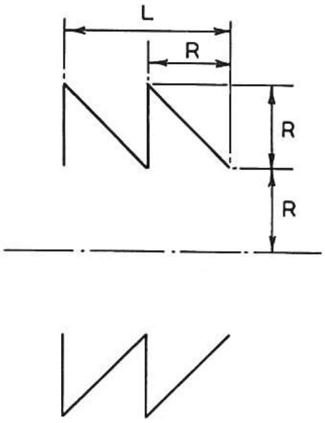

Fig. 7 (CLM-P172)
Type D – Macro-rough tube

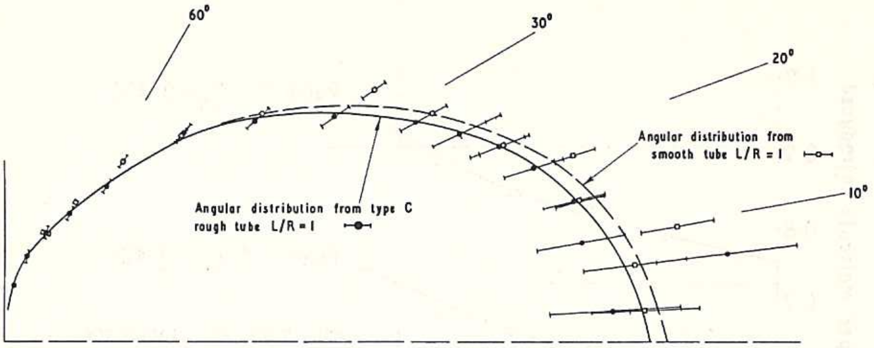

Fig. 8 (CLM-P172)

Angular distribution of molecules from a smooth tube of L/R = 1 and a type C rough tube L/R = 1

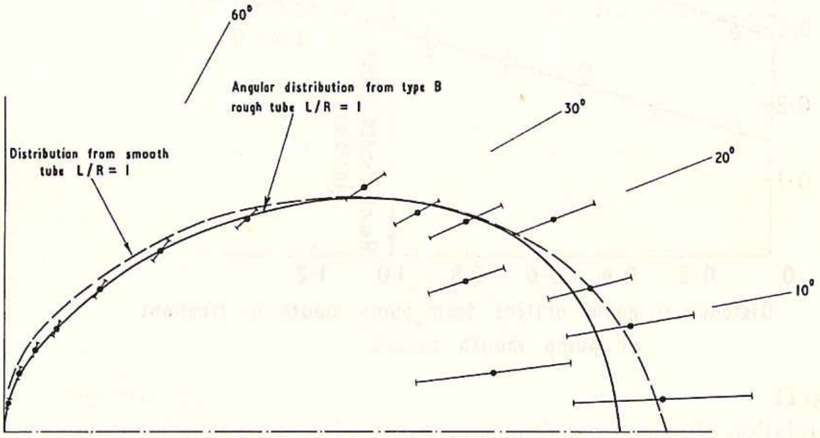

Fig. 9 (CLM-P172)

Angular distribution of molecules from a smooth tube of L/R = 1 and a type B rough tube L/R = 1

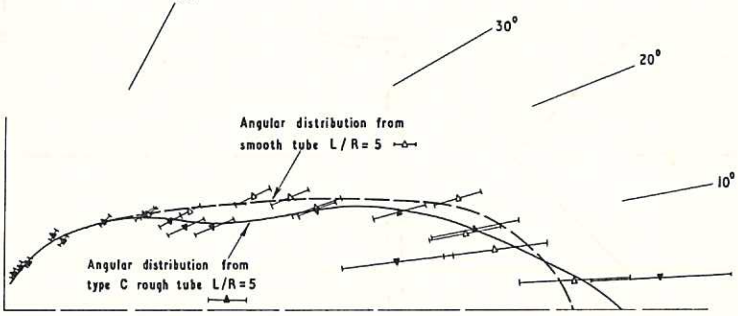

Fig. 10 (CLM-P172)

Angular distribution of molecules from a smooth tube of L/R = 5 and a type C rough tube L/R = 5

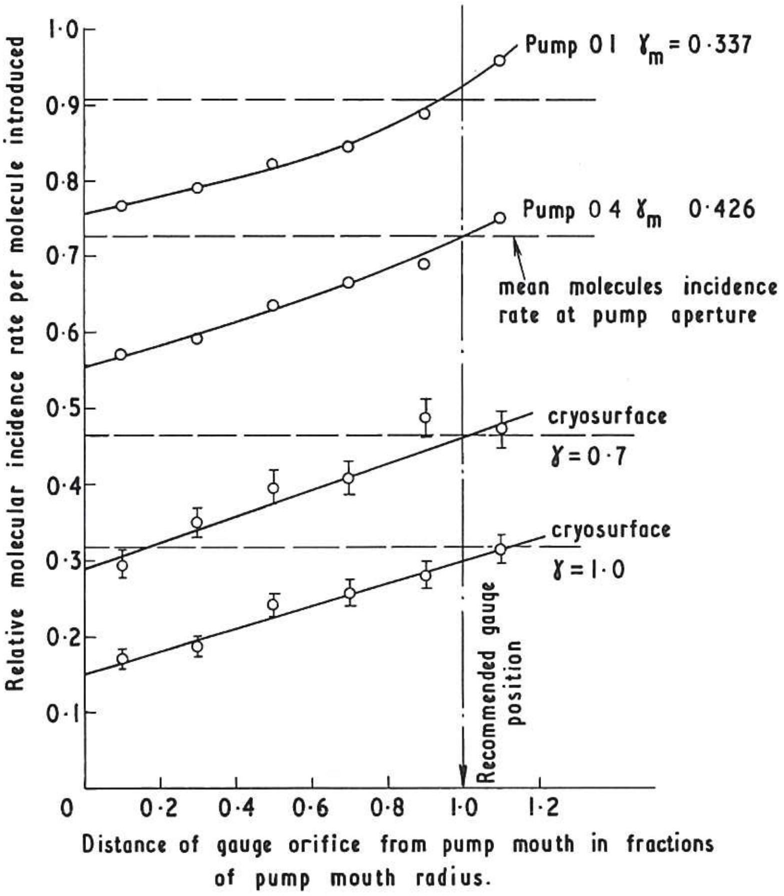

Fig. 11 (CLM-P 172)
Correlation of pumping performance observed at ion gauge location with pumping performance at pump mouth

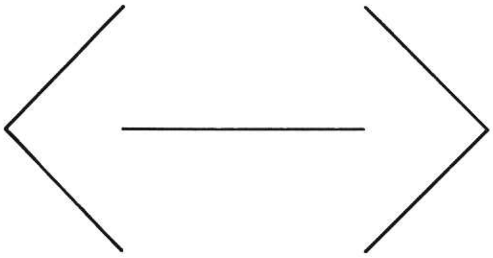

Fig. 12 Type A – vapour trap (CLM-P 172

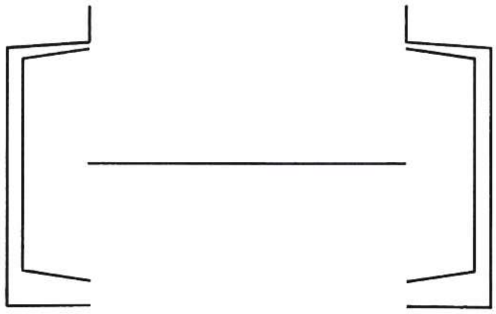

Fig. 13 Type B – vapour trap (CLM-P 172)