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New concepts in molecular gas flow

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This paper will outline several new concepts dealing with molecular flow calculations. One is a simple equation for calculating the "Clausing" transmission probability through circular tubes. A technique will also be demonstrated for developing similar expressions for the short-tube probability of other tube cross sections. Tube conductance will then be compared to transmission probabilities in terms of exit losses, entrance losses, and changes from random gas flow to fully developed tube flow. A format will be presented which assists in converting between short-tube conductance and probabilities. Finally, a correction term is added to Oatley's probability combining equation to compensate for "beaming" effects. This term reduces the normal maximum error for circular tube calculations from 3.7% to 0.28%.

I. INTRODUCTION

The extensive technology available on molecular flow solutions has been reviewed on several occasions (see, in particular Steckelmacher[1]). The current paper is not intended as a review article. However, it will briefly discuss certain important historical developments which are pertinent to understanding several new gas-flow concepts to be presented. We will assume typical molecular-flow conditions, i.e., steady-state flow, constant temperature, random molecular entry to the inlet plane, no gas-to-gas collisions, and a cosine directional distribution following all gas collisions with a wall.

A wide variation of symbols and units has been historically used during the development of vacuum technology. Any attempt to maintain the original nomenclature of the separate contributors would add confusion for the current reader and is not considered warranted. The units and symbols used in this paper will follow the current popular trend. Specifically, Q will be used for the gas throughput in Torr l/s and S for speed in l/s. The conductance C identifies the ratio of the throughput to the total-pressure difference between two points in a system. If P_i and P_j represent two different total pressures, then $C = Q/(P_i - P_j)$, where the pressures are given in Torr. The symbol α has been selected for the molecular transmission probability through any component or group of components connected between two large chambers.

The first equation of interest is that for gas flow through a zero thickness orifice located between two large volumes. The equation is attributed to Knudsen[2] and specifies that the gas flow is proportional to the differential rate at which molecules strike the orifice opening from the two sides

$$Q_{om} = C_{om}(P_1 - P_0) \quad \text{Torr l/s}, \tag{1}$$

with

$$C_{om} = 11.43\,(T/M)^{1/2}a^2 \quad \text{l/s}\,,$$

where subscripts o and m refer to orifice and molecular, respectively. The molecular orifice conductance C_{om} includes the temperature T in Kelvin, the molecular weight M in g/mol, and the orifice radius a in cm. Note that P_1 is the *total* pressure incident on the orifice inlet where total pressure is identified in the classical sense of a pressure measured with the gage looking upstream and including the gas kinetic energy. Static pressure will refer to the pressure measured normal to the flow. Knudsen also developed the asymptotic equation for a very long circular tube:

$$Q_{lm} = \frac{8a}{3l}\,C_{om}(P_2 - P_0)\,, \tag{2}$$

where l is both the tube length in centimeters and a subscript identifying tube flow. This equation was actually first proven many years later by DeMarcus.[3]

Clausing[4] proposed an equation for the more general case of any component connected between two large volumes

$$Q_m = \alpha C_{om}(P_2 - P_0)\,, \tag{3}$$

where α is the transmission probability that a molecule which passes through the inlet plane of the tube, will be transmitted through the tube. Clausing also developed integral equations for the exact solution of α for circular tubes of any length-to-radius ratio and provided a table of approximate numerical values for α vs l/a. These well-known tables are in wide use to this day. More recently, DeMarcus[3] developed mathematical techniques for improved numerical solution of the Clausing integral equations and provided increased-accuracy Clausing-type tables. Cole,[5] using the DeMarcus techniques, further refined the calculations providing tables with from 6 to 9 significant figures. Six-figured Cole values are given in column 2 of Table I. These are recommended as replacements for the limited-accuracy Clausing tables (errors to 3.84%).

Dushman[6] rationalized that, since α must be asymptotic toward both unity and to $8a/3l$ as the length varies from zero to a very long tube, then α can be represented by the expression

$$\alpha = \frac{1}{1 + 3l/8a}\,. \tag{4}$$

He attributed this behavior to the combination of two series conductances: the normal long tube conductance $[C = (8a/3l)C_{om}]$, and a so-called "entrance loss," $(C = C_{om})$. When combined in series, as reciprocals, they yield Eq. (4). We will shortly show that this entrance loss effect becomes an "exit" loss (pressure drop) when total pressure measurements are considered. The magnitude of the error in the Dushman equation is well known, reaching over 12% relative to the Cole data. This is illustrated in the last column of Table I.

TABLE I. Transmission probability data.

l/a	Cole data	Eqs. (10)–(12)	% error	Dushman Eq.	% error
0.1	0.952 399	0.9525	−0.0149	0.9639	−1.20
0.3	0.869 928	0.8707	−0.0924	0.8989	−3.33
0.5	0.801 271	0.8027	−0.1752	0.8421	−5.10
0.7	0.743 410	0.7451	−0.2316	0.7921	−6.55
0.9	0.694 044	0.6958	−0.2538	0.7477	−7.73
1.0	0.671 984	0.6737	−0.2530	0.7273	−8.23
1.2	0.632 228	0.6337	−0.2318	0.6897	−9.08
1.4	0.597 364	0.5985	−0.1908	0.6557	−9.77
1.6	0.566 507	0.5673	−0.1368	0.6250	−10.33
1.8	0.538 975	0.5394	−0.0754	0.5970	−10.77
2.0	0.514 231	0.5143	−0.0107	0.5714	−11.12
3.0	0.420 055	0.4188	0.2874	0.4706	−12.03
4.0	0.356 572	0.3548	0.4862	0.4000	−12.18
5.0	0.310 525	0.3087	0.5935	0.3478	−12.01
6.0	0.275 438	0.2737	0.6368	0.3077	−11.71
7.0	0.247 735	0.2462	0.6384	0.2759	−11.35
8.0	0.225 263	0.2239	0.6136	0.2500	−10.98
9.0	0.206 641	0.2055	0.5726	0.2286	−10.61
10.0	0.190 941	0.1899	0.5221	0.2105	−10.26
20.0	0.109 304	0.1093	−0.0071	0.1176	−7.63
30.0	0.076 912	0.0772	−0.3273	0.0816	−6.14
40.0	0.059 422	0.0597	−0.5023	0.0625	−5.18
50.0	0.048 448	0.0487	−0.6002	0.0506	−4.51
60.0	0.040 913	0.0412	−0.6528	0.0426	−4.01
70.0	0.035 415	0.0357	−0.6816	0.0367	−3.62
80.0	0.031 225	0.0314	−0.6949	0.0323	−3.31
90.0	0.027 925	0.0281	−0.6984	0.0288	−3.05
100.0	0.025 258	0.0254	−0.6960	0.0260	−2.83
1000.0	0.002 646	0.0027	−0.2775	0.0027	−0.51

Kennard[7] suggested a modified equation for very short tubes:

$$\alpha = \frac{1}{1 + l/2a} . \tag{5}$$

This expression was later derived by Santeler *et al.*[8] from probability theory by combining a large number of very short tubes and assuming that each element has a random gas entry. Equation (5) is limited to l/a ratios less than 2 since random gas flow at the entrance changes to fully developed tube flow after a few pipe diameters.

Figure 1, taken from Ref. 8, compares Eqs. (4) and (5) to the Clausing transmission probability. The transition from the short-tube equation for small values of l/a is readily apparent. The bottom sketch further illustrates this concept. At any point in a tube, gas molecules arrive from the inlet end from two different sources. One source is the random gas entering directly through the inlet area through solid angle ϕ. The second source is the molecules transferred from the pressure gradient along the walls of the tube through solid angle θ. The relative fractions of Eq. (4) vs Eq. (5), which are combined at any particular section, depends on the l/a ratio which defines the two solid angles at that section. It is important to note that the change in flow pattern at the inlet (from random gas flow to fully developed tube flow) is totally different and independent from the exit loss (pressure drop) effect to be discussed later.

There is a natural desire to replace the Clausing-type tables with reasonably simple approximate equations. The first attempt was that of Kennard[7] who gave the following approximation to the Clausing data:

$$\alpha = \frac{20 + 8l/a}{20 + 19l/a + 3(l/a)^2} . \tag{6}$$

This is a better approximation than the Dushman equation since the maximum error is reduced to about 5% relative to the Cole tables.

Berman[9] did far better by giving an equation which agrees with the Cole data to 0.13%. The only problem with the Berman equations is the complexity:

$$\alpha = 1 + (l/a)^2/4 - (l/4a)[(l/a)^2 + 4]^{0.5} - N/D , \tag{7}$$

where

$$N = \{[8 - (l/a)^2][(l/a)^2 + 4]^{0.5} + (l/a)^3 - 16\}^2 ,$$

and

$$D = 72(l/a)[(l/a)^2 + 4]^{0.5} - 288 \ln \{l/a + [(l/a)^2 + 4]^{0.5}\} + 288 \ln (2) .$$

Henning[10] gave a solution in the form

$$\alpha = \frac{1}{A + B(l/a)^B} . \tag{8}$$

By selecting special values for parameters A and B, he obtained accuracies to a few tenths of a percent over limited l/a ranges. Unfortunately, several equations are required in order to cover the entire range of l/a from zero to infinity. This is more difficult for a general computer solution than using the more accurate Berman equations.

One intent of the current paper is to introduce a new approximation for the Cole/(DeMarcus/Clausing) data; one which is relatively simple, which covers the entire l/a range, which has a relatively high accuracy, and which is compatible with a new simplified approach to the solution of molecular gas-flow problems to be discussed later.

II. A NEW SHORT-TUBE TRANSMISSION PROBABILITY EQUATION

Evaluation of Fig. 1 suggests that a simple way to obtain a reasonably accurate representation for the transmission probability of a circular tube is to use a mathematical function to transfer between Eqs. (4) and (5) as a function of l/a. One such function is

$$\alpha = \frac{1 + k(l/a)^e}{1/\alpha_1 + k(l/a)^e/\alpha_2}, \tag{9}$$

where α_1 is given by Eq. (5) and α_2 is given by Eq. (4). Note that α approaches the short-tube approximation for small l/a and the Dushman equation for large l/a as required. After substitution of Eqs. (4) and (5) into Eq. (9), a computer search for the best value of parameters k and e to minimize either the maximum absolute error or the maximum percent error in α relative to the Cole data gave:

$k = 0.128\,089$, $e = 1.106\,69$,

Max absolute error $= 0.001\,165$,

$k = 0.168\,958$, $e = 0.935\,413$,

Max percent error $= 0.428\%$.

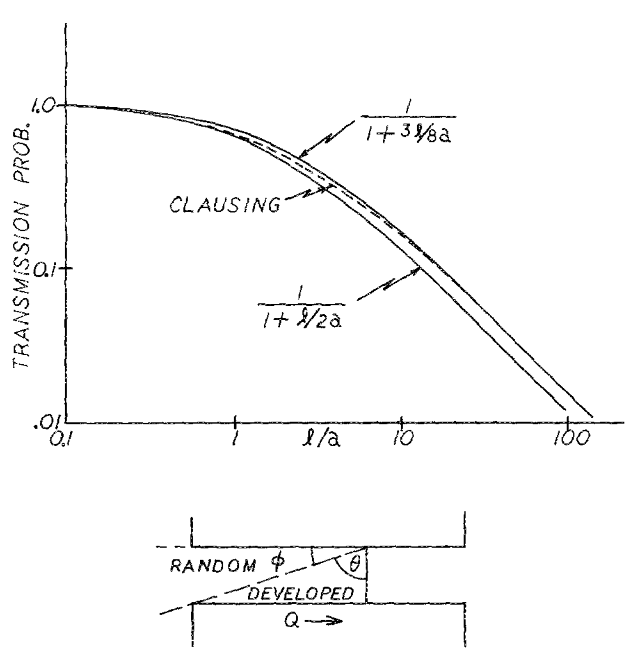

FIG. 1. Transmission probability comparison.

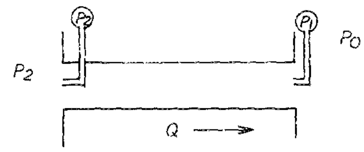

FIG. 2. Tube flow.

After substitution of α_1 and α_2, Eq. (9) may be rearranged into a more usable form

$$\alpha = \frac{1}{1 + 3l'/8a}, \tag{10}$$

with

$$\frac{l'}{l} = \frac{4/3 + k(l/a)^e}{1 + k(l/a)^e}, \tag{11}$$

where either pair of k and e values may be used to obtain the stated accuracies. Note that a reasonable and simplifying compromise is to let $k = 1/7$ and $e = 1$. This results in a further simplification of Eq. (11) to

$$\frac{l'}{l} = 1 + \frac{1}{3 + 3l/7a}. \tag{12}$$

The foregoing change increases the maximum error from 0.43% to 0.7%, which is probably more accurate than required for most purposes. A tabulation of the computed values of the transmission probabilities and their accuracies for Eq. (10) and (12) is given in columns 3 and 4 of Table I.

Equation (10) has the familiar form of the Dushman equation except with an equivalent length l' in place of the true length l. This format allows us to separate the tube conductance from the exit conductance.

III. THE CONDUCTANCE EQUATION OF A CIRCULAR TUBE

Transmission probability identifies the relationship between the flow through a component connecting between two large volumes and the pressure drop between the two volumes; including the pressure drop at the tube exit. What, then, is the relationship between the flow and the pressure drop for just the tube or for any section of the tube? Consider Fig. 2, which illustrates the flow through a tube connecting between two large volumes. This figure contains three different pressures:

$P_2 =$ the normal *total* pressure incident on the tube inlet;

$P_1 =$ the *total* pressure at the tube exhaust measured inside the tube proper. (Note that this pressure is the same as the inlet *total* pressure for gas flow through an orifice.);

$P_0 =$ the *total* pressure in the downstream volume.

Pressure P_0 may be arbitrarily set as close to zero as we desire by using sufficiently high-speed pumping on the exhaust volume; however, P_1 can never be set to zero in a flowing system. A positive gas pressure is required at P_1 in order to exit the gas from the tube. In fact, since the gas flow through the exit equals the gas flow through the tube, the total pressure at the exit can never be less than Q_{lm}/C_{om}; the gas flow through the tube divided by the conductance of an orifice of the same area as the tube. We will select the gas flow through the tube to be given by

$$Q_{lm} = \beta C_{om}(P_2 - P_1)\,. \tag{13}$$

Eliminating pressure P_1 between Eqs. (1) and (13) and setting $Q_{lm} = Q_{om} = Q_m$ in Eq. (3) results in

$$1/\alpha = 1 + 1/\beta\,. \tag{14}$$

This is Dushman's combination of two series components except that the entrance loss is shown to be a pressure drop at the exit when using total pressure measurements.

Combining the foregoing concepts, we suggest that gas flow through a circular tube can best be represented by a tube flow from P_2 to P_1 in which there is a steady change in the inlet gas flow pattern from a random gas flow conductance $(2a/l)C_{om}$ at the entrance to a fully developed tube conductance $(8a/3l)C_{om}$ for long lengths. This behavior can be represented by

$$Q_{lm} = \frac{8a}{3l'}C_{om}(P_2 - P_1)\,, \tag{15}$$

where the equivalent length l' is given by Eq. (11) or Eq. (12). In the event that the tube exists to a large volume, there is an additional exit pressure drop from P_1 to P_0, given by Eq. (1). Eliminating P_1 between Eqs. (1) and (15) gives Clausing's transmission probability relationship, Eq. (3), with α given by Eq. (10). This approach allows us to separately identify the tube conductance βC_{om}, the exit conductance C_{om}, and the overall transmission probability α.

A simple example may serve to clarify the foregoing. Figure 3 illustrates a pump connected through a short tube to a large chamber. We will assume that the tube has a length of 5 cm and a radius of 2.5 cm. The value of C_{om} for air at 300 K would be 229.8 l/s. We will assume that the pump has a net speed of 100 l/s (equivalent to a Ho coefficient of 0.435).

In order to calculate the net system speed in the current approach, we first compute the equivalent length of the tube ($l' = 6.296$), from Eq. (12) and use this to calculate the tube conductance $(8a/3l')C_{om} = 243.3$ l/s. This is combined with the pump speed as reciprocals to get $1/100 + 1/243.3 = 1/70.9$.

In the conventional approach, one would first look up the short tube transmission probability $\alpha = 0.514\,231$ and multiply by C_{om} to get a total transmission conductance of 118.2 l/s. The key step is to then subtract, as reciprocals, the exit conductance of 229.8 l/s in order to get the tube-only conductance of 243.3 l/s. As before, this conductance is then

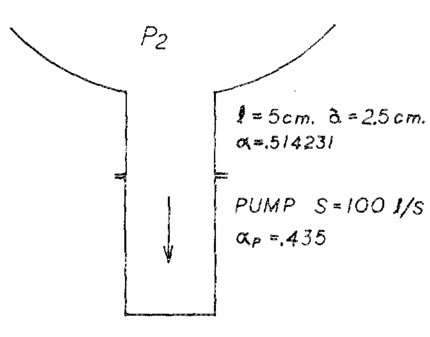

FIG. 3. Pump and tube combination.

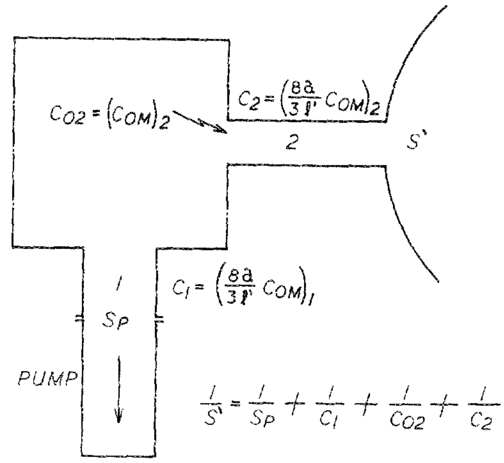

FIG. 4. System speed.

combined with the pump speed to get the net system speed 70.9 l/s. Failure to subtract the exit conductance would result in a tube conductance of 118.2 l/s. If this is combined with the pump speed of 100 l/s, the result is an erroneous system speed of 54.2 l/s, a 23.6% error.

In this example, the correct speed can also be obtained by combining the tube transmission probability with the pump Ho coefficient in the manner of Oatley[11] ($1/0.514231 + 1/0.435 - 1 = 1/0.3083$). The net speed is then obtained from $0.3083\, C_{om} = 70.9$ l/s. Note, however, the Oatley equation should not be used when the tube exits to a large volume.

The principal problem for most users is clarifying the differences between exit and entrance pressure drops and understanding when to make which type of correction. The currently proposed approach removes these uncertainties since the tube conductance is directly calculated, independent of any end effects or transmission probabilities. The system schematic of Fig. 4 further illustrates this point. Tube 1 is the same as the prior example with no exit loss. We assume random gas entry to Tube 1, hence, the tube conductance is $C_1 = [(8a/3l')C_{om}]_1$. The second tube has both a random-gas-entry tube conductance $C_2 = [(8a/3l')C_{om}]_2$, as well as a separate exit conductance $C_{o2} = (C_{om})_2$. The net system speed in the main chamber is easily defined by $1/S = 1/S_P + 1/C_1 + 1/C_2 + 1/C_{o2}$. No question exists as to which short tube transmission coefficient should be corrected for an end effect or whether to use the reciprocal conductance equation or the Oatley probability equation.

The techniques outlined in this report can also be applied to noncircular tube cross sections. Long-tube, molecular-flow equations are already available for a variety of tube sections. The equation for a very short section of the same cross section can be derived from probability theory (see Ref. 8). If a set of data can then be obtained, either by experiment, by Monte Carlo computer analysis, or by integral equation solution, then a transition equation can be written and curve fitted to produce an equation with a good empirical fit over the range of (l/a) equal zero to infinity. Several such solutions are currently in process and will be reported on as they become available. Computer programs for the generalized molecular flow solution of simple multicomponent systems have also been written and will be published. Numerous complications still cloud many of the more complex issues.

Further consideration of the exit behavior in gas flow through vacuum components points out serious difficulties in defining the conductance of components for which we have only theoretical or measured "transmission probabilities." These situations are similar to the Clausing short-tube problem. The reported transmission probabilities of typical vacuum components such as chevrons and H type traps generally include an exit loss. This is certainly true for Monte Carlo calculations where the transmission is based on the molecule striking the exit plane of the component. It is equally true for experimental transmission probabilities where pressures P_2 and P_0 are measured in large volumes at each end of the component, as illustrated on Fig. 5(a).

The product of the transmission probability and the orifice conductance C_{om} results in a combined transmission conductance in the same sense as αC_{om} for a circular tube. Any ensuing calculations are valid only as long as the calculated conductance is used in the same manner, i.e., the gas flow must exit to a large volume. If the trap exits to a tube or to a pump such as in Fig. 5(b), then an exit loss must first be subtracted from the component transmission conductance. The problem is even more complex when the trap exists to an intermediate diameter tube; larger than the trap opening yet not large enough to be a full exit loss [see Fig. 5(c)]. The problem of partial exit losses may be handled in several different ways but further work is required. The principal intent at this point is to indicate the nature of the problem to those individuals having sufficient interest to pursue the matter further.

IV. COMBINING PROBABILITIES

One of the classical problems in molecular flow calculations is that of the beaming effect when combining two conductances in series. Dayton,[12] among others has discussed the fact that the gas exiting the first tube does not produce a random gas entry into the second tube. Under this condition, the transmission probability for the second tube is different from the normal value it has for random gas entry.

This problem can also be visualized by considering the nature of the changing gas flow in a short tube. As we have already seen, the tube conductance is given by $8a/3l'$. Those Δl segments very close to the inlet have a nominal conductance of $2a/\Delta l$, while the segments well removed from the inlet have incremental conductances equal to $8a/3\Delta l$. If we divide a tube into two equal lengths, it is apparent that the half-length closet to the inlet has a lower conductance than the one which is further removed from the inlet. It follows that we cannot obtain the correct composite answer by the *normal* combination of two tube sections each having random-gas-entry conductances.

A new approach is to add a correction factor to the Oatley equation[10] to give

$$\frac{1}{\alpha} = \frac{1}{\alpha_1} + \frac{1}{\alpha_2} - 1 + X, \tag{16}$$

where X is any function of α_1 and α_2 which satisfies the equation. In order to solve for X over the complete range of probabilities, we need to first select an equation format with a minimum number of coefficients and then do a computer curve fit to evaluate the coefficients. The final result is shown on Fig. 6, which gives the correction factor X plotted against

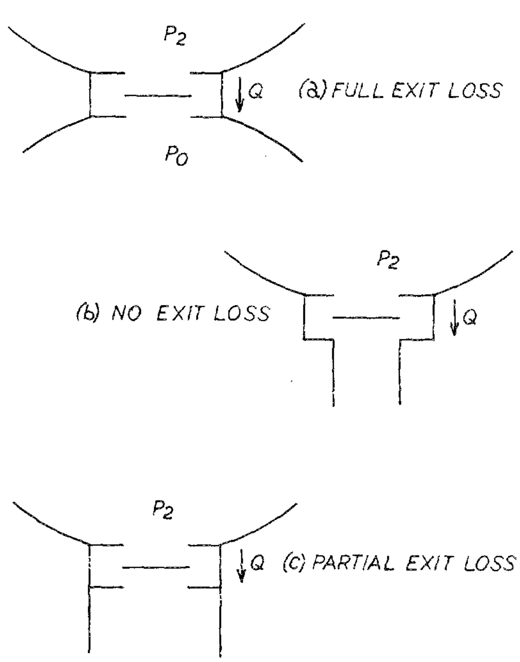

FIG. 5. Trap transition probabilities.

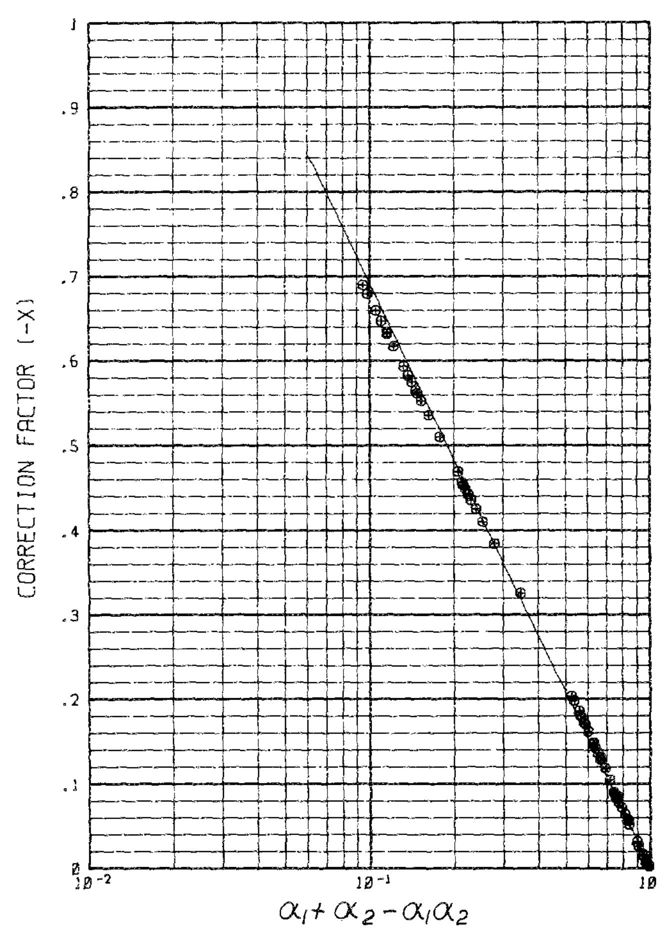

FIG. 6. Beaming correction.

$\alpha_1 + \alpha_2 - \alpha_1\alpha_2$. The excellent curve fit is immediately apparent from the graph. A least squares curve fit gives

$$X = 0.291\,91 \ln (\alpha_1 + \alpha_2 - \alpha_1\alpha_2) - 0.005\,16\,, \qquad (17)$$

with correlation coefficent $R^2 = 0.999\,486$. For further simplicity Eq. (17) can be approximated by

$$X = 0.3 \ln (\alpha_1 + \alpha_2 - \alpha_1\alpha_2)\,. \qquad (18)$$

When Eq. (18) is substituted into Eq. (16), we obtain an improved equation for the transmission probability of two circular tubes in series

$$\frac{1}{\alpha} = \frac{1}{\alpha_1} + \frac{1}{\alpha_2} - 1 + 0.3 \ln (\alpha_1 + \alpha_2 - \alpha_1\alpha_2)\,. \qquad (19)$$

The maximum error in α calculated from Eq. (19) is only 0.282% relative to the Cole data. This is more than a 13 to 1 improvement relative to the 3.7% error which results from using the Oatley equation. It would be nice to conclude that this simple expression would fit other probability combinations such as chevron traps, but this is obviously not so. It may prove to be a good fit for combining rectangular or annular tubes or other geometries, where the gas flow moves steadily from a random behavior at the entrance to a fully developed flow in longer lengths, but it can hardly apply for combinations where each of the components has randomizing elements in its interior. An example of this would be placing two H-type traps in series. In this case, the randomizing effect of the central baffle suggests that the uncorrected Oatley equation would be more accurate.

V. SUMMARY

The lack of clarification between total versus static pressure has led to numerous misunderstandings in vacuum technology. Most of our measurements are static pressure measurements, yet our basic equations for orifice and tube flow can be interpreted as either static or total pressures. This problem has led to differences in pump speed standards between the AVS and other vacuum societies. When we consider total pressures, it becomes obvious that the total pressure at the exhaust of a tube is closely related to the gas flow through an orifice. This explains the fact that a single tube connected between two large volumes has a conductance that can be represented as the combination of a tube conductance and an exit conductance. The tube portion has a changing conductance pattern at the inlet relating to the change from random gas flow to fully developed flow in long lengths. An equation has been presented for the separate calculation of the tube-only conductance, and methods of using this concept in system calculation have been demonstrated.

In addition, a correction has been developed for combining two circular tubes by the Oatley method. Further work is required to apply this type of solution to combining other molecular flow geometries.

Similar new concepts for exit losses in viscous flow have been developed and will be considered in a companion paper also presented at this conference. The separate solution of orifice and tube flow for the molecular-to-viscous transition region has also been developed. This has resulted in a relatively simple computer program for calculating gas flows and pressure drops in short and long tubes for any pressure region. This information will be published in the near future.

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