Comparison between Monte Carlo and analytical calculation of the conductance of cylindrical and conical tubes

J. Gómez-Gonía)
Departamento de Física Aplicada a las Tecnologías de la Información, EUII de Telecomunicación, Universidad Politécnica de Madrid, Crtra. de Valencia, km 7, E-28031 Madrid, Spain

P. J. Lobo
Servicios Informáticos, EUII de Telecomunicación, Universidad Politécnica de Madrid, Crtra. de Valencia, km 7, E-28031 Madrid, Spain

(Received 29 October 2002; accepted 24 February 2003; published 2 July 2003)

The accurate calculation of transmission probabilities of ducts in the molecular flow regime has become a need of vacuum standards on the ultrahigh vacuum region. The usual approach is to simulate a molecular flow of molecules with a Monte Carlo method, because of the difficulties that arise trying to find a solution of the Clausing integral equation in a system of a given geometry. As modern computers increase their speed, the accuracy of Monte Carlo methods is getting higher. It is therefore important to compare simulation results with data obtained by other methods to check that pseudorandom numbers generated are uniformly distributed and not correlated. We have applied both a Monte Carlo method and numerical methods to solve the Clausing integral equation for cylindrical and conical tubes. Both Monte Carlo and numerical methods are consistent within estimated uncertainties. In the case of conical ducts, we obtain values which agree very well with values found in the literature and with uncertainties several orders of magnitude smaller. In the case of cylinders, very accurate transmission probabilities are obtained solving numerically the Clausing integral equation. Comparing with other values found in the literature using a variational method, our values are near the upper bound and quite far away from the lower bound. © 2003 American Vacuum Society.

I. INTRODUCTION

The calculation of the transmission probabilities of vacuum ducts with high precision has interest in metrology and in molecular beam formation studies. This high precision is required to estimate the conductance in dynamic expansion vacuum gauge calibration systems.

In this work we have calculated the transmission probabilities of conical and cylindrical ducts, using both numerical and Monte Carlo methods. We have determined these values with a very high accuracy and compared with values published in the literature.1–3

II. THEORETICAL BASIS

A. Molecular flow

In a previous article4 the characteristics of the calculation of transmission probabilities under molecular flow conditions were described. The basic assumptions are:

1. the flow is assumed to be molecular, i.e. there are no collisions between gas molecules;
2. the flow is assumed to be steady;
3. the adsorption of molecules on the system surface is neglected;
4. molecules have equal probability of entering at any point at the entrance of the duct and they arrive with a distribution of directions according to a cosine law; and
5. the collisions with the system walls are taken as if gas molecules are diffusely reflected, i.e., their velocity directions follow a cosine law.

These conditions have to be applied both for Monte Carlo and for numerical calculation of transmission probabilities.

B. Monte Carlo calculation of Clausing factors

The computer program uses a Mersenne–Twister random number generator.5 The generated pseudorandom numbers are uniformly distributed and are not correlated in the range of numbers we need to perform the simulation. The uncertainties are calculated using the standard deviation σ of a binomial distribution, that can be approximated by Eq. (1), when N is large enough

\[ \sigma = \sqrt{\frac{W(1-W)}{N}}, \]

where W is the transmission probability and N is the number of molecules generated. We have taken an uncertainty of ± 2σ, thus a confidence level of 95%.

C. Numerical calculation of Clausing factors

The theory of transmission probabilities (or Clausing factors) through cylindrical tubes was developed by Clausing6 and reformulated for conical tubes by Iczkowski.3 For com-
With the formalism of Clausing, we can define, \(w_{sr}\), that is inside the cone as the cross section perpendicular to its axis, we can define the area of the plane the wall of the tube. Cutting the cone with just one plane \(r\) parallel planes close to each other, we obtain a "ring" as

From \(w\) parameters, we can calculate the end radius \(x\) as the molecule entering the cone at \(w\) and the rebounding from the surface of the cone at the \(w\) of the function \(w\) is not a continuous function when \(x = y\). The resulting integral equation is

\[
W' = w_{ss}(L, 0) + \int_0^L w_{sr}(L, y)[1 - w(y)]dy.
\]

For cylinders, defined probabilities \((w_{rs}, w_{rr}, w_{sr}, w_{ss})\) are simpler, because \(R\) is constant. In this case, the expressions given by Iczkowski \(et al.\)\(^3\) coincide with Clausing expressions, given in Ref. 6.

### III. RESULTS AND DISCUSSION

#### A. Conical ducts

In the case of conical ducts, the probabilities \(w_{sr}, w_{rs}, w_{rr}\), and \(w_{rr}\) are not continuous and it is necessary to calculate the transmission probabilities using a method described by Iczkowski.\(^3\) Clausing integral equation [Eq. (2)] is solved by a Gauss–Legendre quadrature with \(n\) points. With this approximation, the integral equation can be converted into a system of \(n\) linear equations. The Clausing integral equation has to be rewritten, because the kernel \(w_{rr}(x, y)\) is not a continuous function when \(x = y\). When the resulting integral equation is

\[
w(x) \left[1 - \int_0^L w_{rr}(x, y)dy\right] = w_{rs}(x, L) + \int_0^L w_{rr}(x, y)x[w(y) - w(x)]dy.
\]

Once this system is solved, we will obtain a set of points \(\{x_i, i = 1,n\}\) between 0 and \(L/R_0\) and the approximate values of \(w\), \(\{w_i, i = 1,n\}\) evaluated at every \(x_i\). With these approximate values, \(W\) and \(W'\) are evaluated from Eqs. (8) and (9). We have performed these calculations using figures with 80 digits precision, because due to the discontinuity on the kernel of the equation, using double precision numbers (i.e., 16 digits precision) is not enough to make an accurate calculation. We have determined that our results are not modified using representations up to 200 digits. The libraries used to increase the precision were written by Haible and Kreckel\(^7\) and the algorithms to obtain Gauss–Legendre quadrature and to solve a system of linear equations are described in Ref. 8.

To obtain the Clausing factors, we have computed values of both \(W\) and \(W'\) for different ratios length to aperture radius \((L/R_0)\) and for a number of points \(n\) of 200 and 300. These numbers were found to give the best relation between accuracy and computing time. The accuracy of the calculations was determined comparing the obtained values of \(W\) with those calculated using \(W'\). Both values are related by the following equation:

\[
W_{calc} = W' \left(1 + \frac{L}{R_0} \tan \alpha\right)^2.
\]

Using these values of \(W_{calc}\), we take the calculated value of \(W\) as the mean value of \(W\) and \(W_{calc}\) for 200 and 300 points. The uncertainty we quote is the maximum difference between these values increased to the next decade, i.e., \(1.2 \times 10^{-11}\) is finally \(1 \times 10^{-10}\).

The values of the transmission probabilities are listed in Table I. We have written both numerical and Monte Carlo values. The numerical values have an uncertainty of \(\pm 1\) in
Compared with values by Iczkowski et al., the only discrepancies correspond to the apex angles of 1°, 5°, 10°, and 60°, while Iczkowski et al. give 0.9955 (±1 in the last figure). However, at the same point, our calculation agrees well with the value obtained by Szwemin and Niewinski, using a Monte Carlo simulation. Their value is 0.995 641 60±8.7×10⁻⁷.

For $L/R_o$ of 10 and for angles of 5° and 10° we obtain 0.408 601 27 and 0.580 299 24 (±1 in the last figure), while Iczkowski et al. quote 0.408 600 and 0.580 298, respectively (±1 in the last figure). In all these three cases, the discrepancy is small because if we take the same number of significant figures as Iczkowski et al., we would coincide with their calculations.

For an angle of 1° and a ratio $L/R_o$ of 10, the deviation is higher. We obtain 0.236 831 67 (±1 in the last figure), whereas Iczkowski et al. have 0.236 829 (±1 in the last figure).

Monte Carlo data coincides well with numerical results, but the calculated uncertainties are higher than those from Iczkowski et al., so that no conclusions can be drawn from this comparison. Our data agree well with that of Szwemin and Niewinski, except for an apex angle of 40° and $L/R_o$ of 10 in which we quote for the numerical method a transmission probability of 0.960 081 77 with last figure uncertain and Szwemin and Niewinski give 0.960 068 5±2.8×10⁻⁶. At this point, Icz-
kowski et al.\textsuperscript{3} give 0.960 08 (± 1 in the last figure), which is consistent with our result.

### B. Cylindrical ducts

In the case of cylinders, the probabilities $w_{xx}$, $w_{rr}$, and $w_{rr}$ are continuous so that it is possible to solve numerically Clausing integral equation [Eq. (2)] using an algorithm developed by El-gendi\textsuperscript{10} implemented by the Numerical Algorithm Group (NAG) function D05ABF.\textsuperscript{11} This function is able to solve a Fredholm integral equation of the second kind with a smooth kernel.

In this algorithm, the solution of the equation is approximated by a Chebyshev series of order $n$, so that it can be written in the form

$$w(x) = \sum_{n=0}^{N} c_n T_n(x), \quad (7)$$

where ‘$\sum_{n=0}^{N}$’ indicates that the first term is halved in the sum.

Once the Clausing integral equation is solved, we can compute the transmission probability $W$ using Eq. (3) for different number $n$ of Chebyshev polynomials and several number $m$ of points to evaluate the numerical integral. The accuracy of the method is estimated by calculating the transmission probability $W$ for different numbers $n$ of Chebyshev polynomials and with different number of points $m$ to calculate the integral. We have done this systematically for 3000 and 5000 Chebyshev polynomials and for $1 \times 10^6$ and $1 \times 10^7$ points to calculate the integral expressed in Eq. (3). To check the consistency of the method we also calculate $W'$ from Eq. (4). In the case of cylinders $W$ has to be the same as $W'$ because the transmission probability of the cylinder does not depend on the circulation sense of molecules. Any differences between $W$ and $W'$ come from numerical errors. The uncertainty is calculated as the maximum value of the difference between calculated $W$ and $W'$ with 3000 and 5000
Chebyshev coefficients and $1 \times 10^6$ and $1 \times 10^7$ points to calculate the integral. The final value of the uncertainty is increased to the next decade, i.e., $1.2 \times 10^{-11}$ takes the final value of $1 \times 10^{-10}$.

The values of the transmission probabilities are shown in Table II, where we show the numerical results obtained using the same method applied for conical ducts for the same ratios $L/R$ as Iczkowski et al. (Method 1 in Table II) and those obtained by the El-gendi algorithm described above (Method 2 in Table II). They are accurate within ±1 in the last figure. These uncertainties are very small as compared with previous data, ranging from $1 \times 10^{-11}$ to $1 \times 10^{-8}$ of absolute uncertainty. This corresponds to a relative uncertainty from $1 \times 10^{-11}$ to $4 \times 10^{-6}$. We also give our Monte Carlo simulation results using a number $N$ of molecules and taking the uncertainty as $2\sigma$, as described in Sec. II. Comparing the data obtained by these three methods, all of them agree within estimated uncertainties. They also agree with Monte Carlo simulation results of Szwemin and Niewiński.9

The table also includes data from Cole1,2 using variational techniques. In his calculation, Cole quotes lower ($L$) and upper ($U$) bounds of the transmission probabilities. The mean value is $(U+L)/2$ and the uncertainty is $(U-L)/2$. These values are shown in Table II.

We compare our data to Cole data1,2 in Fig. 2, where the difference between our numerically calculated value (by Method 2), our Monte Carlo simulation results, and the mean value of Cole data1,2 are shown. We also show the difference between the upper bound and the mean value of Cole calculation.1,2 Although this last difference is given at discrete points, we have joined them with lines for clarity. The difference between the lower bound and the mean value is not drawn but it is symmetric to the upper one, with respect to the abscissas axis.

From the figure, we can see that our values agree quite well with Cole upper bound, as already pointed out by Szwemin and Niewiński.9 This was also previously found by Neudachin et al.12

All our results agree with those of Cole,1,2 except for $L/R=1000$. In this case, using an approximation by 3000 and 5000 Chebyshev polynomials we observe a big difference between calculated $W$ and $W'$. To understand this discrepancy, we have performed a series of approximations using from 500 to 10,000 polynomials with a step of 500. We have studied the convergence of calculated values of only $W$ and established that a convergence is found at 7000 polynomials. We then take the average of $W$ calculated with 7000–10,000 polynomials and estimate the uncertainty taking the maximum difference between them. This leads to the number and the accuracy of Table II. This number is not compatible with Cole data, but it is compatible with our Monte Carlo simulation result, as seen both in Table II and in Fig. 2. We would need further study to understand this discrepancy. The origin could be either that we do not have enough precision and an algorithm with a larger number of digits is needed or that the polynomial approximation starts to fail, because of the long length of the duct.

IV. CONCLUSIONS

We have calculated the transmission probabilities for cylindrical and conical ducts with numerical and Monte Carlo simulation methods, assuming a molecular flow regime. All methods agree within estimated uncertainties.

In the case of conical segments, using a numerical method based on Gauss–Legendre quadrature and subsequent resolution of a linear system of equations, we obtain transmission probabilities with uncertainties that are several orders of magnitude smaller than previously published data.

In the case of cylindrical ducts, besides the method described above, the solution can also be approximated with a series of Chebyshev polynomials. The values obtained with both methods have uncertainties which are several orders of magnitude smaller than previously published data. The only discrepancy appears for long tubes, where more study is needed to properly estimate the uncertainty.

ACKNOWLEDGMENTS

The authors want to thank Dr. I. A. Rocha for his help with integral equations. This work has been supported by the Spanish Ministry of Science and Technology under Grant No. DPI2000-3199-E.

7B. Haible and R. Kreckel, CLN, a Class Library for Numbers (http://www.ginac.de/CLN/).
8W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, Nu-
merical Recipes in C: The Art of Scientific Computing, 2nd ed. (Cam-
www.nag.co.uk.
17, 848 (1972).