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The correct and incorrect generation of a cosine distribution of scattered particles for Monte-Carlo modelling of vacuum systems

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Abstract

Computer modelling of vacuum systems is often performed using the Monte-Carlo technique. One of the assumptions frequently made is that molecules originating at the boundaries of the system have a "cosine distribution". The nature of this distribution is occasionally misinterpreted and consequently, the molecular distribution is physically incorrect.

This article describes the main point of confusion by firstly stating the cosine law and describing one possible method of "generating" the correct distribution. It goes on to describe the distribution that results from the most common misinterpretation of the cosine law. This is illustrated by quantifying the effect on the modelled conductance for circular cylinders of various lengths.

Keywords: Monte-Carlo; Cosine distribution; Gas scattering

1. Introduction

The availability of cheap and flexible computer power has made the technique of Monte-Carlo simulation widely accessible. However, the correct conditions and rules that are appropriate to the physical situation being modelled must first be established before simulation can commence. It is at this stage that Monte-Carlo simulations can go wrong, particularly when the person implementing the model is not fully conversant with any intricacies or counterintuitive details. The author is aware of several examples of this phenomenon in the implementation of the cosine law for the scattering of molecules from a surface. This paper discusses the cosine law and demonstrates how to implement it correctly before going on to describe the common misinterpretation of the law and the consequences for modelling the conductance of tubes.

2. The cosine law

In terms of gas molecules leaving a surface, the cosine law (sometimes called the Knudsen cosine law) can be stated [1] as follows:

> the molecular flux dn across a plane surface element A, due to all molecules having velocity vectors with directions within a small solid angle dω, whose axis makes an angle θ with the normal to A, is given by the cosine law formula.

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Hence

$$dn = \left(\frac{Nv_a}{4}\right)\frac{1}{\pi}A\cos\theta d\omega, \quad (1)$$

where N is the number density of molecules and $v_a = \langle v \rangle$, the average molecular velocity. Although the individual processes that result in molecules leaving a surface do not necessarily produce Maxwell–Boltzmann velocity distributions, for equilibrium conditions, the *overall* distribution of molecular flux will obey the cosine law (see [1], p. 20, for comment and references).

In the system of spherical polar co-ordinates (see Fig. 1) the solid angle, $d\omega$ is given by

$$d\omega = \sin\theta d\theta d\phi. \quad (2)$$

Hence, the expression for dn can be written in terms of the polar and azimuthal angles (θ, ϕ)

$$dn = \frac{NAv_a}{4\pi}\cos\theta\sin\theta d\theta d\phi. \quad (3)$$

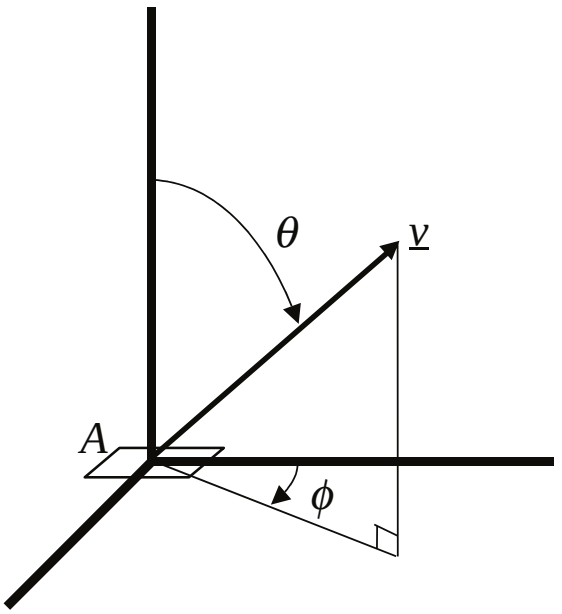

Fig. 1. In the spherical polar co-ordinate system, the direction of a vector, v, is described by the polar angle θ and the azimuthal angle ϕ. In this system θ is defined by the angle between the vector and the normal to some reference plane (for example the plane surface element A) whereas ϕ is defined by the angle in the reference plane between a reference direction and the projection of v onto the plane.

From kinetic theory [1] we have the result that the total molecular flux N_0 from A is

$$N_0 = \frac{NAv_a}{4}. \quad (4)$$

Hence, the cosine law can conveniently be written as

$$dn = \frac{N_0}{\pi}\cos\theta\sin\theta d\theta d\phi. \quad (5)$$

3. Angular probability distributions

Monte-Carlo modelling of the molecules in a vacuum system involves following the progress of a particle from its "origin" until some meaningful event occurs, for example, the particle leaves the system or it is captured. For realistic modelling, the parameters describing the particle's behaviour must be chosen so that they are representative of the real behaviour of molecules in the system. In terms of the molecule's scattering behaviour, this means that the angular distribution of the particles should be chosen so that the overall flux distribution obeys the cosine law.

The angular probability distributions for molecules scattered with a cosine distribution can be determined from Eq. (5) as follows:

3.1. Azimuthal angle

Molecules with a particular azimuth, ϕ, occur with a range of polar angles, θ. Therefore, to discover the azimuthal angular-probability distribution function, $f(\phi)$, which is the probability that a molecule will have a velocity vector of any allowed θ value in the azimuthal angular range $\phi - \phi + d\phi$, Eq. (5) should be integrated over all θ to determine the molecular flux dn_ϕ in this range, i.e.

$$dn_\phi = \frac{N_0}{\pi}d\phi\int_0^{\pi/2}\cos\theta\sin\theta d\theta. \quad (6)$$

The integral evaluates to 12; hence after rearrangement, we can specify

$$f(\phi) = \frac{1}{N_0}\frac{dn_\phi}{d\phi} = \frac{1}{2\pi}. \quad (7)$$

3.2. Polar angle

Molecules with a particular polar direction, θ, occur with a range of azimuthal angles, ϕ, therefore, to discover the polar angular-probability distribution function, $g(\theta)$, Eq. (5) should be integrated over all ϕ, i.e.

$$dn_\theta = \frac{N_0}{\pi}\cos\theta\sin\theta d\theta \int_0^{2\pi} d\phi, \tag{8}$$

i.e.

$$dn_\theta = 2N_0\cos\theta\sin\theta d\theta. \tag{9}$$

Therefore

$$g(\theta) = \frac{1}{N_0}\frac{dn_\theta}{d\theta} = 2\cos\theta\sin\theta = \sin 2\theta. \tag{10}$$

Thus $g(\theta)\,d\theta$ gives the fraction of molecules that have velocity vectors between θ and $\theta + d\theta$.

4. "Generation" of angular distributions

Random number generation of the angular distributions of Eqs. (7) and (10), to produce a cosine distribution of molecular flux can be achieved in a number of ways.

4.1. Azimuthal angle

Generating the azimuthal angle is mathematically trivial. The simplest approach is to generate a uniformly distributed random number, y, in the range $(0 < y \leqslant 2\pi)$ then to assign $\phi = y$. (Alternatively, if the random number can only be generated in a limited range, for example $(0 < y \leqslant 1)$, then $f(\phi)$ can be generated by scaling y i.e. $\phi = y2\pi$.)

4.2. Polar angle

The polar angle can be generated from a single, uniformly distributed random number, say x, in the range $(0 \leqslant x \leqslant 1)$.

Following Suetsuga [2], integrating the polar angular-probability distribution gives

$$x = \frac{\int_0^\theta g(\theta)d\theta}{\int_0^{\pi/2} g(\theta)d\theta} = \frac{\int_0^\theta \sin 2\theta d\theta}{1}$$
$$= 1 - \cos^2\theta = \sin^2\theta, \tag{11}$$

i.e.

$$\theta = \sin^{-1}(\sqrt{x}). \tag{12}$$

Thus, a random angle of departure is determined from a random number.

5. Incorrect interpretation of the cosine distribution law

The most common misunderstanding associated with the cosine law arises when it is *erroneously* supposed to state that:

> the probability of a molecule leaving the surface within a narrow angle $d\theta$, in a direction making an angle θ to the surface normal, is $\cos\theta$.

The misinterpretation occurs most often when a system is being modelled in two dimensions. The traditional schematic representation of the cosine law for molecules scattered from a surface is shown in Fig. 2(a). Occasionally this is misinterpreted as being the *polar angular-probability distribution* whereas in fact it is a projection through the *molecular flux distribution*. The actual polar angular-probability distribution is shown in Fig. 2(b).

The *incorrect* statement of the cosine law fails to take into account the three-dimensional nature of the molecular distribution and the inherent fact that the solid angle $d\Omega$ between θ and $\theta + d\theta$ is a function of θ namely $2\pi\sin\theta\,d\theta$.

The misinterpretation effectively states that the polar angular-probability distribution is $h(\theta)$, where

$$h(\theta) = \cos\theta. \tag{13}$$

This distribution can be generated from a single, uniformly distributed random number in the range $(0 \leqslant x \leqslant 1)$ by integrating the distribution as

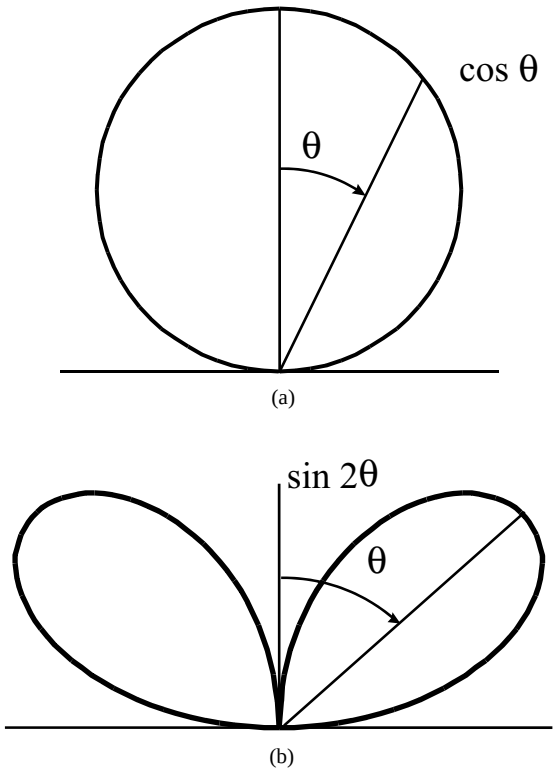

Fig. 2. (a) Projection through the cosine distribution of molecular flux; (b) the polar angular-probability distribution associated with a cosine distribution of molecular flux.

follows:

$$x = \frac{\int_0^\theta h(\theta)\mathrm{d}\theta}{\int_0^{\pi/2} h(\theta)\mathrm{d}\theta} = \frac{\int_0^\theta \cos\theta \mathrm{d}\theta}{1} = \sin\theta. \tag{14}$$

Hence, in this case

$$\theta = \sin^{-1} x \tag{15}$$

in contrast with the correct result of Eq. (12).

An associated azimuthal angle $f(\phi)$ is usually generated using the approach mentioned in Section 4.

6. The effect of the choice of polar angle generator on the molecular flux distribution

To see what effect the choice of the polar angle generator has on the molecular flux distribution (i.e. on the amount of flux *in a particular solid angle*), the angular distribution first needs to be normalised to take account of the changing solid angle (as a function of polar angle), i.e.

$$\mathrm{d}n(\theta, \mathrm{d}\omega) \propto \frac{p(\theta)}{\mathrm{d}\omega(\theta)}, \tag{16}$$

where

$$\mathrm{d}\omega = \sin\theta \mathrm{d}\theta \mathrm{d}\phi. \tag{17}$$

For the *correct* polar distribution $p(\theta) = g(\theta)$, this gives

$$\mathrm{d}n_g(\theta, \mathrm{d}\omega) \propto \frac{g(\theta)}{\sin\theta \mathrm{d}\theta \mathrm{d}\phi} = \frac{2\cos\theta\sin\theta}{\sin\theta \mathrm{d}\theta \mathrm{d}\phi}, \tag{18}$$

i.e.

$$\mathrm{d}n_g \propto \cos\theta, \tag{19}$$

which is the correct cosine distribution as defined at the beginning of this article.

For the *incorrect* polar distribution, $p(\theta) = h(\theta)$, this gives

$$\mathrm{d}n_h(\theta, \mathrm{d}\omega) \propto \frac{h(\theta)}{\sin\theta \mathrm{d}\theta \mathrm{d}\phi} = \frac{\cos\theta}{\sin\theta \mathrm{d}\theta \mathrm{d}\phi}, \tag{20}$$

i.e.

$$\mathrm{d}n_h \propto \cot\theta. \tag{21}$$

The distribution due to Eq. (21) is grossly different from the distribution due to Eq. (19), being very strongly peaked along the surface normal ($\theta = 0$).

7. Transmission probability for a cylinder

The effect of choosing the incorrect cosine distribution is demonstrated in the following example where the transmission probability for molecular flow in a cylinder has been calculated for a selection of cylinders with different length to radius ratio, L/R. In each case, the transmission probability has been calculated using both the correct cosine distribution $g(\theta)$ and the incorrect distribution $h(\theta)$ described above.

The transmission probability is modelled by computing the trajectories for a number of non-interacting particles originating in the entrance plane of the cylinder.

7.1. Monte-Carlo model

The starting co-ordinates for each particle are randomly generated from uniform spatial distributions. The initial direction of each particle is determined by randomly selecting an azimuthal angle (from a uniform distribution) and a polar angle from the relevant polar angular-probability distribution where the direction of the normal to the emitting "surface" is parallel to the axis of the cylinder. The particle trajectory is then determined.

If a particle passes through the exit plane of the cylinder, it is defined to have been transmitted. If a particle intercepts the cylinder boundary, it is subsequently "re-emitted" from the point of impact with a new, randomly selected polar angle (from the relevant angular-probability distribution) with the emission-normal being perpendicular to the surface and directed towards the axis of the cylinder. A new azimuthal angle is also randomly generated, relative to the new emission-normal. The trajectory of the particle is then determined once more.

If a particle passes through the entrance plane of the cylinder, it is defined to have been reflected; if it passes through the exit plane, it is defined to have been transmitted. If the particle intersects the cylinder boundary again, it is again re-emitted and its new trajectory is determined. This process is repeated until the particle is either reflected or transmitted.

The transmission probability is here defined to be the ratio of the number of particles that traverse the exit plane of the cylinder to the number of particles that are initially generated.

A summary of the calculation conditions is given in Table 1 and the results are presented in Fig. 3 which, for comparison, also shows the data of Cole [3]. (Cole's data is partly summarised in Table 2.5, p. 89 of [1] where it is treated as being of a sufficiently high accuracy that it can be used for comparing the quality of other results.)

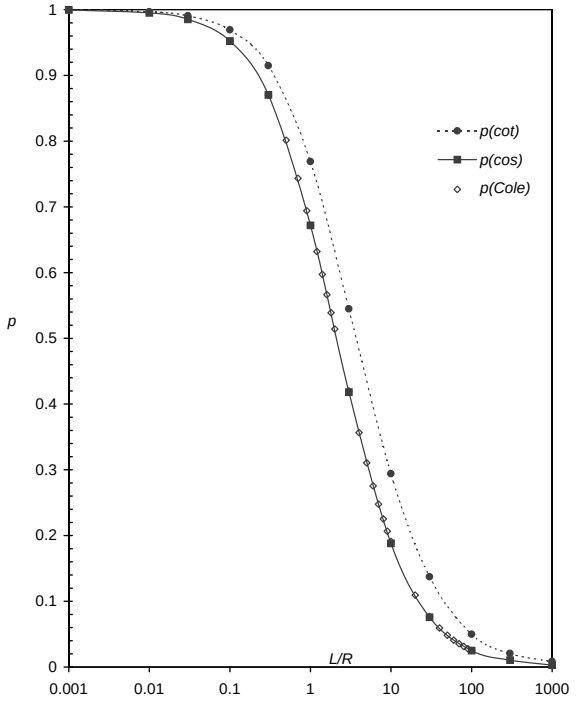

Fig. 3. Transmission probability, p(cos) and p(cot), for various cylinders with length to radius ratio, L/R. Results are shown for Monte-Carlo simulations using the correct (p(cos)) and the incorrect (p(cot)) polar angular-probability distributions together with data due to Cole (p(Cole)) which was determined using variational methods. (The lines joining the modelled data points are given as a visual aid; calculations were only performed at the identified data points.)

8. Summary

The correct interpretation of the cosine law distribution *for molecular flux* results in a $\sin 2\theta$ polar angular-probability distribution. This distribution can be generated from uniformly distributed random numbers in the range $(0 \leqslant x \leqslant 1)$ using the relation $\theta = \sin^{-1}(\sqrt{x})$.

Incorrect interpretation of the cosine law usually arises when it is *erroneously* supposed to state that the polar angle-probability distribution is a $\cos\theta$ distribution. This results in a $\cot\theta$ distribution for molecular flux, which is very strongly peaked along the surface normal.

Use of the incorrect polar angle-probability distribution can produce grossly different results to those generated with the correct distribution.

The results presented clearly demonstrate the significant difference between calculations performed using the correct and the incorrect

Table 1
Summary of calculated data for a range of cylinder dimensions

L/R	n	p(cos)	sd p(cos)	p(cot)	sd p(cot)	dp% p(cos)
0.001	10,000,000	0.99949	0.00001	0.99968	0.00001	0.02
0.01	10,000,000	0.99505	0.00005	0.99680	0.00006	0.18
0.03	10,000,000	0.9853	0.0001	0.9907	0.0001	0.54
0.1	10,000,000	0.9522	0.0002	0.9693	0.0001	1.8
0.3	10,000,000	0.8702	0.0003	0.9148	0.0002	5.1
1	10,000,000	0.6718	0.0005	0.7688	0.0003	14.4
3	10,000,000	0.4183	0.0004	0.5449	0.0004	30
10	1,000,000	0.188	0.001	0.2939	0.0013	56
30	1,000,000	0.076	0.001	0.137	0.001	82
100	10,000	0.025	0.002	0.050	0.002	99
300	10,000	0.011	0.001	0.021	0.001	93
1000	10,000	0.0028	0.0003	0.0083	0.0005	196

L/R is the ratio of cylinder length to radius, n is the total number of particles in the 10 calculation runs made for each cylinder configuration.
p(cos) is the mean transmission probability calculated for 10 runs using the correct cosine distribution $g(\theta)$ (Eq. (3)), sd p(cos) is the standard deviation associated with p(cos). p(cot) is the mean transmission probability calculated over 10 runs using an incorrect cosine distribution $h(\theta)$ (Eq. (4)), sd p(cot) is the standard deviation associated with p(cot). dp% p(cos) is the difference between p(cot) and p(cos) expressed as a percentage of p(cos) (calculated from unrounded data).

distributions as well as illustrating an excellent agreement between the correct cosine distribution and the results of Cole.

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