COMPUTATION OF THE TRANSMISSION PROBABILITY OF COMPLEX SYSTEMS

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The transmission probability in any direction through a duct connecting two large vessels is defined as the ratio of numbers of emerging to entering molecules. Usually it is determined under the following assumptions: the molecules pass through the duct independently of each other, their inter-collision is negligible, the reflection on the walls of the duct is diffusive (the angle of the reflection is independent of that of the incident). These assumptions are seldom realized in real physical circumstances, but the deviations can generally be taken into account, for this reason it is worth to determine the transmission probability under the assumed "clear" circumstances. Theoretical computations are, however, rather laborious even under these restricting assumptions and only a few results are available even for the relatively simple case of a cylindrical tube. A usual computation method is by a Monte Carlo model on a computer, but on account of the high computing time it must be restricted to a few parameters. Therefore it is worth to search for simple methods giving acceptable results either by interpolation between available results or by tracing the problem back to the results on cylindrical tubes.

OATLEY [1] was the first to show an acceptable method for computing the transmission probability of two interconnected cylindrical tubes. The application of his method to combinations of cylindrical tubes of different cross-sections or to combinations of a tube and an orifice of different cross-sections is a little difficult. BALLANCE [2] presented an additive formula as the generalization of OATLEY's result considering that the transmission probabilities through an element in direct and in the opposite direction generally are different. He takes the ratio of the two kinds of transmission probabilities equal to the ratio of the entrance areas of the element. It appears that his generalization is not consistent in every respect. In the following a descriptive model of the addition of transmission probabilities is shown, emphasizing the basic assumptions, to make the deviations from the OATLEY—BALLANCE method obvious.

The new computing method

The transmission probability can be defined as follows:

$$(N_1 - N_2)\, A\, \alpha = I\,, \tag{1}$$

where I is the net number of molecules per unit time that flow from a large reservoir into another one; N_1 and N_2 are the numbers of molecules per unit time per unit cross-section that enter the openings of the system; A is the opening area.

Our assumptions for the computation of the transmission probability of a complex system from those of their elements are the following:

1. Along the junction area of the connected elements the distribution of the molecules is uniform as if coming from a large reservoir.

2. For each connected element it is true that

$$A_L\, \alpha_R = A_R\, \alpha_L\,, \tag{2}$$

where R and L mean *right* and *left* and α_R means the transmission probability of the element to the right.

In computing the transmission probability of a complex system, notations in Fig. 1 are applied where elements 1 and 2 are not necessarily cylindrical

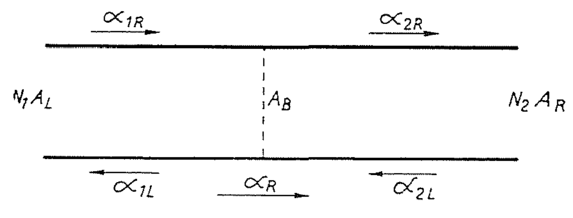


Fig. 1. Diagram of composite system

tubes, but any element with known transmission probability; A_B is the junction area.

α_R can be determined by (1) as follows:

$$(N_1 - N_2)\, A_L\, \alpha_R = (N' - N_2)\, A_B\, \alpha_{2L}\,, \tag{3}$$

where N' is the number of molecules per unit time and unit area that flows to the right through the junction area.

On the right side of (3) the number of molecules $N' A_B$ is composed of two parts, the one that arises from N_1A_L and the other from N_2A_R. The part from N_1A_L is

$$(N' A_B)_I = N_1 A_L \alpha_{1R} + N_1 A_L \alpha_{1R} (1 - \alpha_{2R}) (1 - \alpha_{1L}) + \\ + N_1 A_L \alpha_{1R} (1 - \alpha_{2R})^2 (1 - \alpha_{1L})^2 + \ldots = \\ = N_1 A_L \alpha_{1R} \frac{1}{\alpha_{1L} + \alpha_{2R} - \alpha_{1L} \alpha_{2R}} . \tag{4}$$

The sum in (4) means that in equilibrium, among the molecules crossing A_B at any time there are the ones crossing for the first time, the ones crossing for the second time and so on.

Similarly, the part from N_2A_R considering (2) is

$$(N' A_B)_{II} = - N_2 A_B \frac{\alpha_{1L} \cdot \alpha_{2R}}{\alpha_{1L} + \alpha_{2R} - \alpha_{1L} \alpha_{2R}} . \tag{5}$$

Eq. (3) considering (4), (5) and (2) is

$$(N_1 - N_2) A_L \alpha_R = (N_1 - N_2) A_B \frac{1}{\frac{1}{\alpha_{1L}} + \frac{1}{\alpha_{2R}} - 1} .$$

Thus the transmission probability of the system is

$$\frac{1}{\alpha_R} = \frac{A_L}{A_B} \left[\frac{1}{\alpha_{1L}} + \frac{1}{\alpha_{2R}} - 1 \right] . \tag{6}$$

(6) gives the known Oatley formula if $A_L = A_B$, $\alpha_{1L} = \alpha_{1R} = \alpha_1$ and $\alpha_{2R} = \alpha_{2L} = \alpha_2$, that is true for cylindrical tubes.

Transmission probabilities computed by (6) are equal to those obtained by OATLEY or BALLANCE for simple geometries. However, deviation can be found in the most complicated geometry examined by BALLANCE, that of a cylindrical pipe with restricted openings and a central blocking plate (Fig. 2).

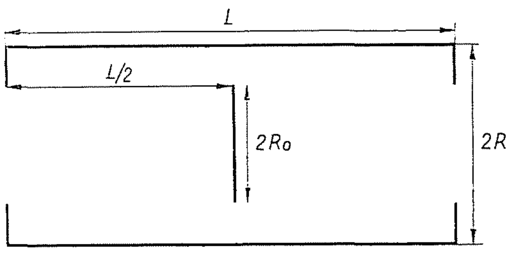


Fig. 2. Cylindrical pipe with the openings at both ends restricted and with a central blocking plate

The transmission probability for this system can be determined in the following steps with the new formula (6):

a) α_{Ra} of the system in Fig. 3a from (6) — as $\alpha_{1L} = \alpha$, $\alpha_{2R} = \frac{A_1}{A_2}$ $\left[\text{Eq. (2) being true for both elements: } A_1 \cdot 1 = A_2 \cdot \frac{A_1}{A_2}\right]$ is expressed as:

$$\frac{1}{\alpha_{Ra}} = \frac{1}{\alpha} + \frac{A_2}{A_1} - 1 . \tag{7}$$

b) α_{Rb} of the system in Fig. 3b — as $\alpha_{1L} = \frac{A_2 - A_1}{A_2}$, $A_B = A_2$ and α_{2R} is given by (7) — is

$$\frac{1}{\alpha_{Rb}} = \frac{A_2 - A_1}{A_2}\left(\frac{1}{\alpha} - 2\right) + \frac{A_2 - A_1}{A_1} + 1 . \tag{8}$$

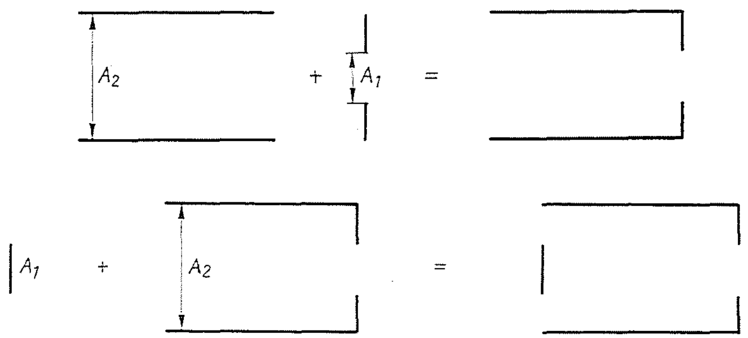


Fig. 3. Diagram for the construction of the system shown in Fig. 2

c) The transmission probability of the cylindrical pipe with restricted orifice and central blocking plate in Fig. 2 — as $\alpha_{1L} = \alpha_{2R}$ is given by (8) and $A_B = A_2 - A_1$ — is

$$\frac{1}{\alpha_R} = 2 + \frac{1}{F\alpha} - \frac{4}{F} + \frac{1}{F-1} , \tag{9}$$

where $F = \frac{A_2}{A_1}$.

BALLANCE's formula for this geometry is

$$\frac{1}{\alpha_B} = 2 - \frac{3}{F} + \frac{1}{F\alpha} + \frac{1}{(F-1)\alpha} . \tag{10}$$

The difference of (10) and (9) is

$$\frac{1}{\alpha_B} - \frac{1}{\alpha_R} = \frac{1-\alpha}{F(F-1)\alpha}. \tag{11}$$

(11) is positive for all values of $F > 1$ and $\alpha < 1$, therefore $\alpha_R > \alpha_B$.

The α values obtained from (9) and (10) for the geometry in Fig. 2 are shown in Figs 4a and 4b as compared to the Monte Carlo data of DAVIS [3].

A proper approximate formula for short cylindrical tubes is [4]

$$\alpha = \frac{2}{L/R + 2} \tag{12}$$

which approximates the exact values from below, for this reason it can be

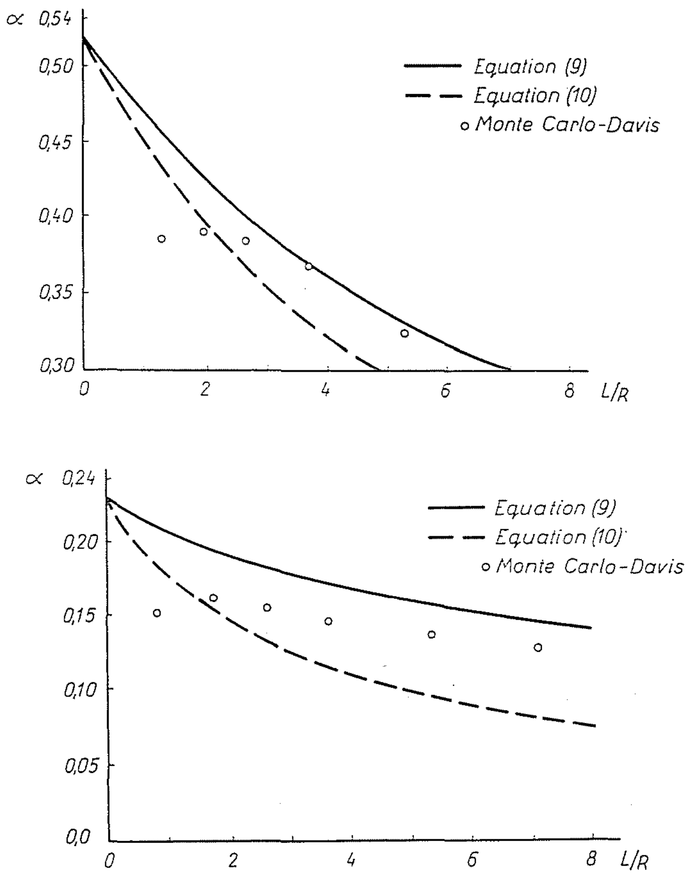


Fig. 4. Transmission probabilities of the system shown in Fig. 2. a) $F = 2.25$; b) $F = 1.25$

used in (9). From (9) and (12)

$$\alpha_R = \frac{2F(F-1)}{(F-1)(4F+L/R)-2(F-2)}, \tag{13}$$

if L/R is given according to Fig. 2.

Correction for short tubes

The transmission probabilities of composite systems, obtained from (9), (10) or (13) are inadequate for short geometries. The reason of this is the assumption in the derivation of (6) that the distribution of the molecules along any cross-section of the system is uniform, which is far from true in the case of short systems.

To consider the real distribution is far more difficult and a simple method to get suitable results is to correct the formulae obtained by (6). The correction can be done by interpolation, prescribing the known values of α. [For example for $\alpha = 1$, that is $L/R = 0$, let $\alpha_R = 0$ in (9).] A correction of (10) by this method fairly approximates the known Monte Carlo data [5].

A proper correction for (13) can be given by the factor

$$\frac{L/R}{L/R + 0{,}2} \tag{14}$$

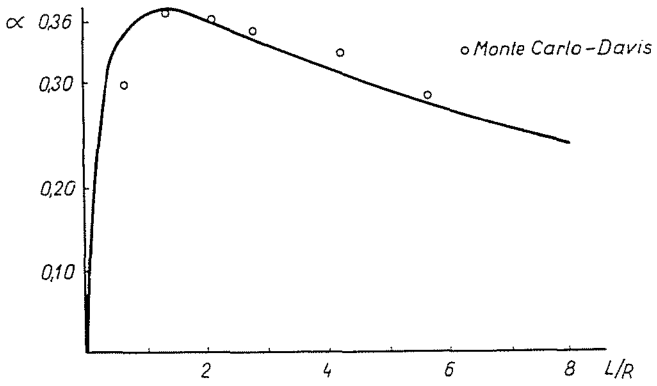
The results are shown in Figs 5a and 5b compared to DAVIS's data. To get the suitable factor, our intention was to find a simple formula for $\alpha_R = 0$ where $L/R = 0$ and α_R will be unchanged if $L/R \to \infty$.

Conclusions

To obtain proper formulae for the computation of the transmission probabilities of complex systems of various geometries it is necessary to define clearly the physical assumptions in the derivation. This gives the possibility to determine the range of validity of the formula, and the influence of the approximation upon the final result.

The evaluation of the obtained result is most effective, if it is possible to compare it with some Monte Carlo data.

In the knowledge of the limits of the formulae obtained from simple physical assumptions it is possible to derive correction factors extending their practical validity.



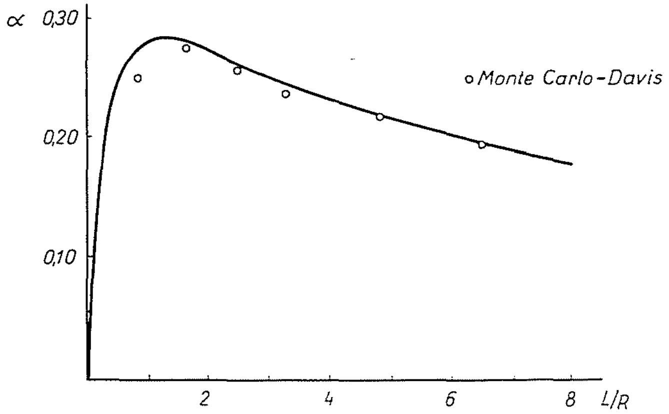


Fig. 5. Transmission probabilities of the system shown in Fig. 2 calculated by (13) corrected by (14). a) $F = 2$; b) $F = 1.5$

Summary

A general procedure is given to compute the transmission probability of composite systems from data of cylindrical tubes. The obtained results are compared to known Monte Carlo data, and to the results of other approximate methods. The errors of the procedure are explained and corrected with proper interpolation formulae.

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