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Molecular flow transmission probabilities of any regular polygon tubes

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ABSTRACT

Research on the molecular flow transmission probabilities of tubes is important in vacuum science and technology, as well as in some special applications in space technology. This study examines an algorithm based on Monte Carlo method to calculate the molecular flow transmission probabilities of any regular polygon tubes. This method fully utilizes the symmetries of regular polygons to simplify calculation. The results show that when the cross-sectional areas and lengths L of tubes remain constant, the molecular flow transmission probabilities of regular polygon tubes increase and approach those of cylindrical tubes with an increase in the number of sides. Moreover, any regular polygonal or cylindrical cross-section tube has nearly the same transmission probability within 2.8% of the maximum difference in the range of $L \leq 100$ (the cross-sectional area of each tube is π).

1. Introduction

The accurate calculation of duct conductance in the molecular flow state is important in many applications in vacuum science and technology, such as in flash-desorption experiments, accurate pressure measurements performed in dynamic conditions of gas flow, design of molecular beam apparatuses, and studies on thermal transpiration [1,2]. It is also important for some special applications in space technology, such as in the use of multi-hole plates with straight holes for air intake to collect space gas as the propellant of air breathing ion engines [3,4]. The relative speed between the space gas and the low-earth orbit satellite is approximately 7700 m/s, which is much faster than the speed of molecular thermal motion (a few hundred meters per second). Therefore, gas flow can be regarded as a molecular beam that can highly pass through straight pipes of multi-hole plates with a high gas collection efficiency. The transmission probability of reflux molecules is low, which leads to a high gas utilization efficiency. Multi-hole plates can be composed of cylindrical tubes, which have already been studied extensively in vacuum science and technology [1,5–7]. However, circles cannot be close-packed on a flat surface unlike in the case of regular triangles, squares, and regular hexagons. The porosity of multi-hole plates that are composed of such regular polygon tubes is theoretically 100%. Thus, studies on the molecular flow and molecular beam transmission probabilities of regular polygon tubes are necessary. Gas-surface interactions are complicated, and the reflection of a molecular beam from the surface does not follow a cosine law in space

because of its high kinetic energy (7700 m/s) [8,9]. Therefore, the transmission probabilities of molecular beams in tubes will not be discussed in this paper. Instead, we only discuss the molecular flow transmission probabilities of regular polygon tubes in normal conditions (The cosine law can be used), which include the molecular reflux of multi-hole plates.

Monte Carlo method, which involves a clear physical process, a simple algorithm, and an acceptable accuracy, was used for the first time by Davis to calculate the molecular flow transmission probabilities of tubes in 1960 [10]. Subsequently, molecular flow transmission probabilities were examined in cylindrical tubes [2], rectangular tubes [11], conical tubes [12], elliptical tubes [13], thin slit [14] and in other tubes [15,16]. In this paper, a Monte Carlo algorithm on regular polygon tubes is studied. The algorithm fully utilizes the symmetries of regular polygons, so the calculation process is simplified, and the calculation time is shortened. Calculation results show that any regular polygon tubes nearly have the same conductance as cylindrical tubes with the same cross-sectional area and length in the molecular flow regime.

2. Details of the calculation

The Monte Carlo method of calculating the conductance of a duct in molecular flow state consists of an evaluation of the fraction of N particles entering one end and leaving the other end of a duct. This evaluation is achieved by calculating the path of each particle between successive collisions with the walls of the duct, with the particle being reflected after each collision according to conditions that will be explained in Appendix. The computer program uses a Mersenne-Twister random number generator. The

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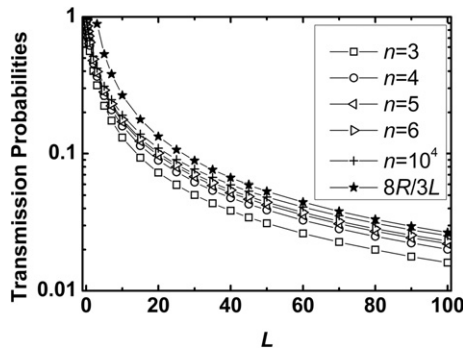E-mail address: xuekchen@163.com (X. Chen).

Fig. 1. Transmission probabilities P versus tube lengths L. The length from the center of each regular polygon to each vertex is 1. The molecular flow transmission probability of a long cylindrical tube is $8R/3L$, where radius $R = 1$. The number of simulated molecules is 3×10^7.
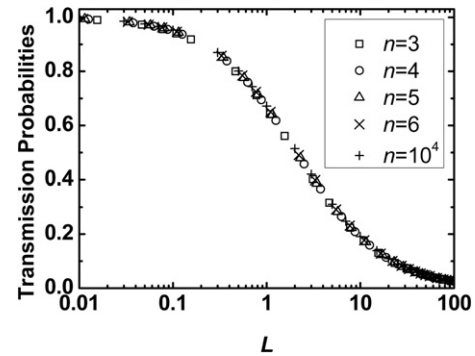

Fig. 2. Transmission probabilities P versus tube lengths L. The molecular flow transmission probability is a function of $L/S^{1/2}$, where S is the cross-section area of the tube. Hence, the transmission probabilities of regular polygon tubes with cross-section area π could be obtained from Table 1 and shown in Fig. 2.

generated pseudorandom numbers are uniformly distributed and are not correlated with one another [17]. The basic assumptions for the calculation are as follows [1,2,10,12,15]: (1) The molecules in the pipe move independently from one another, i.e., no intermolecular collisions exist in the pipe. (2) The molecules possess equal probabilities of entering any point in the entrance of the tubes and arrive with a cosine distribution of directions; in the collisions with the system surface, gas molecules are diffusely reflected, and their velocity directions follow a cosine law. (3) The flow is assumed to be steady, and the adsorption of molecules on the system surface is negligible.

3. Results and discussions

Fig. 1 and Table 1 show the molecular flow transmission probabilities of regular polygon tubes. The number of simulated

molecules is 3×10^7. The number of sides n is 3, 4, 5, 6, 10, 30, 100, and 10000. The distance from the center of each regular polygon to each vertex is 1. The numerical calculation values of transmission probabilities of cylindrical tubes with radiuses of 1, which are accurate within ±1 in the last figure, were reported by Gómez-Goñi and Lobo [1] and are shown in Table 1. When tube lengths L are constant, as illustrated in Fig. 1 and Table 1, the molecular flow transmission probabilities of regular polygon tubes increase and become close to those of cylindrical tubes with an increase in n. Table 1 indicates that if $n \geq 10$, the transmission probabilities of regular polygon tubes no longer increase significantly. This condition is attributed to a small n, which also makes the cross-sectional area of the pipe small. As n increases, the cross-sectional area and shape of the regular polygon tube infinitely approach a circle with radius of 1. The cross-sectional area of a regular polygon tube with 10 sides is 93.55% of that of a cylindrical tube. In Figs. 1 and 2,

Table 1

Molecular flow transmission probabilities of the tubes. The length from the center of each regular polygon to each vertex is 1. The number of simulated molecules is 3×10^7. The numerical calculation values of cylinders with radiuses 1 are accurate within ±1 in the last figure.[a] The differences between the values of regular polygon tubes with 10000 sides and those of cylinders are all less than 2σ.[b]

L	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 10$	$n = 30$	$n = 100$	$n = 10^4$	2σ for $n = 10^4$	Cylinder
0.01	0.99033	0.99307	0.99391	0.99428	0.99478	0.99498	0.99500	0.99499	0.00003	
0.03	0.97248	0.97979	0.98210	0.98324	0.98457	0.98512	0.98520	0.98520	0.00004	
0.05	0.95589	0.96720	0.97083	0.97248	0.97463	0.97558	0.97566	0.97565	0.00006	
0.07	0.94016	0.95507	0.95983	0.96207	0.96490	0.96606	0.96615	0.96620	0.00007	
0.1	0.91833	0.93761	0.94388	0.94682	0.95050	0.95216	0.95230	0.95236	0.00008	0.95239890732
0.3	0.80034	0.83838	0.85138	0.85769	0.86592	0.86950	0.86989	0.86999	0.00012	0.86992814758
0.5	0.71171	0.75969	0.77655	0.78490	0.79573	0.80054	0.80117	0.80116	0.00014	0.80121742018
0.7	0.64200	0.69520	0.71479	0.72422	0.73695	0.74269	0.74329	0.74343	0.00015	0.74340979004
1	0.56138	0.61834	0.63993	0.65048	0.66456	0.67113	0.67178	0.67186	0.00017	0.67198390192
2	0.40154	0.45787	0.47994	0.49095	0.50622	0.51340	0.51412	0.51425	0.00018	0.5142305345
3	0.31568	0.36672	0.38736	0.39792	0.41234	0.41920	0.41996	0.42004	0.00018	0.4200554493
5	0.22357	0.26498	0.28235	0.29129	0.30375	0.30967	0.31031	0.31043	0.00016	0.3105252831
7	0.17390	0.20883	0.22345	0.23122	0.24180	0.24712	0.24764	0.24770	0.00015	0.2477356957
10	0.13096	0.15891	0.17093	0.17724	0.18609	0.19049	0.19088	0.19092	0.00014	0.1909424319
15	0.09322	0.11413	0.12331	0.12817	0.13503	0.13840	0.13884	0.13875	0.00012	
20	0.07252	0.08926	0.09665	0.10067	0.10617	0.10901	0.10934	0.10934	0.00011	0.1093207144
25	0.05931	0.07339	0.07954	0.08290	0.08765	0.08995	0.09019	0.09030	0.00010	
30	0.05016	0.06223	0.06770	0.07064	0.07466	0.07668	0.07689	0.07696	0.00009	0.0769377994
35	0.04354	0.05423	0.05891	0.06147	0.06501	0.06681	0.06700	0.06702	0.00009	
40	0.03846	0.04789	0.05214	0.05442	0.05766	0.05922	0.05941	0.05940	0.00008	0.0594504191
45	0.03439	0.04303	0.04678	0.04881	0.05175	0.05321	0.05339	0.05344	0.00008	
50	0.03117	0.03897	0.04245	0.04435	0.04697	0.04827	0.04838	0.04845	0.00007	0.0484764500
60	0.02627	0.03280	0.03577	0.03739	0.03970	0.04078	0.04095	0.04091	0.00007	0.0409393067
70	0.02270	0.02837	0.03091	0.03224	0.03430	0.03528	0.03541	0.03536	0.00007	0.0354393800
80	0.01995	0.02500	0.02722	0.02846	0.03024	0.03110	0.03120	0.03123	0.00006	0.0312472930
90	0.01778	0.02237	0.02439	0.02550	0.02702	0.02784	0.02791	0.02789	0.00006	0.0279452038
100	0.01607	0.02013	0.02205	0.02304	0.02449	0.02520	0.02528	0.02524	0.00005	0.0252763636

[a] Gómez-Goñi and Lobo [1] computed the molecular transmission probabilities through cylindrical tubes to high numerical precision by using an algorithm developed by El-gendi [18]. This algorithm basically approximates the solution of the Fredholm equation with a series of Chebyshev polynomials.

[b] Using 2σ as the uncertainty of regular polygon tubes with 10000 sides (see text for details).