Comment on "Data on Internal Rarefied Gas Flows" [J. Phys. Chem. Ref. Data 27, 657 (1998)]

Cite as: J. Phys. Chem. Ref. Data **44**, 036101 (2015); https://doi.org/10.1063/1.4929914
Submitted: 10 April 2015 . Accepted: 28 July 2015 . Published Online: 16 September 2015

Oleg Sazhin

Comment on "Data on Internal Rarefied Gas Flows" [J. Phys. Chem. Ref. Data 27, 657 (1998)]

Oleg Sazhin

Institute of Natural Sciences, Ural Federal University, Ekaterinburg 620000, Russia

(Received 10 April 2015; accepted 28 July 2015; published online 16 September 2015)

[http://dx.doi.org/10.1063/1.4929914]

Reference 1 is a comprehensive review of an important rarefied gas dynamics problem. Researchers actively use the review, which is confirmed by its high citation rate. The review presents data on various internal gas flows from hydrodynamic to free-molecular flow regime. In particular, Sec. 5.2 of the review discusses gas flow through capillaries of finite length under free-molecular regime. Under this regime, gas flow through a capillary is commonly described with a so-called transmission probability W. The physical significance of this value is that when a molecule arrives at the entrance cross section of a capillary connecting containers I and II, this molecule will pass through the capillary from container I to container II with the probability of $W_{I\to II}$. Similarly, $W_{II\to I}$ is the probability that the molecule will pass the same capillary in the other direction. The review postulates condition (5.5), according to which in the case of isotropic capillary $W_{I\to II} = W_{II\to I}$.

Section 5.2.4 of the review examines the influence of the capillary's wall roughness on the transmission probability. It is claimed that if the wall roughness has the sawlike shape, then an asymmetric "saw" can make the capillary anisotropic, and, consequently, condition (5.5) can be violated. In our opinion, this statement is debatable.

Let us consider an isolated system of two equal containers, both initially filled with an equal amount of gas molecules. The containers are connected to each other with a narrow rough-surfaced capillary, for which condition (5.5) is false. It is not difficult to demonstrate that when a sufficiently long period of time passes after opening up the capillary, the ratio of the quantity of molecules in the containers will be described by the equation $N_{II}/N_I = W_{I\to II}/W_{II\to I}$, where N_I and N_{II} are the quantity of molecules in containers I and II, respectively. If the values of transmission probability $W_{I\to II}$ and $W_{II\to I}$ differ significantly, the quantities of molecules in the containers will be noticeably different as well. Since the system is isolated, this conjecture comes into contradiction with the second law of thermodynamics and, therefore, with the representation of the equilibrium state of the gas.

This paper aims to conduct a numerical experiment in order to evaluate the correctness of the claim made in section 5.2.4 concerning violation of condition (5.5) in the case of anisotropic capillary. To this end, the test particle Monte Carlo method[2] (TPMC) will be used. The TPMC method relies on the physical nature of molecular transport and can be regarded as a numerical experiment. The total number of generated particles in each individual computation equals 10^9, which allows for the computation error of less than 0.1%.

The geometry of the modeled rough-surfaced capillary is demonstrated in Fig. 1. For our computations, we have chosen the rectangular shape of the capillary (channel) and limited the model to two dimensions. As shown in the figure, the channel of length l and height h has the wall roughness in the shape of an asymmetric saw with uniform teeth; Λ is the height of a tooth, whereas α and β are the tooth's inclination angles. For the gas-surface scattering law, the diffuse and specular as well as Maxwell[3] and Cercignani–Lampis[4] models have been used.

In our computations, the values of the diffuse fraction ε in the Maxwell model as well as the accommodation coefficient for the part of the kinetic energy corresponding to the motion normal to the wall α_n and the accommodation coefficient of the tangential momentum α_t in the Cercignani–Lampis model are equivalent to the values commonly encountered in reality.[5] The roughness height used in computations is also close to real values.

Table 1 presents the results of computations for rough-surfaced channels with the length to height ratio $l/h = 1$ and 10 in the case of the relative height of the roughness $\Lambda/h = 1 \times 10^{-4}$ and inclination angles $\alpha = 90°$ and $\beta = 10°$ (asymmetric "saw"). Table 1 consists of two parts, upper and lower. The upper part shows the parameters of the free-molecular gas flow through the channel from container I to container II, and the lower part shows the same for the opposite direction of the flow. The following parameters have been computed: transmission probability W, mean path $\langle S\rangle$ in the channel and time $\langle t\rangle$ of traveling through the channel for the particles that

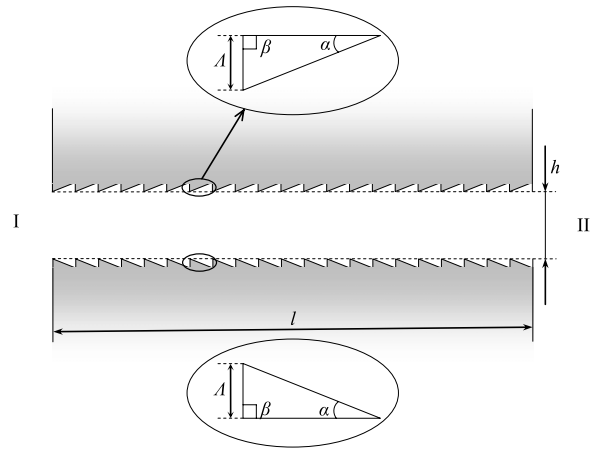

FIG. 1. Geometry of the rough-surfaced channel being modeled: l—channel's length, h—channel's height, Λ—height of roughness, α and β—inclination angles.

TABLE 1. Parameters of the free-molecular gas flow through a rough-surfaced channel depending on the flow direction, length to height ratio l/h, and the gas-surface scattering law in the case of the relative height of the roughness $\Lambda/h = 1\times10^{-4}$ and inclination angles $\alpha = 90°$ and $\beta = 10°$: W—transmission probability of the channel, $\langle S\rangle$—particle's mean path in the channel, $\langle t\rangle$—mean time of the particle's travel through the channel, and $\langle n\rangle$—mean quantity of particle's collisions with the rough surface

Flow direction	l/h	Gas-surface scattering	W	$\langle S\rangle$, h	$\langle t\rangle$, h/v_m	$\langle n\rangle$
I → II	1	Diffuse	0.653 21	1.9027	1.6862	1.1785
		Maxwell ($\varepsilon = 0.8$)	0.679 20	1.8830	1.6688	1.1443
		CL ($\alpha_n = \alpha_t = 0.8$)	0.677 55	1.8840	1.6631	1.1435
		Specular	0.734 94	1.7052	1.5113	1.0223
	10	Diffuse	0.204 42	40.3038	35.7189	1.2128
		Maxwell ($\varepsilon = 0.8$)	0.220 78	37.9084	33.5958	1.2058
		CL ($\alpha_n = \alpha_t = 0.8$)	0.218 65	38.1497	33.7800	1.2028
		Specular	0.223 81	38.1719	33.8296	1.1427
II → I	1	Diffuse	0.653 24	1.9027	1.6862	1.1784
		Maxwell ($\varepsilon = 0.8$)	0.679 21	1.8830	1.6687	1.1443
		CL ($\alpha_n = \alpha_t = 0.8$)	0.677 59	1.8840	1.6633	1.1435
		Specular	0.734 92	1.7051	1.5112	1.0223
	10	Diffuse	0.204 41	40.3045	35.7191	1.2128
		Maxwell ($\varepsilon = 0.8$)	0.220 80	37.9049	33.5913	1.2058
		CL ($\alpha_n = \alpha_t = 0.8$)	0.218 66	38.1540	33.7839	1.2028
		Specular	0.223 81	38.1752	33.8351	1.1427

passed through the entire channel and made at least one contact with the wall; also, the mean quantity of particle's collisions $\langle n\rangle$ with the rough surface during contact.

The physical significance of n may be gathered from the equation offered by Roberts,[6] who first pointed out the effect of the surface's roughness upon the value of the energy accommodation coefficient. Representing the relationship between the energy accommodation coefficient for a smooth surface α_E^1 with the effective energy accommodation coefficient α_E for a surface of such roughness that each molecule on the average strikes it in n different places before returning to the body of the gas, Roberts' equation is as follows: $\alpha_E = 1 - (1 - \alpha_E^1)^n$. Also, v_m in Table 1 is the most probable molecular velocity.

Let us recall that, in the case of a smooth-surfaced channel and diffuse scattering, the value of transmission probability W can be arrived at using the reliable Berman's formula,[7] according to which the value of W equals 0.684 38 and 0.240 80 for $l/h = 1$ and 10, respectively.

As it is obvious from Table 1, in each computation the parameters of gas flow from container I to container II coincide with the parameters of the opposite direction flow within computation error. In particular, this is true for the values of transmission probabilities $W_{I\to II}$ and $W_{II\to I}$. Thus, in the case of anisotropic capillary, condition (5.5) has not been violated.

It is understood that a numerical experiment cannot be accepted as a rigorous proof of our statement. However, upon conducting numerous computations with other geometrical parameters of the asymmetric saw, at no time was a violation of condition (5.5) observed, even in the case of the saw height Λ approaching the channel height h.

It should be noted that a violation of condition (5.5) occurred upon examination of the thermal transpiration phenomenon.[8] However, in this case the containers I and II have different temperatures, meaning that the entire system cannot be considered isolated.

The support by the Ministry of Education and Science of the Russian Federation through the base part of the State task for high educational institutions (the Research Project No. 2189) is gratefully acknowledged.

[1]F. Sharipov and V. Seleznev, J. Phys. Chem. Ref. Data **27**, 657 (1998).
[2]G. A. Bird, *Molecular Gas Dynamics and Direct Simulation of Gas Flows* (Oxford University Press, Oxford, 1996).
[3]J. C. Maxwell, *The Scientific Papers of James Clerk Maxwell* (Dover, New York, 1890).
[4]C. Cercignani and M. Lampis, Transp. Theory Stat. Phys. **1**, 101 (1971).
[5]O. V. Sazhin, S. F. Borisov, and F. Sharipov, J. Vac. Sci. Technol. A **19**, 2499 (2001); Erratum, **20**, 957 (2002).
[6]J. K. Roberts, Proc. R. Soc. A **129**, 146 (1930).
[7]A. S. Berman, J. Appl. Phys. **36**, 3356 (1965); Erratum, **37**, 2930 (1966).
[8]O. Sazhin, A. Kulev, S. Borisov, and S. Gimelshein, Vacuum **82**, 20 (2008).