Using a Thin Wire in a Free-Molecular Flow for Determination of Accommodation Coefficients of Translational and Internal Energy


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Abstract. A new experimental-computational method for determination of the translational and internal energy accommodation coefficients on a thin wire in a free-molecular flow is elaborated. The base of the method is a numerical solution of the heat balance equation of the wire. Measurements were performed in a low-density wind tunnel with Ar, He, H2, N2, CH4, CO2. Besides, the proposed method provides determination of thermophysical properties of the wire.

I. INTRODUCTION

The accommodation coefficient (AC) of energy is determined as ratio

\[ \alpha = \frac{E_i - E_r}{E_i - E_w}. \]  

Here \( E_i \) and \( E_r \) are the energies of incident and reflected molecules and \( E_w \) is the average energy of reflected molecules corresponding to the surface temperature. It is this value usually used as a measure of energy exchange between gas and surface from the times of M. Knudsen [1]. Such a definition assumes an equal accommodation for the translational and internal energy. By using in formula (1) the translational (internal) energy, one can obtain the definition for partial accommodation coefficients of translational (internal) energy \( \alpha' \) (\( \alpha'' \)). Some theoretical and experimental results show that AC’s of translational and internal energy may differ considerably [2 – 4].

Probing with a thin wire has been widely used at high Knudsen numbers for measurements of total energy AC’s in the quiescent gas [5]. The attempt to measure partial AC’s for translational and internal energy of polyatomic molecules in the quiescent gas on early fifties was called in questions later in [6]. The theory of energy AC calculations in studying heat transfer of a cylinder in a free molecular flow was essentially elaborated in [7]. Using of a thin wire anemometer for diagnostics of rarefied gas flows in combination with other instruments allowed to determine the total AC on the base of simplified calculation of wire heat balance [8]. It was shown in [9, 10] that idea of thorough analysis of a heat balance for cylinder in a free molecular flow can work at the determination of partial AC’s for translational and internal energy. In these works the AC’s were determined using an analytical solution of a simplified heat balance equation proposed in [11]. Those simplifications are unacceptable for a wide range of the wire temperature. They bring essential uncertainties into analysis. Our paper presents results of determination of AC’s by accurate numerical solving the heat balance equation with consideration of influence of electro-thermophysical parameters of the wire.

II. METHOD

The heat balance for the wire of a unit length is defined by the following equation:
The dependencies of resistance capacity, gradient at the wire end, can obtain the values of this temperature is one of the main difficulties in solving the considered problem. It is common for the holder to reduce the influence of uncertainties, which are inevitable in experiments. To solve the equation (2) it is necessary to know the heat transfer coefficient \( h \) and the recovery temperature \( T_r \). The expressions for \( h \) and \( T_r \) for a cylinder located perpendicular to the flow are given in [9] for a gas with internal degrees of freedom:

\[
h = \frac{1}{4\sqrt{\pi}} nk\xi \cdot \exp\left(\frac{-S^2}{T}\right) \cdot \frac{U}{S} \left[I_0 + S^2(I_0 + I_1)\right].
\]

\[
T_r = \frac{T}{\xi} \left\{ \alpha'(2S^2 + 5 - \frac{1}{1 + S^2(1 + I_0/I_b)}) + \alpha'' j \right\}.
\]

Here \( n, U, T \) are the number density, velocity, and static temperature of the gas flow; \( S = U/(2kT/m)^{1/2} \) is the speed ratio; \( m \) is the molecular mass; \( k \) is the Boltzmann constant; \( \xi = 4\alpha' + \alpha'' j \); \( j = \frac{S^2}{T} \) is the number of internal degrees of freedom; \( \gamma \) is the adiabatic exponent; \( I_0 \) and \( I_1 \) are the modified Bessel functions of zero and first order for argument \( S^2/2 \).

It is worth noting that in a quiescent gas (\( U = 0 \)) the equation (4) is reduced to the form of \( T_r = T_0 \) and the wire resistance depends only on complex \( \xi = 4\alpha' + \alpha'' j \) of the equation (3). So it is possible to separate the AC’s of translational and internal energy only in the case when there is a directional movement of gas.

In all cases of determination of AC’s, we used the trial-and-error method with thoroughly minimization of errors. A series of experimental measurements of the wire resistance \( R_s \) is performed by different currents \( I_k, k = 1..N \). Scanning of all suitable pairs of AC’s \( (\alpha', \alpha'') \) has been accomplished. For each such a pair \( (\alpha', \alpha'') \) and for each current \( I_k \) the equation (2) is numerically solved and the temperature distribution along the wire \( T_w(x) = T_0(x, \alpha', \alpha'', I_k) \) is found. Given the temperature distribution, the integral wire resistance is calculated \( R(\alpha', \alpha'', I_k) = \frac{\rho_0}{\pi r_0^2} \int_0^L [1 + \alpha' T_w(x, \alpha', \alpha'', I)] dx \) (\( L \) is the wire length). Then the discrepancy between the computed and experimental resistance \( \Delta_k = R(\alpha', \alpha'', I_k) - R_s \) is calculated, and the function \( F(\alpha', \alpha'') = \sum_1^N \Delta_k^2 \) is considered. As the sought-for AC’s, such a pair of \( (\alpha', \alpha'') \) is chosen for which \( F(\alpha', \alpha'') \) takes the minimum value. Such an approach allows reducing the influence of uncertainties, which are inevitable in experiments.
III. EXPERIMENTS, RESULTS AND DISCUSSION

The experiments were performed in a low-density wind tunnel, where rarefied gas flow was created by free jet expansion of gas through a sonic nozzle. The nozzle diameter is \(d_* = 6\) mm. The stagnation pressure is \(P_0 = 1000 \pm 2100\) Pa, the background pressure is about 2.7 Pa. The stagnation temperature is \(T_0 = 290 – 300\) K. A thin wire probe was placed on the jet axis at distances of \(2 + 7 d_*\) from the nozzle exit. Given such experimental conditions, the flow near the wire is free from influence of the background gas [13]. So the flow parameters on the jet axis for the considered distances correspond to those calculated for expansion of nonviscous gas [14]. It was confirmed by results of numerical modeling of viscous gas expansion that was graciously presented by P. A. Skvorodoko.

A gilded tungsten wire with the diameter of 8.3 \(\mu\)m was used as the probe. With such a diameter, a free molecular flow was provided at the above mentioned conditions. The wire was welded to a stainless steel holder in the form of a cylinder with the diameter 0.6 mm tapered to the size 0.2 mm. The typical wire length \(L\) was of 3 – 10 mm.

One of the most important requirements to experiments in the wind tunnel and calibration procedures is a high precision of measurement of the voltage and amperage. These strict requirements are inevitable, as well as main results are extracted by precise numerical calculation of the temperature distribution along the wire. A voltmeter and a source of electric current with accuracy of 0.1 % were used for our measurements.

The experiments in a free jet were preceded by determination of electro-thermophysical properties of the wire: the specific resistance \(\rho\), the heat conductivity coefficient \(\lambda\), and the emissivity \(\varepsilon\), with taking into consideration their dependence on temperature. In these experiments, the wire tips were clamped between solid copper terminals to provide an ideal heat contact between the wire and the terminals as much as possible. The dependence \(\rho = \rho(T_w)\) is determined by the measurements in a thermostat in air by atmospheric pressure. When measuring electric resistance in the thermostat, a low amperage is used to eliminate the electric heating of the wire.

The surface emissivity \(\varepsilon(T_w)\) is found by preliminary calculation (by solving the equation (2) for vacuum) of dependence \(R = R(\varepsilon)\) for the wire with \(L = 100\) mm for two constant values of the heat conductivity coefficient \(\lambda\) of 120 and 150 W/(m·K). For such a length, the heat flux through radiation is by one order higher than through the holders. The range of \(\lambda\) reasonably covers the spread of these values known from the literature. The emissivity \(\varepsilon\) is determined by the value of \(R\) known from the experiments. The emissivity determined by this means is used to calculate a more definite heat conductivity coefficient with the length wire \(L = 10\) mm, when the heat flux from the wire to the holder dominates. After this, the emissivity can be defined more accurately from the determined heat conductivity.

In the results of these calibration procedures, the following characteristics for the tested wire were determined:

\[
\varepsilon = 0.05 \cdot [1 + 0.00335 \cdot (T_w - 273)] ,
\]

\[
\rho = 5.65 \cdot 10^{-3} [1 + 0.0041 \cdot (T_w - 273)] \text{Om} \cdot \text{m} ,
\]

\[
\lambda = \begin{cases} 145 - 0.11 \cdot (T_w - 273) \text{ W/(m} \cdot \text{K)} , & T_w \leq 250\degree \text{C} \\ 117 - 0.06 \cdot (T_w - 523) \text{ W/(m} \cdot \text{K)} , & T_w \geq 250\degree \text{C} . \end{cases}
\]

At the first stage, the AC’s were determined for monoatomic gases Ar and He. One of the typical experimental dependencies of the wire resistance on current is presented in fig. 1 (solid line) for argon flow (\(L = 3.45\) mm, \(S = 5.84\)). By looking through the appropriate AC’s, a minimal discrepancy between experimental and computational dependencies for this case has been obtained for \(\alpha' = 0.85\). The final fitting of computational dependence (dashed line) to the experimental one is shown in fig. 1.

In experiments with polyatomic gases (\(H_2, N_2, CH_4, CO_2\)) performed at the room stagnation temperature and temperature of the wire below 400°C, only rotational degrees of freedom as internal ones are active. So the above procedure was performed for a set of pairs of AC’s (\(\alpha', \alpha''\)). The figure, presenting discrepancy \(\Delta = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \Delta_i^2}\) in dependence on AC’s, is three-dimensional one. Fig. 2 shows projection of this figure on (\(\alpha', \alpha''\)) plane for nitrogen flow (\(L = 9.4\) mm, \(S = 4.64\)).
FIGURE 1. The final fitting of computational dependence of the wire resistance $R$ on the current $I$ to the experimental one for Ar by $\alpha' = 0.85$ ($P_0 \approx 2100$ Pa, $L = 3.45$ mm, $S = 5.84$).

FIGURE 2. The field of discrepancy $\Delta$ of experimental and computational dependencies of the wire resistance $R$ by determination of AC's for N$_2$ ($P_0 \approx 2100$ Pa, $L = 9.4$ mm, $S = 4.64$; $\alpha' = 0.67$, $\alpha'' = 0.57$).
AC’s averaged over many measurements with different wire probes, gas pressures, and at different distances from the nozzle are presented in the table I. The comparison of results of different research groups for AC’s is usually questionable, since it is difficult to find the results for identical or similar conditions on many key parameters (the energy of incident molecules, interaction angle, original structure of the surface, characteristics of the surface sorbate, the surface temperature). This task is completely indefinite for surfaces of engineering interest. In table II, some data from literature is given at least at close interaction energy. Comparison of tables I and II shows qualitative agreement for our data and those from literature.

**TABLE I. Accommodation coefficients.**

<table>
<thead>
<tr>
<th>Gas</th>
<th>$\alpha'$</th>
<th>$\alpha''$</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>0.29 ± 0.05</td>
<td>—</td>
</tr>
<tr>
<td>Ar</td>
<td>0.8 ± 0.05</td>
<td>—</td>
</tr>
<tr>
<td>$N_2$</td>
<td>0.67 ± 0.04</td>
<td>0.56 ± 0.08</td>
</tr>
<tr>
<td>$CH_4$</td>
<td>0.78 ± 0.1</td>
<td>0.73 ± 0.16</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>0.9 ± 0.23</td>
<td>0.79 ± 0.15</td>
</tr>
<tr>
<td>$H_2$</td>
<td>0.44 ± 0.04</td>
<td>-0.15 ± 0.05</td>
</tr>
</tbody>
</table>

**TABLE II. Data on AC’s from literature.**

<table>
<thead>
<tr>
<th>Gas</th>
<th>Surface</th>
<th>$T_1$</th>
<th>$\alpha'$</th>
<th>$\alpha''$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>W, covered by O</td>
<td>330</td>
<td>0.18</td>
<td>—</td>
<td>[15]</td>
</tr>
<tr>
<td>He</td>
<td>Pt</td>
<td>310</td>
<td>0.24</td>
<td>—</td>
<td>[16]</td>
</tr>
<tr>
<td>Ar</td>
<td>W, covered by gas</td>
<td>300</td>
<td>1.0</td>
<td>—</td>
<td>[17]</td>
</tr>
<tr>
<td>Ar</td>
<td>Pt, burning in vacuum</td>
<td>410</td>
<td>0.76</td>
<td>—</td>
<td>[16]</td>
</tr>
<tr>
<td>$N_2$</td>
<td>W, burning in vacuum</td>
<td>450</td>
<td>0.36</td>
<td>—</td>
<td>[18]</td>
</tr>
<tr>
<td>$N_2$</td>
<td>Au, covered by gas</td>
<td>293</td>
<td>0.89</td>
<td>0.78</td>
<td>[4]</td>
</tr>
<tr>
<td>$CH_4$</td>
<td>Pt</td>
<td>373</td>
<td>0.81</td>
<td>—</td>
<td>[17]</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>W, covered by $CO_2$</td>
<td>330</td>
<td>0.99*</td>
<td>—</td>
<td>[15]</td>
</tr>
</tbody>
</table>

* AC obtained for total energy.

From the presented above experiments for $N_2$, $CO_2$ and $CH_4$, the conclusion can be made that for low energies of molecules (corresponding to the room stagnation temperature) the AC’s of translational energy are slightly higher than the AC’s of internal energy. It is confirmed by known theoretical [3] and experimental [4] works.

Determination of AC of internal energy is of particular interest in the proposed method. The available data on such AC’s are very scanty. It is known that the molecular beam facilities are main instruments for experimental study of the gas-surface interactions on the level of information on translational and internal energy distribution function. In numerous molecular beam experiments, AC is not presented usually, and often there is not enough experimental data for calculation of those coefficients. Besides, the most interesting experimental data for molecular beams are obtained for conditions with well-cleaned oriented crystal surface.

Analysis of the papers where the authors provided enough data for calculation of the AC revealed that those coefficients for translational and internal energy might be different significantly. So at a very high translational energy of incident molecules, the rotational AC can be much higher than unity [19, 20]. The effect may be accounted for translational-rotational energy transition during inelastic molecule-surface interaction.

This challenge to the traditional definition of internal energy AC is forced by our experiments with hydrogen. The peculiarity of the hydrogen jet adiabatic expansion at our conditions ($d_*=6$ mm, $P_0=1300$ ÷ $1400$ Pa, $T_0=290$ ÷ $300$ K) is the freezing of the rotational energy just close to the nozzle exit. The probe was placed at distance of $4d_*$ from the nozzle exit. The obtained negative value of rotational AC has been verified by reiterated experiments with different computational treatment. The qualitative stability of results has led to persuasion that the transition of frozen rotational energy at the lowest energy levels to the translational energy of reflected molecules is responsible for the intriguing result. The indirect evidences of the explanation were found in [21, 22]. Studying of molecular hydrogen interaction with the surface (001) MgO, the authors of [21] have observed scattering corresponding to deactivation of rotational energy on definite low levels by inelastic gas surface collisions. In [22], partial conversion of rotational energy into kinetic energy of the scattered molecules by interaction of NO molecules with graphite surface was shown.
On the base of all the said, the general conclusion on internal energy transitions at the collision with a surface can be expressed. The definition of this process, attendant by rotational-translational energy coupling, as accommodation process contradicts to physical content. At least for polyatomic gases, the definition “transformation coefficient” (TC) of energy, which is not limited by the bounds 0 – 1, quite fits for scientific literature.

III. CONCLUSION

The vast variety of experimental data on accommodation coefficients is very insufficient to cover the practical needs in operation with an engineering surface. That is why the elaboration of this method for study of translational and internal energy exchange by gas–surface interaction under conditions similar to reality of technologies is of paramount interest. The proposed method is quite simple and effective tool in receiving of data useful both for comprehension of gas – surface energy exchange and for simulation of gas – surface interaction in real technological applications.

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REFERENCES