Determination of accommodation coefficients of translational and internal energy using a thin wire in a free-molecular flow

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A new experimental–computational method for determination of translational and internal energy accommodation coefficients on a thin wire in a free-molecular flow is elaborated. The method is based on numerical solution of the heat balance equation of the wire. Measurements were performed in a low-density wind tunnel with Ar, He, N2, CH4, and CO2. In addition, the proposed method provides determination of thermophysical properties of the wire. © 2003 American Institute of Physics. [DOI: 10.1063/1.1533098]

I. INTRODUCTION

The thermal accommodation coefficient is determined as the ratio

$$\alpha = \frac{E_i - E_r}{E_i - E_w}$$

where \(E_i\) 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. This value is often used as a measure of energy exchange between the gas and the surface.\(^1\) Such a definition assumes an equal accommodation for the translational and internal energy. By using in Eq. (1) the translational (internal) energy, one can obtain the definition for accommodation coefficients of translational (internal) energy \(\alpha'\) (\(\alpha''\)). Some theoretical and experimental results show that the accommodation coefficients of translational and internal energy may differ considerably.\(^4\)–\(^6\)

Analysis of the heat balance for a wire located in a free-molecular flow allows the separation of the above-mentioned accommodation coefficients. In Ref. 6 the accommodation coefficients were determined using an analytical solution of a simplified heat balance equation proposed in Ref. 7. Those simplifications are unacceptable for a wide range of the wire temperature. They bring essential uncertainties into analysis. This article presents results of determination of accommodation coefficients by accurate numerical solving the heat balance equation with consideration of influence of electrothermophysical parameters of the wire.

II. METHOD

The heat balance for the wire of a unit length is defined by the following equation:

$$c_g \pi r_0^2 \frac{dT_w}{dx} = \frac{T^2}{\pi r_0^2} + \lambda \pi r_0^2 \left(\frac{1}{r_0} - \frac{1}{r_b}\right) + 2 \pi r_0 h(T_r - T_w)$$

$$- 2 \pi r_0 \varepsilon \sigma (T_{w}^4 - T_{r}^4),$$

where \(x\) is the distance measured along the wire; \(T_w\) is the wire temperature; \(r_0\) is the radius; \(c\) is the specific heat capacity; \(g\) is the density; \(I\) is the electric current; \(\rho\) is the specific electric resistance; \(\lambda\) is the heat conductivity coefficient; \(\varepsilon\) is the surface emissivity; \(\sigma\) is the Stefan–Boltzmann constant; \(T_w\) is the temperature of surrounding surfaces; \(T_r\) is the recovery temperature of the wire; \(h\) is the heat transfer coefficient for the given flow parameters. In this work \(\rho, \varepsilon,\) and \(\lambda\) are considered to depend on the temperature: \(\rho = \rho_0(1 + \alpha_0 T), \\lambda = \lambda_0(1 + \beta_0 T), \\varepsilon = \varepsilon_0(1 + \chi_0 T), \rho_0, \varepsilon_0,\) and \(\lambda_0\) are defined at \(T=0^\circ C\).

The boundary condition for Eq. (2) is the wire-holder junction temperature \(T_r\). A correct determination of this temperature is one of the main difficulties in solving the considered problem. It is common for the holder to be massive compared to the wire. If the holder temperature \(T_b\) at a large distance from the junction is measured or evaluated, one can consider \(T_r\) depending on the wire-to-holder heat flux and the holder heat resistance from the junction to the surface with the known temperature \(T_b\). The heat transfer at small distances from the junction \(r \approx r_0\) is assumed to be as in a plane layer and at large distances \(r \gg r_0\) as in a spherical layer. It allows us to obtain a simple approximate evaluation of \(T_b\):

$$T_b = T_b + \frac{q}{2 \pi \lambda b} \left(\frac{1}{r_0 - \frac{1}{r_b}}\right) + \frac{q}{\pi \lambda b r_0},$$

where \(q\) is the heat flux from the wire to the holder (that is determined in calculation through the temperature gradient at the wire end); \(\lambda_b\) is the heat conductivity coefficient of the holder; \(r_b\) is the holder radius. By \(r_b \gg r_0\) one can obtain

$$T_b = T_b + \frac{3}{2} \frac{q}{\pi \lambda b r_0}.$$

To solve Eq. (2) it is necessary to know the heat transfer coefficient \(h\) and the recovery temperature \(T_r\). The kinetic theory of gases is able to find these quantities at convex surfaces in a free-molecular flow.\(^8\) The expressions for \(h\) and \(T_r\) for a cylinder located perpendicular to the flow are given in Ref. 6 for a gas with internal degrees of freedom:

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\[ h = \frac{1}{4\sqrt{\pi}} nk \xi \exp\left( -\frac{S^2}{2}\right) \cdot \frac{U}{2 \cdot [I_0 + S^2(I_0 + I_1)]}, \]  
\[ T_r = \frac{T}{\xi} \left[ \alpha' \left( 2S^2 + 5 - \frac{1}{1 + S^2(1 + I_1/I_0)} \right) + \alpha'' j \right]. \]

where \( n, U, \text{ and } T \) are the number density, velocity, and static temperature of the gas flow; \( S = U/(2kT/m) \) is the speed ratio; \( m \) is the molecular mass; \( k \) is the Boltzmann constant; \( \xi = 4\alpha' + \alpha'' j \); \( j = (5 - 3\gamma)/(\gamma - 1) \) is the number of internal degrees of freedom; \( I_0 \) 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 (\( U = 0 \)) Eq. (4) is reduced to the form of \( T_r = T \), and the wire resistance depends only on complex \( \xi = 4\alpha' + \alpha'' j \) of Eq. (3). So it is possible to separate the accommodation coefficients of translational and internal energy only in the case when there is a directional movement of gas.

In all cases of determination of accommodation coefficients, the trial-and-error method is used with a thorough minimization of errors. A series of experimental measurements of the wire resistance \( R'_k \) is performed by different currents \( I_k \), \( k = 1 \rightarrow N \). Scanning of all suitable pairs of accommodation coefficients \( (\alpha', \alpha'') \) has been accomplished. For each pair \( (\alpha', \alpha'') \) and for each current \( I_k \) Eq. (2) is numerically solved and the temperature distribution along the wire \( T_w(x) = T_w(x, \alpha', \alpha'', I_k) \) is found. Given the temperature distribution, the integral wire resistance is calculated \( R(\alpha', \alpha'', I_k) = \rho_0 / \pi r^2 \int_0^L [1 + \alpha_0 T_w(x, \alpha', \alpha'', J) \] dx \) (\( L \) is the wire length). Then the discrepancy between the computed and experimental resistance \( \Delta_k = R(\alpha', \alpha'', I_k) - R'_k \) is calculated, and the function \( F(\alpha', \alpha'') = \sum_k \Delta_k^2 \) is considered. As the sought-for accommodation coefficients, 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. RESULTS AND DISCUSSION

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

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 of 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 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 electrothermophysical properties of the wire: the specific resistance \( \rho \), the heat conductivity coefficient \( \lambda \), and the emissivity \( \varepsilon \), taking into consideration their dependence on temperature. In these experiments, the wire tips were clamped between the 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 with the isothermal wire. 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 Eq. (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 \( R \) shown in 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:

\[ \varepsilon = 0.05[1 + 0.0035 \cdot (T_w - 273)], \]
\[ \rho = 5.65 \times 10^{-8}[1 + 0.0041 \cdot (T_w - 273)] \text{Om m,} \]

![FIG. 1. 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, \( S = 5.84 \)).](image-url)
At the first stage, the accommodation coefficients 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 accommodation coefficients, a minimal discrepancy between experimental and computational dependencies 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 ($N_2$, $CH_4$, $CO_2$), 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 accommodation coefficients ($\alpha'$, $\alpha''$). The figure, presenting discrepancy

$$\Delta = \sqrt{\frac{1}{N} \sum \Delta^2_i}$$

in dependence on accommodation coefficients, is the three-dimensional one. Figure 2 shows projection of this figure on the $(\alpha', \alpha'')$ plane for nitrogen flow ($L = 9.4$ mm, $S = 4.64$).

Accommodation coefficients averaged over many measurements with different wire probes, gas pressures, and at different distances from the nozzle are presented in Table I. The comparison of results for accommodation coefficients 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 are given at close interaction energy. Comparison of Tables I and II shows qualitative agreement for our data and those from literature.

Determination of accommodation coefficient of internal energy is of particular interest in the proposed method. The available data on such accommodation coefficients are very scanty. In numerous molecular beam experiments, accommodation coefficients are not usually presented, 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 articles where the authors provided enough data for calculation of the accommodation coefficient revealed that those coefficients for translational and internal energy may be different significantly. So at a high energy of incident molecules, the rotational accommodation coefficient can be much higher than unity. This effect may be accounted for translational–rotational energy transition during inelastic molecule–surface interaction.

From the performed experiments, the conclusion can be made that for low energies of molecules (corresponding to the room stagnation temperature) the accommodation coefficients of translational energy are slightly higher than the accommodation coefficients of internal energy. It is confirmed by known theoretical and experimental works.

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 elabo-
ration of this method for the study of translational and inter-

nal energy exchange by gas–surface interaction under con-

ditions 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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