

Interpretation of Impact and Static Pressure Measurements in Non-Equilibrium Supersonic Flow by the DSMC Method

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Abstract. The treatment of impact and static pressure measurements by the DSMC method allows not only to find the corrections to pressure measurements, but to optimize the Pitot tube design. In the result of computational analysis of static pressure values on different surfaces in the supersonic nonequilibrium flow of tetrafluoroethylene, the simple gasdynamic method of determination of polyatomic gas relaxation constants over a wide range of temperature is originally developed. The promising approach is the using measurements in a supersonic nozzle.

Keywords: static pressure, relaxation constant, polyatomic molecule, hypersonic flow, DSMC, tetrafluoroethylene.

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INTRODUCTION

The presented study pursues two main objectives: 1) the extension of works on justification of the direct simulation Monte Carlo (DSMC) method as a powerful instrument for the interpretation of impact and static pressure measurements in non-equilibrium rarefied gas flows; 2) the development of gasdynamic method for determination of relaxation constants of polyatomic molecules at high temperature by static pressure measurements in nonequilibrium flows. The correction factor for the Pitot tube as the ratio of the measured pressure to the pressure behind the shock wave can be calculated for any axisymmetrical probe for any rarefaction, when such correction is essential. The theory of Pitot tube for supersonic rarefied flows has long-run history, well known for specialists in gas dynamics. Here we cite only some of works in this field [1-4]. During last years the studies have appeared where the correction factors are determined by the DSMC method [4, 5]. In our work such calculations have exposed the peculiarities of the supersonic flow formation past the Pitot tube for a wide range of the Knudsen number. The search calculations by the DSMC method were performed on the example of the tetrafluoroethylene (C_2F_4) flows.

A large body of researches of polyatomic gas relaxation time for low-lying states was performed by ultrasonic, optic acoustic, and shock wave methods [6]. Kantroviz work [7] has given impetus to our searches. The conception of [7] is outlined in [8]. It was based on the determination of the relaxation rate on the Pitot tube indications in a subsonic flow, when vibrational energy is partially frozen in the front of the tube. In the present work the use of measurements of the static pressure during polyatomic gas expansion has been studied for assessment of the relaxation constants.

ABOUT USING THE DSMC METHOD

The numerical simulations performed in this study employ the DSMC method [9]. Macroscopic flow quantities (velocity, density, temperature, etc.) are obtained by sampling particle properties over a large number of time steps once a steady state has been achieved. The usual radial weight factor scheme is modified in such a way that particles are discarded during translation phase and multiplied during collisions phase. Collisions are calculated using the majorant frequency scheme [10] with corrections concerning the radial weight factor scheme.

To account for the internal degrees of freedom, the Larsen-Borgnakke model is used [9]. The relaxation rate was recalculated based on recommendations [11]. The local translational temperature T_t and vibrational energy E_V are

determined in each cell as time averaged values through the entire steady part of the calculation. These values are used to calculate the number of collisions necessary for vibrational energy relaxation $Z_V(T_v, T_v)$ and the number of vibrational degrees of freedom $\xi_V(T_v)$. Rotational relaxation is calculated independently using fixed relaxation collision number Z_R and the number of rotational degrees of freedom ξ_R . Only rotational-translational (RT) and vibrational-translational (VT) energy transfer are considered.

ANALYSIS OF SUPERSONIC GAS FLOWS PAST THE PITOT TUBE

High quality experiments were performed by V. A. Suhnev [3] in transition regimes of supersonic air flow with different design of the Pitot tube facade. Fig 1 presents the original data [3] and values calculated by the DSMC method. The correlation between computational and experimental results looks satisfactory.

As a rule the experimental corrections point on excessive values of displayed pressures. In some cases, especially for thin wall tubes for the Knudsen number $Kn = \lambda_f/D \sim 0.1$, the corrections underread the pressure (here λ_f is the mean free path in the flow, D is the external tube diameter). In such cases there is a vortex motion in the open internal part of the tube (Fig.2) (here $d/D = 1$, where d is the internal tube diameter). There is no vortex for $Kn \sim 0.1$. According to experiments [3] at $d/D = 0.1$ in the range of $Kn > 0.03$ the Pitot tube always gives overestimation of pressure.

Basing on previous experiments and our computational analysis for different values of ratio d/D , one can recommend Pitot tubes either with the thin wall ($d/D \sim 1$) mouth or with a small internal diameter ($d/D \sim 0.1$)

The DSMC method allows calculate the static pressure on the tube surface. The correlation of static pressures on the tube surface is the subject of separate studies out of this paper topic.

CONSTRUCTION THE C₂F₄ MOLECULE RELAXATION MODEL

The relaxation model for C₂F₄ gas is constructed on the base of known characteristics of C₂F₄ molecules and properties of gas. The molecular mass is 100 amu. The known dependency for the saturated C₂F₄ vapor pressure in the temperature range of 140 – 300 K [12] shows that the vapor can be considered as an ideal gas. Parameters of the Lennard-Jones (LJ) model are $\sigma = 4.8$ Å, $\varepsilon = 209$ K [13]. The parameters of the variable soft sphere (VSS) model (which was used in DSMC simulation) were determined from temperature dependence of viscosity for LJ model:

for $T_{ref} = 1000$ K: $\alpha = 1.30$; $\omega = 0.71$; $d_{ref} = 5.01$ Å;

for $T_{ref} = 300$ K: $\alpha = 1.50$; $\omega = 0.94$; $d_{ref} = 6.70$ Å.

The C₂F₄ molecule has 12 vibrational degrees of freedom with the following frequencies: 190, 218, 394, 406, 508, 551, 558, 778, 1186, 1337, 1340, 1872 cm⁻¹ [14]. For each vibrational mode, there are energy

$$\varepsilon_v = \frac{R\Theta}{\exp \varphi - 1}$$

and heat capacity

$$C_v = \frac{d\varepsilon_v}{dT} = \frac{R\varphi^2 \exp \varphi}{(\exp \varphi - 1)^2},$$

where R is the universal gas constant, $\Theta = hv/k$ is the characteristic vibrational temperature, h is the Plank constant, v is the vibrational frequency, $\varphi = \Theta/T$. Summing over all the modes, we can calculate the vibrational heat capacity

$C_{vTB} = \sum_v C_v$ and, correspondingly, the total heat capacity $C_p = \frac{5}{2}R + \frac{j_R}{2}R + C_{vTB}$. Given $j_R = 3$, in the range from

50 K to 1000 K, the heat capacity obtained with the use of the vibrational frequencies can be approximated by the polynomial

$$C_p = 22.6 + 0.258 T - 2.63 \cdot 10^{-4} T^2 + 1.25 \cdot 10^{-7} T^3 - 2.23 \cdot 10^{-11} T^4 \text{ J/(mole K)}.$$

The number of active vibrational degrees of freedom is calculated as $j_V = \varepsilon_V/(RT)$.

The model was constructed for the temperature range 100-1000 K with the following assumptions: 1) the molecule is non-polar; 2) the lowest mode is considered as harmonic one; 3) vibrational-translational energy transfer occurs through the lowest mode (with frequency $v = 190$ cm⁻¹); 4) intramolecular equilibrium is set up instantaneously; 5) rotational-vibrational energy transfer is considered as negligible, and rotational-translational relaxation is accounted independently; 6) rotational relaxation collision number Z_R is taken equal to 5 according to [15]; 7) the relaxation rate (the number of collisions necessary for the lowest frequency mode de-excitation) of the C₂F₄ lowest mode is governed by Landau-Teller law, i.e. $\log Z_{10} = A \cdot T^{-1/3} + B$ [16].

Dependence $Z_{10}(T)$ is constructed on the basis of experimental measurements of vibrational relaxation time for relatively low temperature (300 – 400 K). The collision number Z_{10} is determined by relation [16]

$$Z_{10} = c\tau_1 \left(1 - \exp\left(-\frac{\Theta_1}{T}\right) \right),$$

where c is the collision frequency, τ_1 is time for vibrational relaxation of the lowest mode, Θ_1 is the characteristic vibrational temperature of the lowest mode. Time τ_1 is determined as [16]:

$$\tau_1 = \tau_{VIB} C_1 / C_{VIB},$$

where τ_{VIB} is the overall vibrational relaxation time and C_1 is heat capacity of the lowest mode. The collision frequency c was estimated based on the VSS model parameters as [9]

$$c = 4d_{ref}^2 n \sqrt{\frac{\pi k T_{ref}}{m}} \left(\frac{T}{T_{ref}} \right)^{1-\omega}.$$

Here we use the model with $\omega = 0.7$ and $d_{ref} = 5.8 \text{ \AA}$ at $T_{ref} = 300 \text{ K}$ as “intermediate” for 300–1000 K range. As a result, for $T = 300 \text{ K}$ we have $Z_{10} = 15.5$ from relaxation time $\tau_{VIB} = 17 \text{ ns}$ [16], for $T = 373 \text{ K}$, $Z_{10} = 8.2$ from time $\tau_{VIB} = 14 \text{ ns}$ [6]. Given these two values of Z_{10} , the temperature dependence is obtained as

$$\log Z_{10}(T) = 26.4 T^{-1/3} - 2.76.$$

This formula is used for preliminary analysis.

Knowing Z_{10} dependence, the number of collision necessary for relaxation of the overall vibrational energy is:

$$Z_V = c\tau_{VIB} = \frac{Z_{10}(T_t)}{1 - \exp\left(-\frac{\Theta_1}{T_V}\right)} \frac{C_{VIB}(T_V)}{C_1(T_V)},$$

where T_t is the translational temperature and T_V is the vibrational one.

ANALYSIS OF STATIC PRESSURE MEASUREMENTS IN C₂F₄ FLOWS

The following numerical experiments were performed for jet flows behind the sonic nozzle with the critical section diameter $d^* = 10 \text{ mm}$ at the stagnation temperatures $T_0 = 300 \text{ K}$ and 1000 K at different pressures corresponding to $Kn_0 = \lambda_0/d^* = 9.3 \cdot 10^{-4}$ (here λ_0 is the mean free path in the stagnation chamber). The flow in the critical section is assumed to be plane parallel. The temperature of the nozzle surfaces is taken equal to the stagnation temperature.

Fig. 3 shows the stream lines of the jet flow of C₂F₄ past the Pitot tube. The calculations have shown that the stagnation temperature variation for the same Knudsen number has negligible effect on the static pressure distribution on the tube surface. Strong shock effect on the tube nose can be possible reason of this result.

The reduction of shock effect is seemingly possible on the surface of a very sharp cone. Fig. 4 shows the flow structure along the cone with half angle 5° . The cone apex is located on the distance 30 mm from the nozzle, where the Mach number $M \sim 4.5$. The peculiarity of the flow is formation of the shock layer in the vicinity of the cone surface. Stream lines are almost parallel to the cone profile. It was found that for $Kn_0 = 9.3 \cdot 10^{-4}$, temperature variation in the range $T_0 = 300 - 1000 \text{ K}$ practically has no effect on the relative static pressures on the cone surface.

The encouraging results were obtained from analysis of flow around and inside of the short tube with zero thickness of the wall, with diameter 10 mm and length 30 mm , being distant 30 mm from the nozzle. One can see the flow structure (Fig. 5) and the static pressure distribution on the internal surface of the tube (Fig. 6). It is worth noting that the static pressure of the external surface proved to be not sensible to change of T_0 . At $T_0 = 300 \text{ K}$ and 1000 K and fixed $Kn_0 = 9.3 \cdot 10^{-4}$ in both cases the transonic flow is established inside of the tube with shock wave in the open part. It is possible that just forming such a flow is responsible for the difference of static pressure on the internal surface of the tube at above T_0 and different tube temperature. Fig. 6 presents the distribution of the static pressures along the internal generatrix of the cylinder for all cases: 1, 2) $T_0 = 1000 \text{ K}$; $T_w = 1000 \text{ K}$, 300 K ; 3, 4) $T_0 = 300 \text{ K}$; $T_w = 1000 \text{ K}$, 300 K . Here T_w is the wall temperature. In cases 1, 3, 4 shock wave is straight, in the case 2 it is oblique. One can see that the pressure difference at some points of the inner surface of the tube at different stagnation temperatures can be measured by precise instrument (baratrons) with high accuracy. Results of these measurements can be used for determination of relaxation constants.

ANALYSIS OF C₂F₄ FLOW IN THE SUPERSONIC NOZZLE

The difficulties of static pressure measurements in a free flow have pushed authors to analyse behavior of the static pressure on the wall of the Laval nozzle supersonic part. For the search numerical experiment, the conical nozzle with angle of expansion 40°, critical diameter 10 mm, and length 50 mm was chosen.

The search computational modeling was performed for the cases at T_0 equal to 300 K and 1000 K and $Kn_0 = 9.3 \cdot 10^{-4}$. Fig. 7 shows the results of calculations of the static pressures for mirror reflecting walls with the extracted relaxation effect (curve 1,2) and for the case of full accommodation (curves 3,4). In the first case the difference of the static pressures close to the nozzle exit reaches more that 100% (higher pressure for higher temperature). In the second case (with influence of boundary layer) the difference of pressures in the same region reaches about 35%.

Analysis of this effect has shown that it is not only the influence of V-T relaxation, but changing the flow in the nozzle due to displacement by the boundary layer. One can make an important conclusion: for reasonably known accommodation coefficient of vibrational energy on the wall and negligible slip of the flow, it is possible to calculate not only the relaxation constants, but the effective collisional cross-section of polyatomic molecules at different temperatures.

Modern precise instruments for low pressure measurements (baratrons) have the error not higher than 1%. It allows to expect that experimental data can be used for determination of relaxation constants.

Thus the obtained results show that measurements of static pressure in the nozzle and their treatment by the DSMC method open new way for collisional kinetic studies.

Experiments with supersonic nozzle are highly attractive for the following reasons:

- 1) the effect of relaxation is traced in the flow over a wide range of temperature in one experiment, the whole run of static pressure along the nozzle is valuable for analysis;
- 2) the technique of pressure measurements on the nozzle wall is simple in realization.

CONCLUSION

The DSMC method is a powerful instrument for treatment of impact and static pressure measurements. From experiments and calculations, the recommendation on the pressure probe design can be formulated.

As far as the static pressure is the most sensible parameter to the influence of relaxation in flows, its direct or indirect measurement allows to evaluate the relaxation constants and their dependences on temperature.

The most promising method for determination of relaxation constants of polyatomic gases over a wide range of temperature without solution huge problems with sophisticated technique is analysis the static pressure behavior along the supersonic nozzle.

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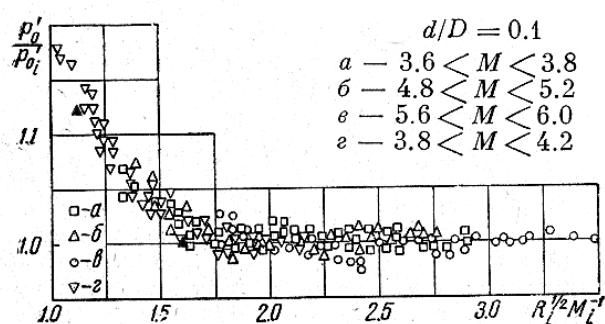


FIGURE 1. Correction factors for the Pitot tube ($d/D = 0.1$) obtained by the DSMC calculation (filled symbols) in comparison with experimental data [3] (hollow symbols). R_i and M_i are the Reynolds and Mach numbers.

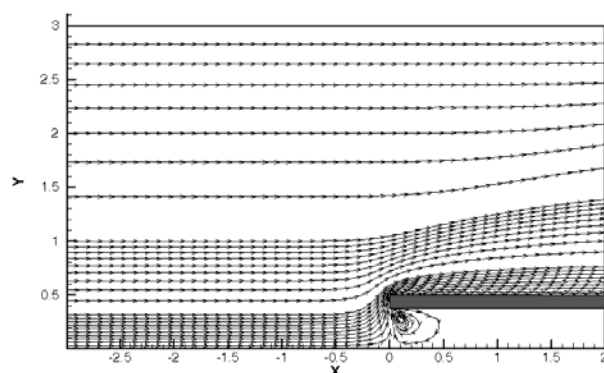


FIGURE 2. Stream lines around the Pitot tube ($d/D = 0.75$) placed into the plane-parallel flow of air for $M_\infty = 5$, $T_0 = 300$ K, $Kn_\infty = 0.114$.

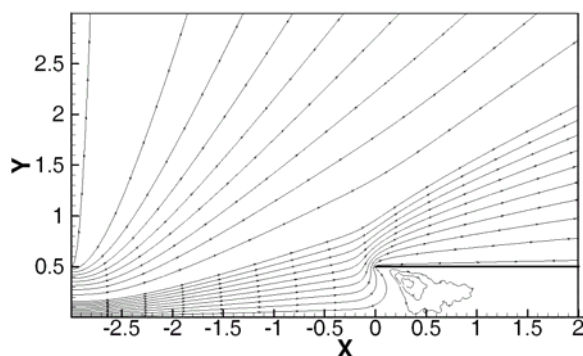


FIGURE 3. Stream lines in C_2F_4 jet flow past the $d/D = 1$ Pitot tube; $T_0 = 1000$ K; $P_0 = 10$ torr ($Kn_0 = 9.3 \cdot 10^{-4}$).

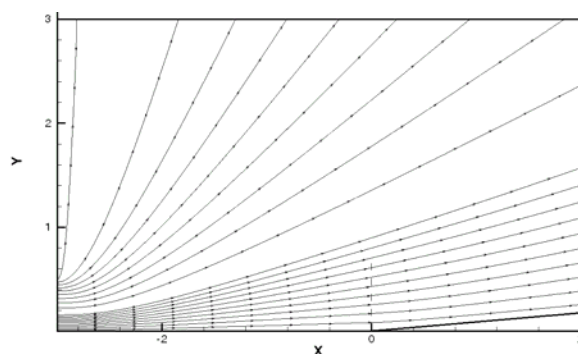


FIGURE 4. Stream lines around the 10° cone in the C_2F_4 jet; $T_0 = 1000$ K; $P_0 = 10$ torr ($Kn_0 = 9.3 \cdot 10^{-4}$).

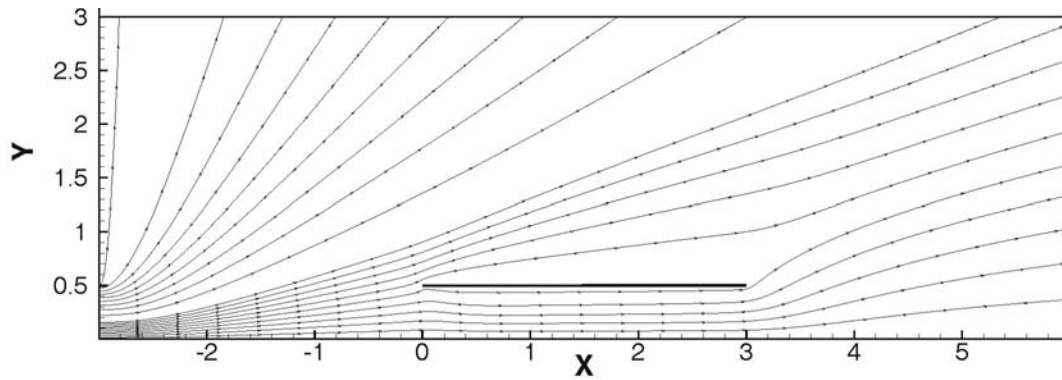


FIGURE 5. Stream lines around the open $L/d = 3$ tube in the C_2F_4 jet; $T_0 = 1000$ K; $P_0 = 10$ torr ($Kn_0 = 9.3 \cdot 10^{-4}$).

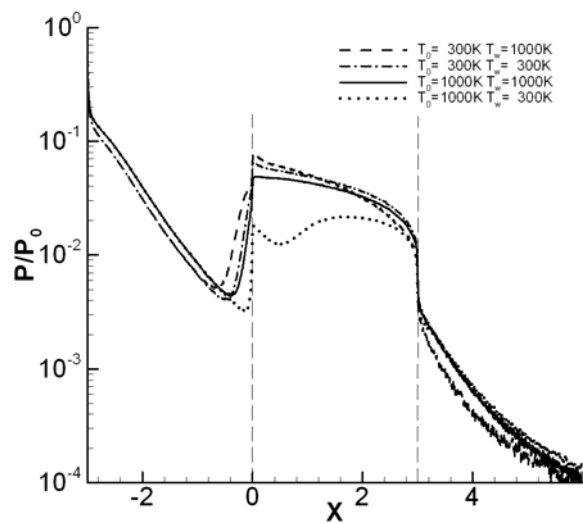


FIGURE 6. Static pressure on the inner wall of the tube and in the flow along the tube generatrix. Tube is placed into the C_2F_4 jets with different temperatures for $Kn_0 = 9.3 \cdot 10^{-4}$.

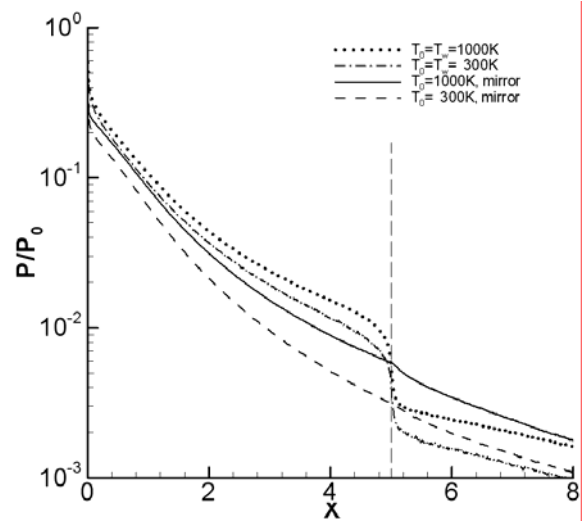


FIGURE 7. Static pressure of C_2F_4 on the wall of the 40° cone nozzle and farther in the flow parallel to axis for $Kn_0 = 9.3 \cdot 10^{-4}$ with $T_0 = 300$ K and 1000 K.