Stability of axisymmetric supersonic submerged microjet of nonequilibrium sulphur hexafluoride

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Abstract. The influence of vibrational excitation and relaxation of molecules of gaseous sulphur hexafluoride (SF$_6$) on the gas-dynamic structure and stability of high-velocity microjets flowing out of axisymmetric convergent micronozzles is studied numerically. The present numerical simulations are performed with allowance for vibrational relaxation of molecules with the use of a two-temperature model of relaxing flows by means of solving unsteady Navier-Stokes equations in a 3D formulation. The effects of vibrational relaxation of gas molecules on the gas-dynamic structure, intensity of disturbances, and length of the supersonic core of microjets are considered.

1. Introduction

Supersonic jet microflows of polyatomic gases may involve physical effects associated with internal degrees of freedom of molecules. In particular, in supersonic microflows of some vibrationally excited gases, the characteristic spatial scale of vibrational relaxation becomes comparable with the jet flow scale. Effects associated with vibrational relaxation of molecules may lead to changes in the gas-dynamic structure of microjets, loss of stability of the gas flow, and reduction of the supersonic core length. The influence of vibrational relaxation on jet microflows has to be studied because of potential applications of such microflows in macroflow control problems, thermal protection of various surfaces, intensification of mixing, and creation of devices for local thermal actions.

The present paper describes a numerical study of the influence of vibrational excitation and relaxation of molecules of gaseous sulphur hexafluoride (SF$_6$) on the gas-dynamic structure and stability of high-velocity microjets flowing out of axisymmetric convergent micronozzles. SF$_6$ was chosen as a test gas because these molecules ensure large contributions of vibrational degrees of freedom to the internal energy of the gas already at room temperature or minor heating. The time of vibrational relaxation of SF$_6$ depends on temperature and pressure. At atmospheric pressure, the characteristic time of vibrational-translational relaxation of SF$_6$ is short, which allows the influence of molecule nonequilibrium to be neglected at macroscales. However, this influence should be taken into account in high-velocity microflows. Table 1 shows the spatial scale of relaxation $c\cdot\tau_{vt}$ for different temperatures ($c$ is the equilibrium velocity of sound in the gas and $\tau_{vt}$ is the time of vibrational relaxation). The data are given in accordance with [1]. Table 1 also shows the Reynolds numbers Re$_d$ based on the nozzle diameter $d = c\cdot\tau_{vt}$ equal to the characteristic spatial scale of relaxation and on the parameters of equilibrium nonisobaric exhaustion in the nozzle throat with the use of the data reported in [2]. Here the jet pressure ratio $n$ is equal to 1.363.
Table 1. Spatial scale of vibrational relaxation.

| Temperature (K) | Relaxation length (μm) | Reynolds number |
|-----------------|------------------------|-----------------|
| 300             | 115                    | 8400            |
| 450             | 70                     | 3500            |
| 600             | 50                     | 1450            |

It is seen that both the spatial scale of relaxation and the Reynolds number $Re_d$ corresponding to this scale rapidly decrease with an increase in temperature. For supersonic axisymmetric air microjets, it was experimentally demonstrated in [3] that jet flows with $Re_d$ higher than 2000 are turbulent. Therefore, it is difficult to expect the nonequilibrium state of high-velocity SF$_6$ jets to produce a significant effect on the transition to turbulence at room temperature because the characteristic value $Re_d = 8400$ in Table 1 is too high. At the same time, as the gas is heated to 600 K, the characteristic value is $Re_d = 1600$, which may be close to the Reynolds number of the laminar-turbulent transition, and vibrational nonequilibrium of SF$_6$ molecules can significantly affect the stability and jet penetration distance of these microflows. Therefore, the domain of interest of the present study was limited to the stagnation temperature of 600 K and to the interval of nozzle diameters $d = 13.75 - 110$ μm, which ensure exhaustion into the ambient space with the Reynolds numbers $Re_d = 400 - 3200$. The effects of the diameter of the convergent micronozzles on the gas-dynamic structure, stability, and penetration distance of supersonic microjets with and without allowance for vibrational relaxation (equilibrium microjets) was studied. The influence of vibrational relaxation of the gas on the microflow was determined through comparisons of the mean flow parameters, oscillations, and supersonic core length for nonequilibrium and equilibrium jets.

2. Numerical simulation

In the present work, SF$_6$ flows were numerically simulated by using the ANSYS Fluent software for solving three-dimensional unsteady Navier-Stokes equations with the use of a density-based solver (hereinafter the ANSYS Fluent terminology is used), implicit scheme of the second-order accuracy in space with the Roe-FDS method of convective flux splitting, and explicit Runge-Kutta method in time. The thermal conductivity of the test gas was specified by the formula from the kinetic theory, and the gas viscosity was determined by approximating the data [2] by a polynomial dependence on temperature. The energy of vibrational degrees of freedom was calculated from the characteristic vibrational temperatures in the harmonic oscillator approximation. Sulphur hexafluoride has 15 vibrational modes characterized by six vibrational temperatures $\theta_n = \{1114, 926, 1364, 885, 753, 499\}$ (K). Two cases (equilibrium and nonequilibrium) were considered in SF$_6$ simulations. In the equilibrium test case, the specific heat at constant pressure $c_p$ was determined as a function of the gas temperature $T$ and characteristic vibrational temperatures $\theta_n$ with the multipliers $r_n = \{1, 2, 3, 3, 3, 3\}$ corresponding to mode degeneration

$$\frac{c_p}{R} = 4 + \sum_{n=1}^{6} r_n \frac{(\theta_n/T)^2 \exp(\theta_n/T)}{(\exp(\theta_n/T) - 1)^2},$$

where $R$ is the specific gas constant.

The nonequilibrium state of vibrational degrees of freedom of SF$_6$ molecules was modeled by the two-temperature model of relaxing flows, where the change in the energy of each vibrational mode in time was determined by the Landau-Teller equation

$$\frac{df_{v,n}}{dt} = \frac{1}{\tau_{vt}} \left( e_{v,n}^{eq} - e_{v,n} \right).$$

Here $e_{v,n}$ is the vibrational energy of the $n$-th mode, $e_{v,n}^{eq}$ is the local value of the equilibrium vibrational energy of the $n$-th mode, and $\tau_{vt}$ is the time of vibrational relaxation, which was assumed to be identical for all vibrational modes in the present study. The equilibrium energy of vibrational degrees of freedom was found by the formula
\[ e_{\text{eq},n} = \frac{\theta_n}{e^{\theta_n/T_{\text{tr}}-1}} R, \]

where \( T_{\text{tr}} \) is the temperature of translational-rotational degrees of freedom.

Using the approaches described in [4] and also the UDS (User Defined Scalar) and UDF (User Defined Function), which are user's modules built into the code, we supplemented the Navier-Stokes equations with the equations of conservation of vibrational energy of SF\textsubscript{6} molecules. The energy exchange between the vibrational and translational-rotational degrees of freedom with a finite relaxation time was also modeled with the use of UDF by means of adding the source term \( q_{\text{tv,n}} \) calculated by the Landau-Teller equation to the built-in equations of conservation of vibrational energy for each vibrational mode. To eliminate energy balance violations in the Navier-Stokes equations, the same expressions with the opposite sign were added to the equations for translational-rotational energy:

\[
\frac{\partial}{\partial t} (\rho E_{\text{tr}}) + \nabla [u(\rho E_{\text{tr}} + P)] = \nabla (\lambda \nabla T_{\text{tr}} + \tau_{\mu} u) - \sum_{n=1}^{6} r_n q_{\text{tv,n}}
\]

\[
\frac{\partial}{\partial t} (\rho e_{\text{v,n}}) + \nabla (u \rho e_{\text{v,n}} - \mu \nabla e_{\text{v,n}}) = q_{\text{tv,n}}
\]

Here \( \rho, P, \) and \( \lambda \) are the density, pressure, and thermal conductivity, \( u \) is the velocity vector, \( \tau_{\mu} \) is the viscous stress tensor, \( E_{\text{tr}} = \int_{T_{\text{ref}}}^{T_{\text{tr}}} c_{p,\text{ref}} dT - \frac{P}{\rho} + \frac{u^2}{2} \) is the translational-rotational energy of the gas, and

\[ q_{\text{tv,n}} = \frac{\rho}{\tau_{\text{tr}}} (e_{\text{eq},n} - e_{\text{v,n}}). \]

The time of vibrational relaxation of SF\textsubscript{6} molecules was calculated by means of approximating the data [1] by the dependence, which has the form

\[ P \cdot \tau_{\text{tr}} = \exp \left( 38.8 T_{\text{tr}}^{-1/3} - 8.126 \right) \text{ [Pa} \cdot \text{s]} \]

The estimates [5] show that the gas pressure exerts minor effects on the physical and thermophysical properties of SF\textsubscript{6} at moderate stagnation pressures of the order of 2 – 3 atm, and the equation of state for a perfect gas can be used.

For modeling axisymmetric microjets with allowance for the flow in the real nozzle duct, we defined a computational domain shown in Figs. 1a and 1b.

\[ \text{Figure 1. Section (a) and isometric pattern (b) of the computational domain contour and fragments of the computational grid near the nozzle throat in the plane (x,y) for z = 0 (c) and in the plane (y,z) for x = 16d (d). 1 – input boundary, 2 – wall, 3 – output boundary.} \]

The computational domain contained a subdomain of the nozzle duct with the settling chamber, which was finalized by the throat cross section with the radius \( d/2 \), and also a subdomain of jet exhaustion with the axial and radial sizes equal to 25\( d \) and 10\( d \), respectively. The domain was covered by a structured hexahedral grid, which was refined in the core flow and mixing region in the radial direction and in the nozzle throat region in the streamwise direction. An example of fragments of the computational grid near the nozzle throat in the plane (x,y) for z = 0 is shown in Fig. 1c, and that in the plane (y,z) for x = 16\( d \).
is shown in Fig. 1d. The computational domain contained approximately $N \approx 10^7$ grid cells. The parameters imposed on the left boundary of the computational domain (settling chamber) were the total pressure and temperature of the gas ($P_0$ and $T_0$). The external boundaries of the ambient space were subjected to the condition of exhaustion of the same gas with $P_{\text{inf}} = 0.1013$ MPa and $T_{\text{inf}} = 300$ K into the atmosphere. The nozzle wall temperature both in the settling chamber and on the boundary with the ambient space was set at $T_w = 600$ K. Nonequilibrium SF$_6$ jets were numerically simulated only at one value of the total pressure $P_0 = 0.2332$ MPa and temperature $T_0 = 600$ K, which corresponded to $n = 1.363$. The computations were performed in a three-dimensional formulation for different diameters of convergent nozzles. Depending on the value of $Re_d$, either the LES or DNS formulation of the problem was used. The criterion for choosing the DNS approach was the value of $Re_d < N$. Both the nonequilibrium and equilibrium exhaustion was considered; in the latter case, the specific heat of the gas was taken to be a function of temperature $c_p = c_p(T)$ and relaxation processes were ignored. The initial flow field was the steady solution of the equilibrium problem. When the nonequilibrium problem was solved, an initial perturbation was imposed on the flow field owing to significant changes in the gas flow parameters. Then an unsteady computation was performed until steady mean parameters of the flow were reached, after which the mean and fluctuating flow characteristics were computed.

3. Results of experiments and numerical simulations of SF$_6$ jets

Figure 2 shows the instantaneous numerical Schlieren visualization (integral $y$-components of the density gradient in the $z$-direction) of the computed nonequilibrium (a) and equilibrium (b) supersonic SF$_6$ jets flowing out of the nozzles of different diameters: 13.75 $\mu$m (1), 20 $\mu$m (2), 27.5 $\mu$m (3), 55 $\mu$m (4), and 110 $\mu$m (5). Flow turbulence is observed in the numerical simulations of both nonequilibrium and equilibrium microjets in the considered range of $Re_d$. However, the length of the laminar region in nonequilibrium jets is appreciably greater than that in equilibrium jets. Thus, the influence of effects associated with the finite time of vibrational relaxation on the development of disturbances and on the laminar-turbulent transition in these flows is observed. It is also seen in Fig. 2 that
the flow fields of all jets contain wave cells corresponding to image brightness variations. However, the number and sizes of these cells visible in the figure are different for equilibrium and nonequilibrium jets. In the equilibrium case, the jet contains a large number of wave cells, but there are only 2-3 cells visible in the image in the nonequilibrium case, and their streamwise sizes and contrast in the image are significantly smaller than in the equilibrium case. Thus, the influence of vibrational relaxation on the gas-dynamic structure of the jet is manifested as smaller variations of flow parameters along the wave cells. These effects can be explained by manifestation of the properties of frequency dispersion of sound in the gas with vibrational relaxation [6]. By analogy with acoustics, where sound propagation in a nonequilibrium gas exhibits dispersion of the velocity of sound depending on the disturbance wave length, here the wave cell size depends on the flow scale. Moreover, as sound dispersion involves the so-called molecular absorption, which reaches the maximum intensity at wave lengths $\lambda \sim c \cdot \tau_{\text{rel}}$, the pressure variations on the wave cells of a similar scale also become smaller.

The effect of attenuation of flow parameter variations is illustrated in Fig. 3a, which shows the mean velocity $U$ at the axis of the jet flowing out of the nozzle with the diameter $d=55 \, \mu m$ for the nonequilibrium (1) and equilibrium (2) SF$_6$ jets. It is seen that the amplitude of variations of the equilibrium jet flow velocity and also the number and sizes of the wave cells are greater than the corresponding values in the nonequilibrium case. Moreover, the characteristic drastic decrease in the mean velocity corresponding to flow turbulization occurs faster. For the nonequilibrium jets, the drastic decrease in velocity occurs in the flow region where the wave cells are absent, i.e., in the isobaric flow region. Attenuation of flow parameter variations in the nonequilibrium jet leads to reduction of the amplitude of disturbances owing to the decrease in the number of the wave cells and attenuation of their intensity as generation sources.

![Figure 3](image-url)

**Figure 3.** Velocity (a) and root-mean-square fluctuations of velocity (b) at the axis of the SF6 jet flowing out of the nozzle with the diameter $d=55 \, \mu m$ for $n=1.363$ and $T_0=600 \, K$ in the nonequilibrium (1) and equilibrium (2) flows.

Another factor affecting the development of disturbances is more intense molecular absorption of sound in the gas with vibrational relaxation as compared to the nonequilibrium gas. Figure 3.b shows the amplitude of the root-mean-square fluctuations of velocity $U'$ at the jet axis. It is seen that the amplitude of equilibrium jet flow velocity fluctuations in the near flow field rapidly increases and becomes greater than the amplitude of velocity fluctuations in the nonequilibrium jet almost by an order of magnitude. The distance between the peak values of the intensity of velocity fluctuations corresponds to the wave cell size. Further downstream, the disturbances are exponentially enhanced and the jets transform to the turbulent state. The disturbance growth rates are also slightly higher in the equilibrium case. Because of the combination of the rapid increase in the amplitude in the near flow field and the higher growth rates of disturbances in the equilibrium jet, the laminar-turbulent transition occurs faster and the supersonic core length is smaller than in the nonequilibrium jets.

Figure 4 shows the supersonic core length $L_c$ for the nonequilibrium (1) and equilibrium (2) microjets as a function of $Re_\theta$. The supersonic core length (jet penetration distance) was calculated from the
condition of equality of the axial values of the mean velocity of the jet to the equilibrium velocity of
sound calculated on the basis of the averaged translational temperature of the gas.

$$L_c/d$$

![Figure 4. Supersonic core length of the nonequilibrium (1) and equilibrium (2) microjets.](image)

It is seen that the supersonic core length in the nonequilibrium microjets at $Re_d > 400$ is greater than that of the equilibrium microjets. The maximum predicted jet penetration distance also turned out to be greater for the nonequilibrium flow. The maximum supersonic core length characterizes the jet stability because it is actually determined by the maximum length of the limiting laminar flow in terms of $Re_d$. Therefore, the value of $Re_d$ corresponding to reduction of the supersonic core length can be considered as a criterion of the laminar-turbulent transition in the jets. In the present numerical simulations these values were estimated to be $Re_d \approx 700$ for the nonequilibrium flow and $\sim 500$ for the equilibrium flow.

Conclusions
The influence of vibrational excitation and relaxation of SF6 molecules on the gas-dynamic structure and stability of moderately underexpanded supersonic microjets flowing out of axisymmetric convergent micronozzle into the ambient space has been numerically studied. For the test conditions of the present study, vibrational relaxation of the gas affects the gas-dynamic structure of the microjets, as well as the intensity of disturbances and their growth rates in the mixing layer. The number and streamwise sizes of the wave cells and also the intensity of pressure fluctuations in the near flow field in the nonequilibrium jets are smaller than the corresponding values for the equilibrium jets. As a result, the Reynolds number of the transition to the turbulent flow and the supersonic core length in the nonequilibrium jets are greater than in the equilibrium gas.

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