This paper presents the results of numerical studies of rotational-translational nonequilibrium, kinetic, and diffusive processes in spherical expanding gas flows. Computations are made using the direct simulation Monte-Carlo (DSMC) method [1, 2] and the solver [3] of the Navier-Stokes equations in terms of classical and quantum concepts [3-7], at the Knudsen numbers \( Kn^* \) from 0.0015 to 0.03 and pressure ratios \( P = p_0/p_a \) from 100 to 10,000.

Fig. 1 Left: Rotational \( T_R \) (filled markers) and translational \( T_t \) (empty markers) temperatures in spherical flow at various pressure ratios: \( P = 17.6 \) (circles), 78.9 (triangles), and 175.7 (squares). Right: \( T_R \) and \( T_t \) at various relaxation parameters: \( B^* = 17 \) and 95.2.

Experimental studies of underexpanded \( N_2 \) jets [8, 9] discovered a delay of rotational temperature \( T_R \) compared to the translational one \( T_t \). A drop in the gas density downstream leads to a decrease in the number of collisions and the \( T_R \) departure from the equilibrium value [6]. The Navier-Stokes equations and relaxation equation, based on the \( \tau \)-approximation [7], are solved by the numerical method [3]. Solutions depend on Reynolds number \( Re^* \), \( P = p_0/p_a \), temperature \( T_a \) and relaxation parameter \( B^* \) that is calculated as a ratio of \( p\tau_R \) and viscosity. Here index "a" refers to background conditions and index * refers to sonic conditions. The distributions of \( T_R \) and \( T_t \) at \( Re^* = 161.83 \), \( B^* = 28.4 \), \( T_a = 295 \) K, and various \( P \) values are shown in Fig. 1 (left). Computations confirm the delay of \( T_R \) compared to \( T_t \). Inviscid flow parameters \( T_R \) and \( T_t \) were estimated in [6]. The decrease of the main relaxation parameter \( B^* \) leads to a faster "frozen" value of \( T_R \) in the supersonic-flow zone (see Fig. 1, right). The spherical flow could be separated by the coordinate \( R_S \), at which the stream parameters are extreme, into two regions with different properties [10]. In the first "internal" region the flow is supersonic. The flow parameters depend on the Reynolds numbers \( Re^* \) and \( Re_S \) (or related Knudsen numbers \( Kn^* \) and \( Kn_S \)) [6]. In the second "external" region, there is a transition of supersonic flow through the spherical shock wave into a subsonic stream. The Reynolds number \( Re_a \) (or related Knudsen number \( Kn_a \)) based on the length scale parameter at infinity, \( R_a = r\sqrt{P/\rho} \) [11], is the major similarity parameter in this region. The similarity factor \( K_2 = Re_a = Re^*P^{1/2} \) [11] can be used to study the flow structure here. The major changes of \( T_R \) and \( T_t \) occur in the shock wave at values of the normalized distance parameter \( t/R_a \) about 1. The shock width decreases with increasing \( K_2 \).
At the decrease of $T_t$, adiabatic collision conditions [12] should be taken into account, and the relaxation time $p \tau_R$ increases due to the sharp decrease of the rotational transfer probabilities. Following [4], $p \tau_R$ values were calculated for $N_2$ at stagnation temperature $T_0 = 295$ K [see Fig. 2, left] under the conditions of aerodynamic experiments in underexpanded jets [6-9]. At $T_t > 273$ K, numerical results correlate well with experimental data [14, 15]. In the expansion of nitrogen, starting at $T_0 = 300$ K, the maximum population of molecules occurs at rotational levels $j^*$ from 6 to 4 [4]. The results of calculating $p \tau_R$ for $j^* = 6, 5,$ and 4 are shown in Fig. 2 (left). The calculations based on the classical concept [13] (see solid line in Fig. 2, left) do not show a tendency of increasing $p \tau_R$ with the decrease of $T_t$ at $T_t < 100$ K.

For qualitative estimations, the energy relaxation time is replaced by the relaxation time of the level $j^*$. Figure 2 (right) shows the distributions of rotational temperature $T_R$ along the axis of $N_2$ jet at $B_j = (pur/p\tau_R)_j = 2730$, $p ur_j = 240$ torr·mm and $T_0 = 295$ K. The result of using the classical mechanics concept [13] (solid line) does not correlate the experimental data (filled squares [8], triangles [9]) for $T_R$, which are lower and upper bounds on the distribution of rotational energy along the $N_2$ jet axis. Numerical results, based on the quantum concept for values of $p \tau_R$ at $j^* = 6$ and 5, correlate with the experimental data [9].

Fig. 2: Left: The rotational relaxation parameters $p \tau_R(T_t)$ in $N_2$ expanding into a vacuum. Right: The rotational $T_R$ temperature in freejet expanding flow of $N_2$.

Fig. 3: Argon mole fraction distributions (left) and species temperatures (right) in spherical expanding flow of $Ar$-$He$ mixture at different Knudsen numbers $Kn$ and pressure ratios $P$.

Kinetic and diffusion effects in spherical expanding $Ar$-$He$ flows (mole fraction $f_{Ar} = 0.5$) were studied using the DSMC method [2] at $Kn$ from 0.0015 ($Re_s = 1240$) to 0.015 ($Re_s = 124$) and $P$ from 100 to 10,000. Both phenomena influence the shock thickness, parallel and transverse species' temperatures, diffusive velocities, and species separation. Distributions of $f(Ar)$ and species temperatures are shown in Fig. 3. The species concent-
ratio changes insignificantly at r < R_a. Accumulation of the light component occurs in the spherical shock (see Fig. 3, left) due to baro-diffusion effects [2]. For near-continuum flow conditions at K_2 =12.4, the DSMC data correlates with solutions of the Navier–Stokes equations [16] (see Fig. 3, left). In contrast to the one-temperature continuum approach [16], the DSMC method allows simulating multi-temperature kinetic media. It is found that T(He) increases more rapidly than T(Ar) in the supersonic zone at r < R_a (see Fig.3, right).

In supersonic flow, the effect of freezing the parallel temperature TX found in [1] is confirmed (see Fig. 4, left). The freezing comes first for heavier molecules (Ar) at smaller values of Kn. The transverse temperature TY for both species follows the temperature in the isentropic expansion [1, 2]. The spherical expansion of a binary gas mixture into a flooded space was analyzed in the case of the presence of a diffusive flux at the infinity r >> R_a. The numerical results were calculated for the case of the expansion of Ar with little He content (f_{Ar,*} = 0.99) into a space filled by He with a small admixture of Ar (f_{Ar,a} = 0.02). The distributions of argon concentration f_{Ar}, number density, and pressure at Kn = 0.014, Re = 78.5, and K_2 = 0.785 are shown in Fig. 4 (right). The case of the expansion of He into a space filled by Ar was analyzed in [2]. The results demonstrate that the background gas does not penetrate through the spherical shock wave into the inner supersonic region of the flow.

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