KINETIC AND QUANTUM PHENOMENA IN EXPANDING GAS FLOWS

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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.

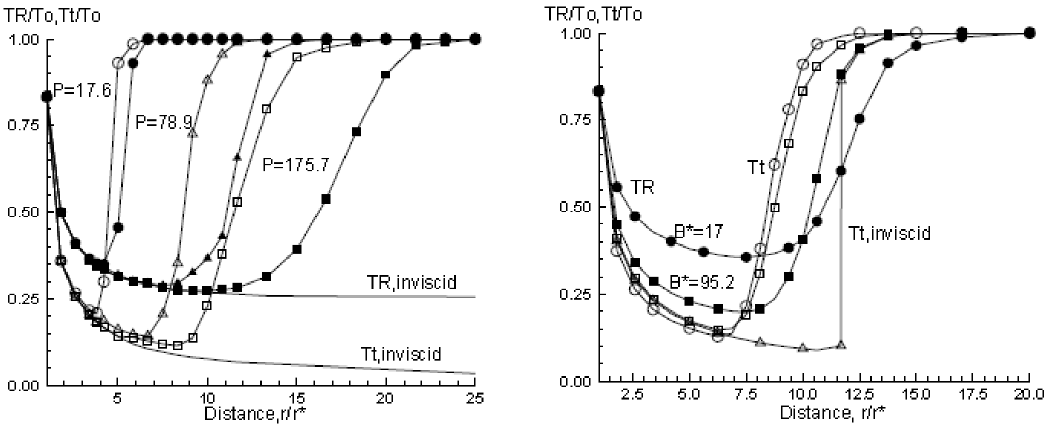

Fig. 1 *Left*: Rotational T_R (filled markers) and translational T_t (empty markers) temperatures in spherical flow at various pressure ratios: P = 17.6 (circles), 78.9 (triangles), and 175.7 (squares). *Right*: T_R and T_t at various relaxation parameters: B_* = 17 and 95.2.

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 τ-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, $R_a = r_* P^{1/2}$ [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 r/R_a about 1. The shock width decreases with increasing K_2.

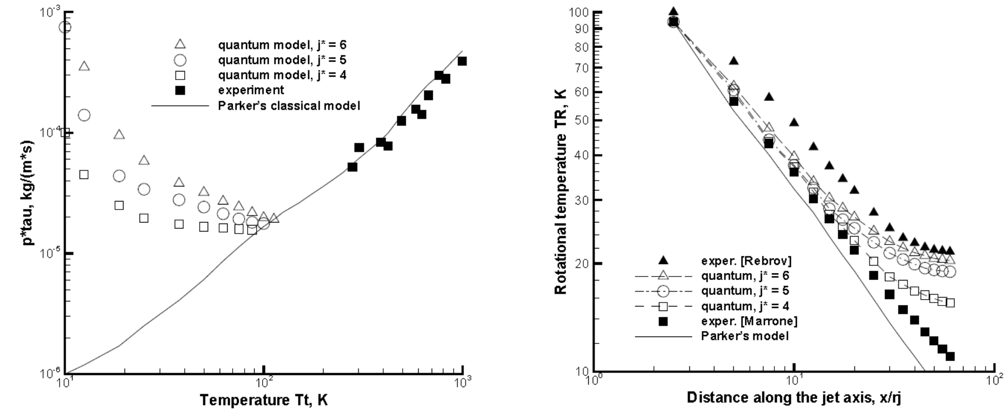

Fig. 2: *Left*: The rotational relaxation parameters $p\tau_R(T_t)$ in N_2 expanding into a vacuum. *Right*: The rotational T_R temperature in freejet expanding flow of N_2.

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 $B_{*j} = (\rho ur/p\tau_R)_{*j}$ = 2730, p_0r_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].

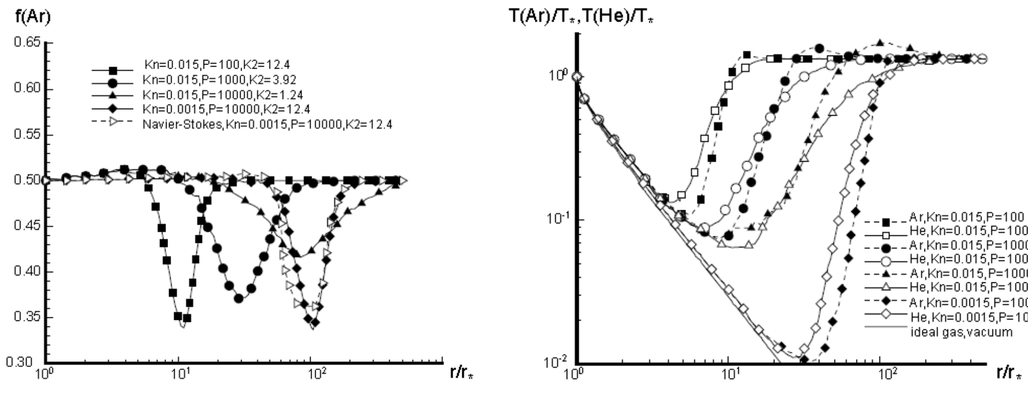

Fig. 3 Argon mole fraction distributions (*left*) and species temperatures (*right*) in spherical expanding flow of *Ar-He* mixture at different Knudsen numbers Kn_* and pressure ratios *P*.

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_* = 1240) to 0.015 (Re_* = 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 concentration 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 Fig3, *right*).

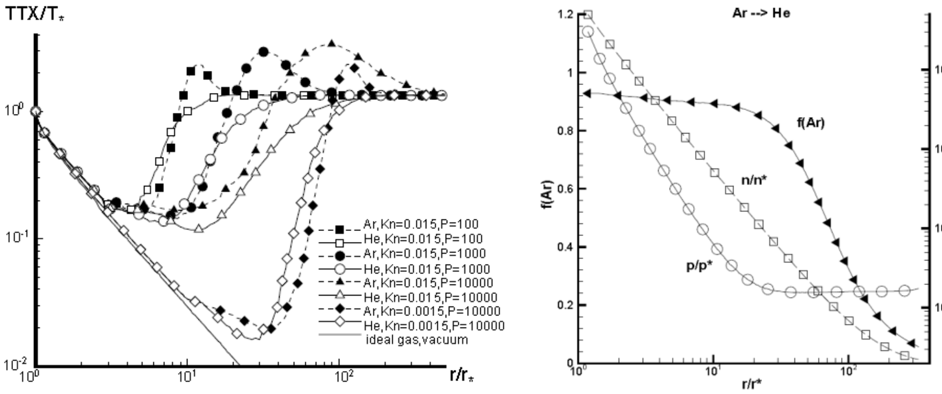

Fig. 4 *Left*: Parallel temperatures of species in spherical expanding flow of *Ar-He* mixture at different Knudsen numbers Kn_* and pressure ratios *P*. Right*:* Argon mole fraction, pressure and number density in expansion of argon into helium at $Kn_* = 0.014$ and $K_2 = 0.785$.

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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