Technical Notes

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Influence of the Physical Model on the Vibration Relaxation in Expansion Flows

J. G. Meolans,* C. Nicoli,† and R. Brun‡
Université de Provence, Laboratoire de Dynamique et Thermophysique des Fluides, Marseille, France

Introduction

A PROBLEM remains concerning the disagreement between the experimental values of the vibrational relaxation times obtained in nozzles and those measured in shock tubes. For N_2, nozzle data first suggested relaxation times 15-70 times shorter than those coming from shock tube data.[1,2] More recent results, however, seem to show that the nitrogen relaxation rate in steady expansion flows cannot exceed five times the one obtained in shock tubes.[3] At any rate, a difference remains, unexplained in the bounds of the simplified Landau-Teller theory. We shall use here a relatively simple analytico-numerical model. The results are compared with those given by previous models and experimental data.

Model Analysis

The relaxation equation and the population of the vibrational levels are derived from the Boltzmann equation.[4] The translation-vibration (TV) efficient collisions may be assumed to be negligible compared to vibration-vibration (VV) ones in the chosen conditions ($T<2300$ K).[5,6] A Treanor distribution of the vibrational population is thus obtained:

$$n_v = n \exp(-\epsilon_v/kT + Kv)/\Sigma \exp(-\epsilon_v/kT + Kv)$$

and a global relaxation equation gives the quantity K[4]. In this equation, only the TV terms appear. These terms include the mean cross sections $\langle\sigma^v_{v+1}\rangle$, characterizing the $v+1 \rightarrow v$ TV transitions. In order to calculate $\langle\sigma^v_{v+1}\rangle$, the interaction potential is taken as $V_1 + V_2 + V$[7]. V_1 and V_2 are the intramolecular potentials for which the Morse potential is chosen to take into account the vibrational anharmonicity. The intermolecular potential V is assumed to have an exponential form, thereby describing an interaction in which the short-range repulsive effects are preponderant. This choice is realistic for homonuclear molecules undergoing nonresonant TV exchanges at relatively high temperatures.[7] According to Herzfeld[8] and Hansen et al.,[9] the angular dependence of V is given by $V = V_0 \Sigma_{s,t} \exp - r_{st}/\ell$, where the r_{st} are the interatomic distances of two interacting molecules. $\langle\sigma^v_{v+1}\rangle$ is analytically derived from a three-dimensional (FODWA) method.[7,8] Taking an approximate analytical expression for the Morse oscillator matrix element,[10] analytic calculation of $\langle\sigma^v_{v+1}\rangle$ can be performed and finally[6] $\langle\sigma^v_{v+1}\rangle = 3\chi_1\chi_2\langle s^v_{v+1}\rangle$. The $\langle s^v_{v+1}\rangle$ cross section was obtained in a previous paper[11] with the spherical potential V used by Schwartz and Herzfeld (S.H.)[12] and with the Morse anharmonic oscillator model. The $\chi_1\chi_2$ factor, close to one, is a slowly decreasing function of v alone.

Steady expansion flows are studied in two axisymmetric convergent-divergent nozzles with hyperbolic profiles:

$$A/A_c = 1 + (x - x_c)^2 (tg\phi/r_c)^2$$

where A is the nozzle section at abscissa x, ϕ is the angle between the asymptote and the nozzle axis, and r is the radius. The subscript c denotes the throat values. The flow is assumed to be one dimensional, the boundary layer is neglected, and the unsteady Anderson method is used.[13] Dimensionless variables are defined: $u/(RT_r)^{1/2}$, p/p_r, T/T_r, e_V/RT_r, ρ/ρ_r, K and the space variable A/A_c, where u, p, ρ, and T are the macroscopic velocity, pressure, density, and temperature respectively. The subscript r denotes the reservoir parameters. The vibrational energy e_V and the gas constant R are defined per mass unit. So transformed, the system depends solely on T_r and $G_r = p_r r_c/tg\phi$. Two values of G_r are considered—$(G_r)_{conv}$ in the convergent part and $(G_r)_{div}$ in the divergent part. Furthermore, writing the entrance conditions (e subscripted) requires knowing the area ratio A_e/A_c.

For nozzle 1, $x_c = 0.5$ cm, $r_c = 0.1$ cm, $tg\phi_{conv} = 0.6$, and $tg\phi_{div} = 0.14$. For nozzle 2, $x_c = 5$ cm, $r_c = 0.48$ cm, $tg\phi_{conv} = 0.63$, and $tg\phi_{div} = 0.13$. The computation is performed with $p_r = 50$ and 100 bars. The T_r values are chosen in the 2000-3200 K range.

Nonequilibrium Effects Upstream of the Throat

In the convergent part the nonequilibrium effects increase as $(G_r)_{conv}$ decreases; thus, for $T_r = 2800$ K, these effects are insignificant for $(G_r)_{conv} = 76$ but noticeable if $(G_r)_{conv} = 8.3$. The upstream nonequilibrium increases as well when T_r decreases, but $(G_r)_{div}$ and A_e/A_c have negligible effects. In order to sustain these conclusions, the quantity

$$\Delta c = 100\left((e_V - e_{Veq})/e_{Veq}\right)c$$

is defined at the throat section and plotted in the $(T_r, (G_r)_{conv})$ plane (Fig. 1). When Δc is about 5, the subsequent effects upon the downstream flow are noticeable; in these conditions, an approximate computation (often performed[14]), assuming equilibrium flow up to the critical point, sensibly distorts the frozen vibrational energy diagram in the $\{e_V, (G_r)_{div}\}$ plane (Fig. 2). Therefore, in the $(T_r, (G_r)_{conv})$ plane, a region is defined where taking into account the nonequilibrium in the convergent part is recommended (Fig. 1). On the other hand, this upstream nonequilibrium is markedly less important here (2-3 times) than for the S.H. model.

Flow in the Divergent Part

1) In the present conditions, the anharmonicity alone is not sufficient to noticeably modify the vibrational energy evolution. Analogous conclusions are derived by Nanbu[14] for similar values of T_r and $(G_r)_{div}$. The profiles of e_V given by the present model, however, are markedly closer to equilibrium profiles than those foreseen by the previous models (Fig. 3). Such an evolution is in agreement with the available experimental data.[1,2] Moreover, Fig. 2 gives a comparison of the frozen vibrational energy e_{Vf} with the one

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*Assistant Professor.
†Postdoctoral Research Student.
‡Maitre de Recherche, C.N.R.S.

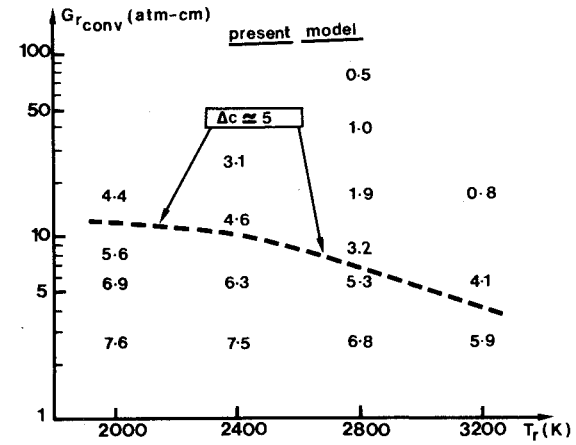

Fig. 1 Δc values ($\Delta c = (e_V - e_{V\ \text{equilibrium}}/e_{V\text{equilibrium}})$ at the throat section.

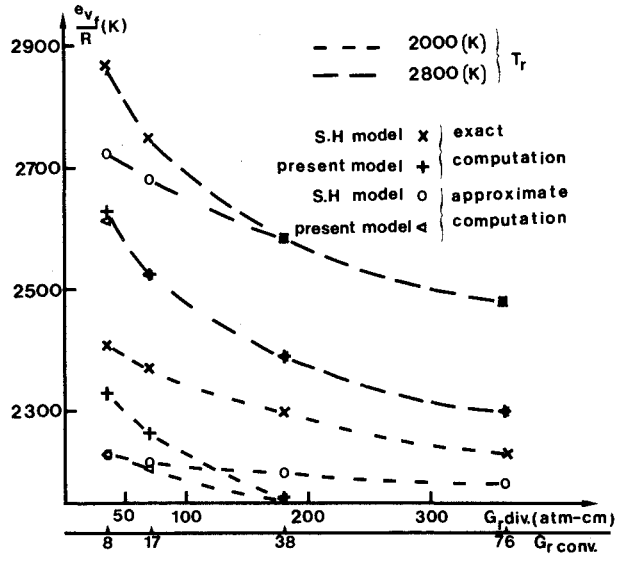

Fig. 2 Frozen vibrational energies vs $(G_r)_{div}$.

derived from the S.H. model. In order to evaluate this improvement, experimental conditions of Hurle et al.[1] are used in the calculation. The measured vibrational temperature T_V is compared with the computed T_V. The theoretical values do not exceed experimental data by more than 16%, as compared to the 30% obtained by these authors or by the S.H. model. These data are generally considered to be underestimated,[2,3] but Hurle et al. claimed that experimental uncertainties alone could not explain such a disagreement. Thus, the present results seem realistic and more satisfying than the previous ones. This conclusion is enhanced by the results concerning the relaxation time to be discussed.

2) A fictitious relaxation time τ_f is defined, a posteriori, from the computed macroscopic quantities by using the classical relaxation equation, $\overline{e_V} - e_V = \tau_f de_V/dt$ ($\overline{e_V}$ is the local equilibrium energy). The ratio τ_0/τ_f, which sensibly increases with T_r, varies little with $(G_r)_{div}$, τ_f is found to be 3-6 times shorter than the time τ_0 obtained with the S.H. model (at $A = 3A_c$, where the freezing has not begun). Moreover, for a high T_r (3200 K), temperatures in the vicinity of the throat ($A/A_c = 1,4$) reach the usual shock tube temperature range (T ≃ 2300 K). In these conditions, for $(G_r)_{div} = 363$, τ_f is about six times shorter than the relaxation time τ_s measured behind a shockwave (in this temperature range τ_s is about equal to τ_0). These results are close to those which Teare et al.[3] obtained from experiments. Indeed, these authors came to a conclusion of a maximal ratio of 5 between τ_s and the relaxation time measured in nozzles.

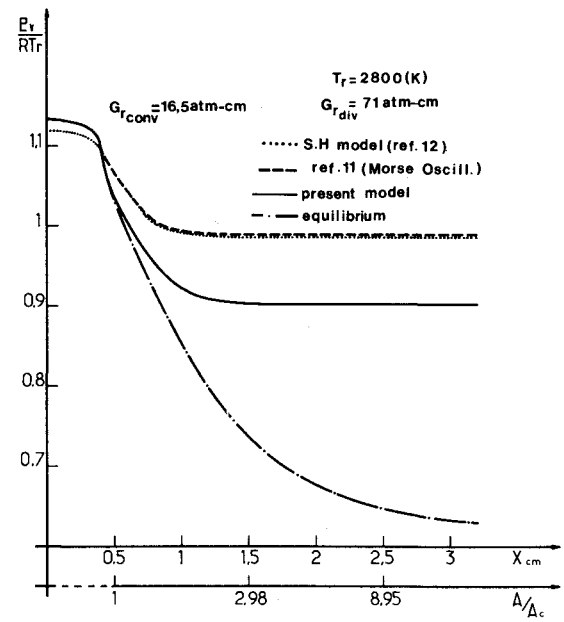

Fig. 3 Vibrational energy evolutions.

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