Entropy in Nonequilibrium Nozzle Flows of Vibrationally Relaxing Diatomic Gases

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Theme

IN nonequilibrium nozzle flows of vibrationally relaxing or chemically reacting gases, the nonequilibrium processes inevitably increase the entropy of gases in nozzles. This increased entropy in turn affects flowfields and relaxation phenomena themselves. The analyses of nonequilibrium phenomena in nozzle flows are, in almost all cases, equivalent to those of flowfields themselves. However, it is regretful that in spite of the large number of researchers, few good studies on this problem[1] have been done because of the difficulties in analyzing theoretically these flowfields. In light of such circumstances, our effort is mainly devoted to investigation of the roles of entropy in the analyses of nonequilibrium nozzle flows. First the maximum and minimum critical mass flows for vibrationally relaxing diatomic gases under the fixed reservoir conditions are obtained. Next a new criterion for the validity of the equilibrium-frozen flow approximation is proposed. Finally the effects due to increasing entropy on the asymptotic behaviors of flows far downstream of a throat are examined. All these analyses are based upon the new system of basic equations which has been derived by the author.

Contents

The system of equations governing the quasi-one-dimensional, inviscid, nonconducting flow may be written in suitably rearranged forms

$$F_V(M)(1+A)/m = F_{V0} \exp G_V(\xi_V;\xi) \tag{1}$$

$$\tfrac{7}{10}M^2 = (1/\phi - \mathscr{E}_V)\xi - \tfrac{7}{2} \tag{2}$$

$$\pi(A,\xi_V;\xi)\, d\mathscr{E}_V/d\xi = -(\mathscr{E}_V - \mathscr{E}) \tag{3}$$

$$(W_2/R)(S-S_0) = \int_{\xi_0}^{\xi} (\xi_V - \xi)(d\mathscr{E}_V/d\xi)\, d\xi \tag{4}$$

where

$$\xi = \theta/T, \qquad \xi_V = \theta/T_V \tag{5}$$

$$F_V(M) = M/(M^2+5)^3 \tag{6}$$

$$G_V(\xi_V;\xi) = -\int_{\xi_0}^{\xi}\left[\xi - \frac{3\phi}{(1-\phi\mathscr{E}_V)}\right](d\mathscr{E}_V/d\xi)\, d\xi \tag{7}$$

$$\mathscr{E} = 1/(\exp\xi - 1), \qquad \mathscr{E}_V = 1/(\exp\xi_V - 1) \tag{8}$$

and where $\pi(A,\xi_V;\xi)$ in the rate equation (3) is assumed to be a known function of A, ξ_V, and ξ. Here x is the distance along a stream measured from a throat, $1+A(x)$ the cross-sectional area ratio, p the pressure of a gas, ρ the density, T the rotational-translational temperature, T_V the vibrational temperature, h the specific enthalpy, S the specific entropy, and constants m, θ, W_2, and R are, respectively, the critical mass flow, the characteristic temperature of vibration, the molecular weight of a molecule and the universal gas constant. Parameters ϕ and F_{V0} are also constants which are determined from the reservoir conditions. Subscript zero denotes the reservoir or the stagnation point. M is the frozen Mach number. Here the independent variable is not x but ξ, and it is assumed that flows start from equilibrium reservoirs.

Equation (1) in conjunction with Eqs. (2, 4, 6, and 7) can also be rewritten in the form

$$(1+A) = \frac{125}{216}\left(\frac{7}{10}\right)^{1/2}\left(\frac{m}{m_f}\right)\frac{\exp\xi_0}{\xi_0{}^3(\exp\xi_0 - 1)}\exp\left(\frac{\xi_0}{\exp\xi_0 - 1}\right)$$
$$\left\{\frac{\xi^{5/2}\left[\dfrac{(\exp\xi_V - 1)}{\exp\xi_V}\right]\exp\left[-\dfrac{\xi_V}{(\exp\xi_V - 1)}\right]}{\left[\dfrac{1}{\phi} - \dfrac{1}{(\exp\xi_V - 1)} - \dfrac{7}{2\xi}\right]^{1/2}}\right\}\exp\left[\frac{W_2}{R}(S-S_0)\right] \tag{9}$$

where subscript f denotes the frozen flow. Equation (9) shows that the degree to which the flow parameters in nozzles are affected by the existence of nonequilibrium is completely determined by the entropy and the vibrational temperature. Thus, an algebraic equation is obtained, relating $A(x)$, ξ, ξ_V, and S, which in conjunction with the remainders of basic equations yields very simple analytical solutions not only for the frozen ($\xi_V = \xi_0$ and $S - S_0 = 0$) flow but also for the equilibrium ($\xi_V = \xi$ and $S - S_0 = 0$) one. With it, we can calculate all the flow quantities for these limiting flows without carrying out the tedious numerical calculations on the electric digital computer. It must be emphasized that using Eq. (1) or Eq. (9) as one of the basic equations describing a nonequilibrium nozzle flow, we can expect considerable merits in investigating analytically nonequilibrium effects on the flowfields, especially in determining the critical mass flow, in estimating the validity or accuracy of the equilibrium-frozen flow approximation, and in analyzing the asymptotic behaviors of nonequilibrium flows far downstream of the throat.

Entropy and critical mass flows. Though it has often been pointed out that the difficulties in determining the critical mass flow greatly complicate the analyses of nonequilibrium nozzle flows, there have been few works on this problem. In almost all cases, the obtained results have indicated that the critical mass flows of general nonequilibrium flows are smaller than the frozen and greater than the equilibrium. But this tendency is rather empirical and has never been exactly proved theoretically. A conclusion can be drawn that, in general, at least theoretically under the fixed reservoir conditions, the maximum critical mass flow is the frozen one, while the minimum is the one which is somewhat smaller than the equilibrium. This conclusion is obviously contradictory to the empirical tendency previously observed.

Now imposing a condition

$$x(dA/dx) \geqq 0 \tag{10}$$

on the nozzle geometry, we can reasonably assume

$$\xi_0 \leqq \xi_V \leqq \xi \tag{11}$$

$$d\xi_V/d\xi \geqq 0 \tag{12}$$

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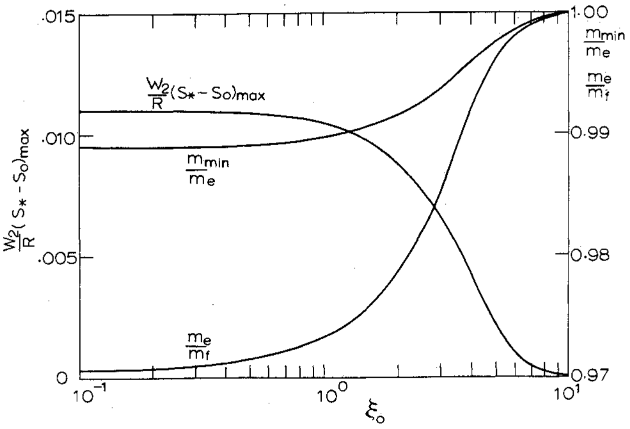

Fig. 1 Critical mass flow and the maximum entropy at the critical point.

for the flows considered here. Assuming (11) and (12) under the condition (10), we can obtain the next relation under the fixed reservoir conditions

$$m_{\min} \leqq m \leqq m_{\max} = m_f \tag{13}$$

where

$$m_e/m_f = [F_V(M_{et})/F_V(1)] \exp(-G_{Vet}) \tag{14}$$

$$\frac{m_{\min}}{m_e} = \frac{1}{(1+A_{e*})} \exp\left\{ -\xi_{e*}(\mathscr{E}_0 - \mathscr{E}_{e*}) - \left[\ln\left(\frac{\exp \xi_{e*}}{\exp \xi_{e*} - 1}\right) + \frac{\xi_{e*}}{(\exp \xi_{e*} - 1)} \right] + \left[\ln\left(\frac{\exp \xi_0}{\exp \xi_0 - 1}\right) + \frac{\xi_0}{(\exp \xi_0 - 1)} \right] \right\} \tag{15}$$

where subscripts e, t, and $*$ denote, respectively, the equilibrium flow, the throat and the critical point ($M = 1$), and ξ_{et} and ξ_{e*} are determined, respectively, by energy equations at the throat and the critical point ($M = 1$). The result (13) is very significant not only physically but also practically in numerical analysis of the subsonic region, in which it often happens that the value of critical mass flow must be guessed beforehand for the given reservoir conditions and nozzle shape and size. Figure 1 shows the critical-mass-flow ratios m_e/m_f and $m_{\min}/m_e$ and the maximum entropy at the critical point. The explicit solution which gives the critical mass flow of general nonequilibrium flow can also be easily obtained. It shows that the critical mass flow is completely determined by the entropy increase in the subsonic region and the vibrational temperature at the critical point.

Entropy and equilibrium-frozen flow approximation. The simplest and most significant approximation to a nonequilibrium flow is the equilibrium-frozen one, in which the upstream equilibrium branch and the downstream frozen branch are joined together at the freezing point. The simple criteria for the freezing point have been proposed by Bray et al. and have been found to agree well with the numerical solutions in many cases. However the equilibrium-frozen flow approximation cannot fully match the exact solution far downstream of the freezing point because of increasing entropy due to nonequilibrium processes in the flow. Even if the freezing point is suitably chosen, this approximation cannot always give a correct prediction of the state of the flow far downstream. Hence it is obvious that we need a new type of criterion for the general and precise validity of this approximation.

Fortunately our new system of basic equations can also provide us with a completely analytical solution for this equilibrium-frozen flow. In order that the equilibrium-frozen flow matches well the exact solution in the whole of the flow region with an acceptable error, the following three conditions must be satisfied:

$$Q_1 = |(\mathscr{E}_{Vef} - \mathscr{E}_V)/\mathscr{E}_V|_{\max} \ll 1 \tag{16}$$

$$Q_2 = |(m_{ef} - m)/m| \ll 1 \tag{17}$$

$$Q_3 = \{\exp[W_2/R)(S_\infty - S_0)] - 1\} \ll 1 \tag{18}$$

where subscript ∞ denotes the downstream limit. We can reasonably expect that the set of these three conditions serves as a new type of criterion for the validity of the equilibrium-frozen flow approximation. It must be noted, however, that these quantities Q_1, Q_2, and Q_3 are not always completely independent of each other, and Q_2 is usually so small that it is less important than the others.

Entropy and asymptotic behaviors far downstream. The equilibrium-frozen flow approximation is completely based upon the freezing phenomenon of relaxing energy at infinity. However, there can be two cases. In one, the entropy of the gas converges to a finite value and in another it diverges to infinity. In the latter case, the equilibrium-frozen flow approximation breaks down far downstream even when the flow does finally freeze.

These discussions suggest the importance of investigation on the final flow patterns. Furthermore it is very interesting not only purely theoretically but also practically to know how the increasing entropy affects the relaxation phenomenon.

Consider the region far downstream of a throat in a nozzle and consider the nozzle geometry described by

$$A = Kx^n \tag{19}$$

where K and n are positive constants and the latter is less than or equal to 2. Then the rate equation can be reduced finally to the form

$$[\alpha\xi^{\kappa} \exp(-l\theta^s \xi^{-s})\Theta - \tfrac{2}{5}\xi^2(\mathscr{E}_V - \mathscr{E})]\, d\mathscr{E}_V/d\xi \approx -(\mathscr{E}_V - \mathscr{E}) \tag{20}$$

for N_2 and O_2 gases, where

$$\Theta = \exp[(1 - 1/n)(W_2/R)(S - S_0)] \tag{21}$$

Parameters 1, s, and κ are constants characteristic to each gas, and α is nearly constant depending upon the reservoir conditions, nozzle shape and size, vibrational temperature, and kind of a gas. It is surely worth noting that when $n > 1$, an increase in entropy has negative effect on the vibrational relaxation phenomenon, when $n < 1$ positive effect and when $n = 1$ no effect.

References

[1] Conner, L. N. and Erickson, W. D., "Entropy Production in Vibrational-Nonequilibrium Nozzle Flow," *AIAA Journal*, Vol. 2, No. 2, Feb. 1964, p. 397.