Computer solutions to the problem of vibrational relaxation in hypersonic nozzle flows

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This report is an extension of an earlier note in which a simple method of estimating the distribution of vibrational temperature along a hypersonic nozzle was described. Results were presented for hyperbolic, axisymmetric nozzles with reservoir conditions $1000 \leqslant p_0 \leqslant 4000$ p.s.i.a., $1000 \leqslant T_0 \leqslant 3000\,^{\circ}$K. The problem was subsequently programmed for the Ferranti Mercury computer at the University of London computing centre, and the results of these computations are given here. The vibrational temperatures are compared with those of the previous simple method. The distributions of pressure and temperature through the nozzle are also given and a simple method of estimating the vibrational temperature is described.

1. Introduction

In a previous note, Stollery & Smith (1962) have discussed the thermodynamic aspects of equilibrium and non-equilibrium vibrating gas flows. The vibrational rate equation was integrated numerically, the perfect-gas values being assumed for pressure and temperature, to find the variation of vibrational temperature along the nozzle. A simple criterion for the freezing point was found to agree well with the numerical solutions.

In a subsequent paper by Stollery & Park (1963) the vibrational rate equation was integrated exactly along with the one-dimensional inviscid flow equations for nozzle flow to find the variation of both temperature and pressure using a digital computer. The present note is a condensed version of that paper.

2. Formulation of the problem

Fundamental equations

The appropriate quasi one-dimensional flow equations of mass, momentum and energy are

$$\rho A v = \text{const.} = \dot{m}, \tag{1}$$

$$-\rho v(dv/dx) = dp/dx, \tag{2}$$

$$Cp_a T_a + \sigma + \tfrac{1}{2}v^2 = \text{const.} = Cp_a Ta_0 + \overline{\sigma}_0. \tag{3}$$

The notation used is standard; σ is the energy stored in vibration and $\overline{\sigma}$ indicates the equilibrium value. Suffix a indicates the active degrees of freedom (i.e. translation and rotation here), whilst suffix 0 denotes reservoir conditions. The equation of state is

$$p = \rho R T_a, \tag{4}$$

and the linear form of the rate equation is used, thus

$$d\sigma/dx = L^{-1}(\bar{\sigma}-\sigma). \tag{5}$$

The relaxation length L is equal to $v\tau$, where τ is the vibrational relaxation time. In order to programme the problem, analytic expressions are required for σ and τ. Those used for air, namely

$$\sigma = \{5974/[\exp(3076/T_i)-1]\}\,\text{cal/mole}, \tag{6}$$

where T_i is the vibrational temperature in °K, and

$$\tau p = 1\cdot402\times10^4\exp(-T_a/401\cdot1)\,\text{atm}\,\mu\text{sec}, \tag{7}$$

agree well with the data given in Stollery & Smith (1962).

Air is here assumed to behave as a hypothetical, pure, diatomic gas with a characteristic vibrational temperature of 3076 °K. This assumption permits the use of a single rate equation in the nozzle flow analysis, but its validity is questionable because the chief constituents of air have markedly different vibrational relaxation times. However, the few experimental data of Gaydon & Hurle (1962) show only one relaxation time and provide the basis for equation (7).

The form of the rate equation used in this paper also requires some justification. The linear form is usually assumed to hold only for small departures from equilibrium (see for example the chapter by Herzfeld 1955). In a more recent paper (Wild 1963), an alternative view is expressed. In the nozzle flows examined here, the departures from equilibrium are large. The linear form of the rate equation is used because it is simple and because no generally accepted improvement is available.

Reduction of equations

By use of the Mach number M_a, based on the frozen sound speed a_F, equations (1) to (5) may be reduced to the form

$$\frac{1}{T_a}\frac{dT_a}{dx} = \frac{\gamma_a-1}{1-M_a^2}\left[\frac{M_a^2}{A}\frac{dA}{dx}+(1-\gamma_a M_a^2)g\right], \tag{8}$$

$$\frac{1}{p}\frac{dp}{dx} = \frac{\gamma_a M_a^2}{1-M_a^2}\left[\frac{1}{A}\frac{dA}{dx}+(1-\gamma_a)g\right], \tag{9}$$

$$g = -(d\sigma/dx)/(\gamma_a RT_a) = -(\bar{\sigma}-\sigma)/(\gamma_a RT_a L), \tag{10}$$

$$M_a^2 = 2(h_0-Cp_aT_a-\sigma)/a_F^2 \tag{11}$$

$$a_F^2 = (\partial p/\partial\rho)_{s,\sigma} = \gamma_a RT_a. \tag{12}$$

When $M_a = 1$, (8) and (9) both give

$$A^{-1}dA/dx = (\gamma_a-1)g. \tag{13}$$

Since g is positive the station at which $M_a = 1$ must be downstream of the throat, and so at the throat M_a is subsonic. With the frozen sound speed as the characteristic parameter, the problem is analogous to that of one-dimensional perfect gas flow with heat addition. If the nozzle shape can be expressed in the form

$A/A^* = f(x/x_0)$, where the superscript * refers to the throat condition and x_0 is a characteristic length, then equations (8) and (9) may be non-dimensionalized using the variables

$$p' = p/p_0, \quad T' = T/T_0, \quad \xi = x/x_0, \quad L' = L/x_0, \quad \sigma' = \sigma/\sigma_0$$

to demonstrate that px_0 is a similarity parameter for the transformed equations.

The computer problem

The computer is programmed to solve equations (8) to (12) for p and T_a given $A(x)$, p_0 and T_0. In these calculations an axisymmetric hyperbolic geometry was used, so that

$$A/A^* = 1 + (x \tan\theta/r^*)^2, \tag{14}$$

where r^* is the throat radius and θ is the semi-angle of the asymptote cone. The similarity parameter for this shape is $p_0 r^*/\tan\theta$. Upstream of the throat, θ was taken as 45°. Two downstream values were used, namely $\theta = 5°$ and $\theta = 15°$. The mass flow $\dot{m}$ is unknown initially, and a solution in the convergent section of the nozzle is only possible by choosing a range of values of $\dot{m}$ and finding the one which satisfies the boundary conditions. These are (i) that the flow is in equilibrium at nozzle entry, and (ii) that equation (13) must be satisfied when $M_a = 1$. Finding the correct value of $\dot{m}$ takes a long time even with the use of a computer. Once it has been found, the solution for the divergent section of the nozzle is straightforward apart from the need to jump through the critical station, $M_a = 1$.

3. Method of calculation

Frozen flow

For frozen flow, $\tau = \infty$ and $d\sigma/dx = 0$ so that g, as given by equation (10), is zero. The solution of the nozzle flow is then identical to that for an isentropic adiabatic perfect gas flow having a reservoir temperature T_{a_0}.

Equilibrium flow

When the flow is in equilibrium, $\tau = 0$ and $T_a = T_i$. The rate equation is replaced by $\sigma = \bar{\sigma}(T_a)$ and equation (8) is transformed to

$$\frac{1}{M_a^2}\frac{dT_a}{T_a}\left[\frac{1-M_a^2}{\gamma_a - 1} + \frac{1-\gamma_a M_a^2}{\gamma_a R}\frac{d\bar{\sigma}}{dT_a}\right] = \frac{dA}{A}, \tag{15}$$

with $M_a^2 = 2(h_0 - Cp_a T_a - \bar{\sigma})/\gamma_a R T_a$. The flow is no longer dependent on the size of the nozzle or on the reservoir pressure, $p_0 r^*/\tan\theta$ is no longer a similarity parameter, and equation (15) may be solved to give T_a/T_{a_0} as a function of nozzle area ratio. At the throat (15) becomes

$$\frac{Cp_a + (d\bar{\sigma}/dT_a)^*}{Cp_a + \gamma_a (d\bar{\sigma}/dT_a)^*} = M_a^2 = \frac{2(h_0 - Cp_a T_a^* - \bar{\sigma}^*)}{\gamma_a R T_a^*}, \tag{16}$$

and, since $d\bar{\sigma}/dT_a = f(T_a)$ from equation (6), it may be solved for T_a^* if h_0 is given. The value of T_a^* is fed into (15) as the initial value and numerical calculation can proceed for both increasing and decreasing values of T_a, that is for both the divergent and convergent sections of the nozzle. Table 1 (*a*) shows a sample equilibrium calculation in which air at reservoir conditions $p_0 = 4000$ p.s.i.a. and $T_0 = 2000$ °K is expanded through a hypersonic nozzle. The solution is compared with the frozen-flow result and with the equilibrium-flow values of both Erickson & Creekmore (1960) and the Ames research staff (1953). In figures 1 and 2, five equilibrium-flow solutions are given for the reservoir temperature range $1000 \leqslant T_0 \leqslant 3000$ °K, with the intention of supplementing the real gas solutions given by the Ames staff.

(*a*) *Nozzle exit conditions* ($A/A^* = 536$)

	M_a	p (p.s.i.a.)	T_a (°K)	T_i (°K)	$\rho \times 10^6$ (slug/ft.^{3})	v (ft./sec)
Frozen flow	10·00	0·094	95·4	2000	4·59	6420
Equilibrium flow	9·40	0·110	120	120	4·25	6870
Non-eq. flow—computer solution	9·70	0·106	104	1270	4·73	6440
Eq. solution of Erickson & Creekmore	9·58	0·106	119	119	4·13	6870
Eq. solution of Ames Research Staff	9·37	0·111	120	120	4·27	6880

(*b*) *Conditions along the nozzle*

	Equilibrium flow			Non-eq. flow			Frozen flow		
A/A^*	M_a	p (p.s.i.a.)	T_a (°K)	M_a	p (p.s.i.a.)	T_a (°K)	M_a	p (p.s.i.a.)	T_a (°K)
4·24	2·80	123	863	2·87	124	811	3	109	714
10·7	3·71	30·5	595	3·85	29·8	543	4	26·4	476
25·0	4·65	8·77	421	4·83	8·57	381	5	7·56	333
53·2	5·60	2·93	308	5·80	2·86	278	6	2·54	244
104	6·55	1·10	228	6·78	1·09	211	7	0·97	185
190	7·51	0·47	182	7·76	0·46	169	8	0·41	145
327	8·45	0·22	147	8·72	0·21	133	9	0·19	116
536	9·40	0·11	120	9·70	0·106	104	10	0·094	95·4

TABLE 1. A comparison of equilibrium, non-equilibrium and frozen flow conditions for hyperbolic nozzle; $2\theta = 10°$, $r^* = 0·125$ in., $T_0 = 2000$ °K, $p_0 = 4000$ p.s.i.a.

Non-equilibrium flow

When τ is finite, equations (12) to (15) must be solved numerically, first for the subsonic section of the nozzle. Two methods of solution are possible. The mass flow rate $\dot{m}$ may be chosen, and downstream numerical integration (from the equilibrium reservoir conditions) permitted until $M_a = 1$, when equation (17) must be satisfied. Alternatively, the station at which $M_a = 1$ and the corresponding value of g are chosen, and the equations integrated for the region upstream as far as the reservoir station ($A/A^* = 100$), where the computed values must match the given reservoir conditions. In both cases a great deal of time is saved by using the simple method described in the earlier paper (Stollery & Smith 1962) to obtain a first approximation for T_i^*. In this work the second method was adopted and matching effected at the reservoir station.

The solution for the supersonic portion of the nozzle with $\dot{m}$ now known is straightforward. Table 1 (*b*) shows the result of a sample calculation and compares it with the equilibrium solutions already described. Figures 3 to 6 portray twelve solutions computed by the present method.

4. Discussion

The reasons for calculating equilibrium-flow values assuming vibration to be the only real-gas effect were, first, that we wished to examine the effects of vibration alone and, secondly, that there was no agreement between the three existing nozzle flow solutions consulted when writing this note. The calculations of Erickson & Creekmore, unlike the other two references, were made using compressibility factors substantially different from unity. Our calculations ignore compressibility. The matching differences are shown in table 1 (*a*). Some recent tables (Evered, Metcalf & McIntyre 1961) suggest that the compressibility effect is negligible for pressures below 5000 p.s.i. Figures 1 and 2 make a further comparison between our results and the three others. A result obtained by Bernstein (1961) for nitrogen is also included and shows that the differences between the frozen and equilibrium properties for nitrogen are rather greater than those for air. Figures 1 and 2 demonstrate that the ratios p_E/p_F and T_E/T_F at exit from any high supersonic, or hypersonic nozzle ($A/A^* \geqslant 10$), are close to 1 for reservoir temperature below 1000 °K, and rise to around 1·30 for $T_0 = 3000$ °K.

Figures 3 to 6 show the non-equilibrium distribution of static pressure and translational temperature through the nozzle for various values of $p_0 x_0 \equiv pr^*/\tan\theta$ and two reservoir temperatures. For a reservoir temperature of 1000 °K, figure 3 shows that at low values of $p_0 x_0$ (i.e. low reservoir pressure, a small nozzle and large divergence angle) the flow is close to being completely frozen. As $p_0 x_0$ is increased, the flow freezes a little further downstream towards the throat (in all the cases considered with $T_0 = 1000$ °K freezing occurred before the throat was reached), and more of the energy stored in vibration reaches the translational modes. At the highest levels of $p_0 x_0$ considered ($p_0 = 4000$ p.s.i.a., $r^* = \frac{1}{8}$ in., $\theta = 5°$), an interesting point emerges: the non-equilibrium static pressure level exceeds the equilibrium value. Thus the greatest discrepancy between perfect and real-gas nozzle pressure distributions is not limited to the difference between the frozen and equilibrium solutions. The heat-addition analogy suggests that the heat added q is proportional to $\overline{\sigma}_0 - \sigma$ in non-equilibrium flow and $\overline{\sigma}_0 - \overline{\sigma}$ in equilibrium flow. Since $\sigma > \overline{\sigma}$ there is 'less heat addition' when the flow is out of equilibrium. The addition of heat at subsonic velocities reduces pressure so we might expect to find $p_E < p$ in the convergent part of the nozzle. At supersonic speeds heat addition increases the static pressure, and whether the equilibrium solution 'overtakes' the non-equilibrium one depends on where freezing occurs in the nozzle. The subsonic branch of the equilibrium solution for the static pressure ratio is shown in figures 3 and 4, and it does fall below one (i.e. $p_E < p_F$

as one might again predict from the heat-transfer analogy since in completely frozen flow $q \equiv 0$).

The earlier work of Stollery & Smith (1962) presented a quick and simple method of calculating the distribution of vibrational temperature throughout a nozzle but did not give explicitly a 'sudden freezing' criterion. In a more recent

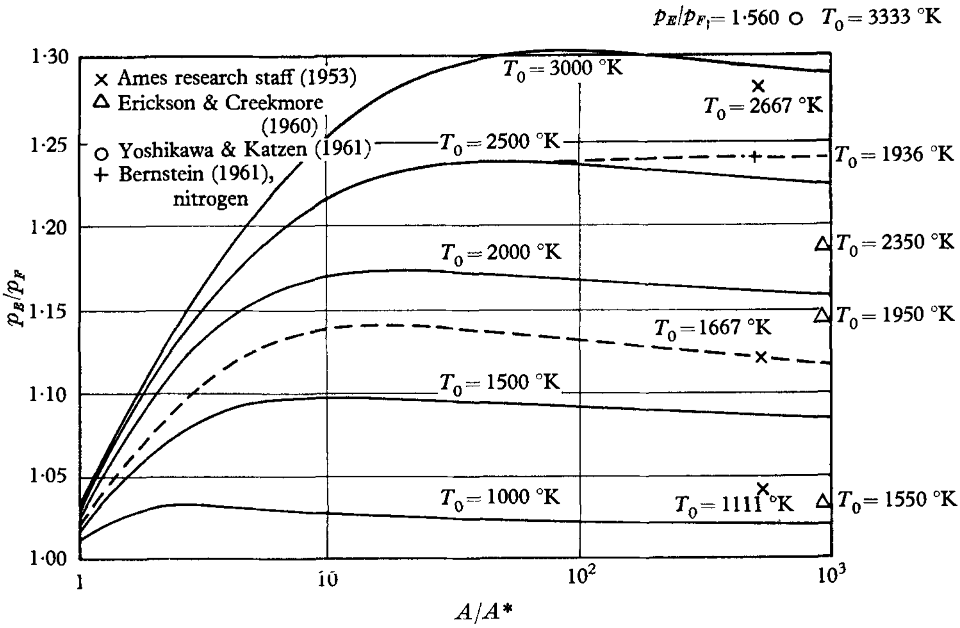

FIGURE 1. Variation of pressure in equilibrium flow.

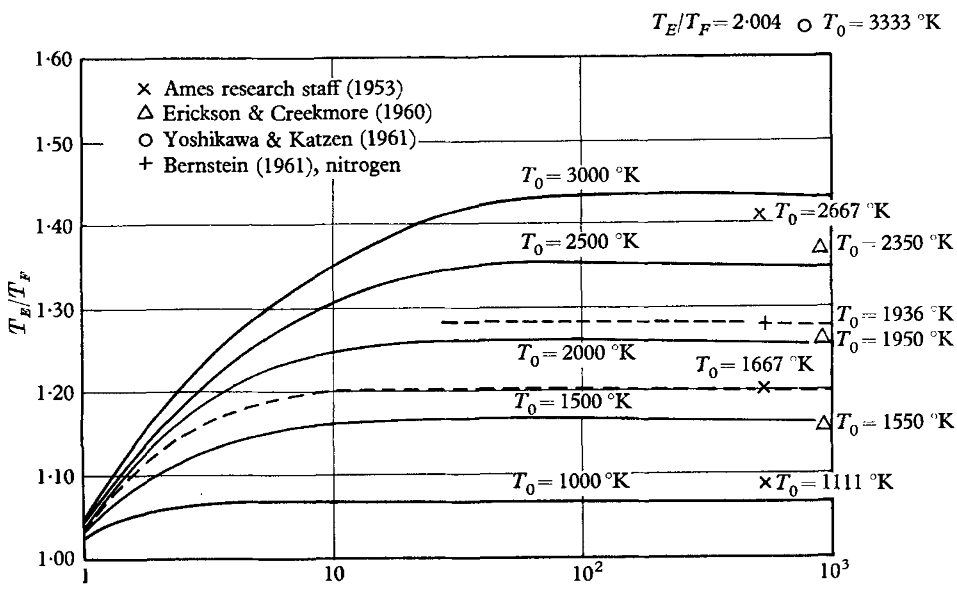

FIGURE 2. Variation of temperature in equilibrium flow.

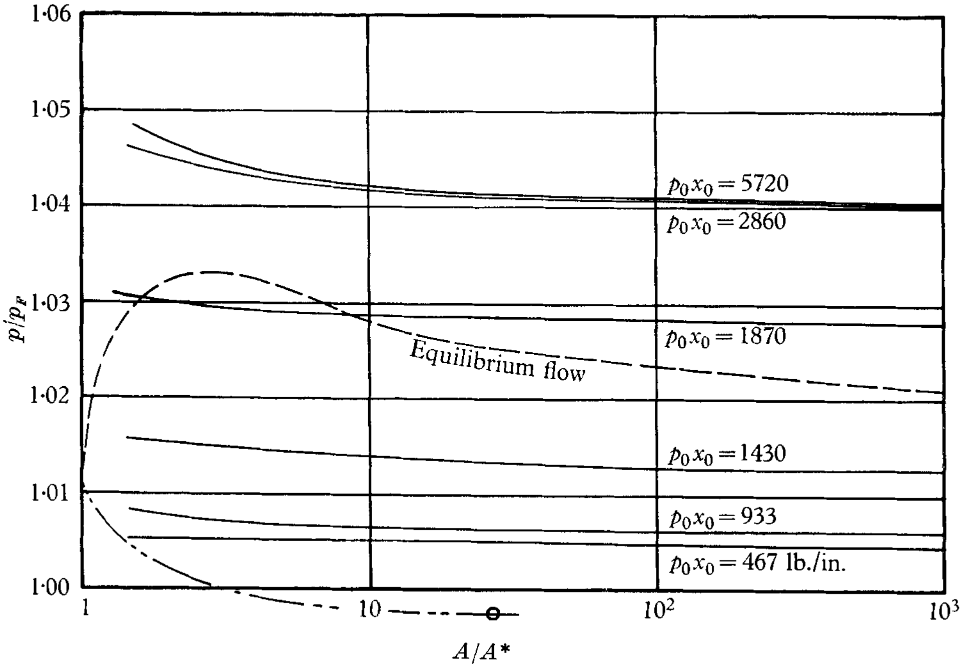

FIGURE 3. Variation of pressure in non-equilibrium flow, exact solution, $T_0 = 1000\,°K$.

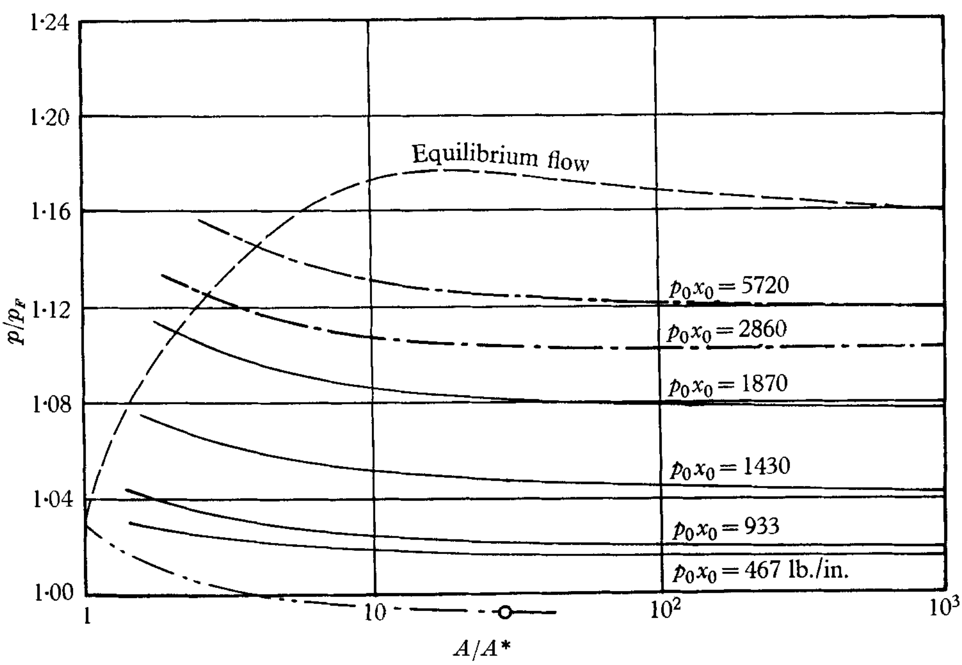

FIGURE 4. Variation of pressure in non-equilibrium flow, exact solution, $T_0 = 2000\,°K$.

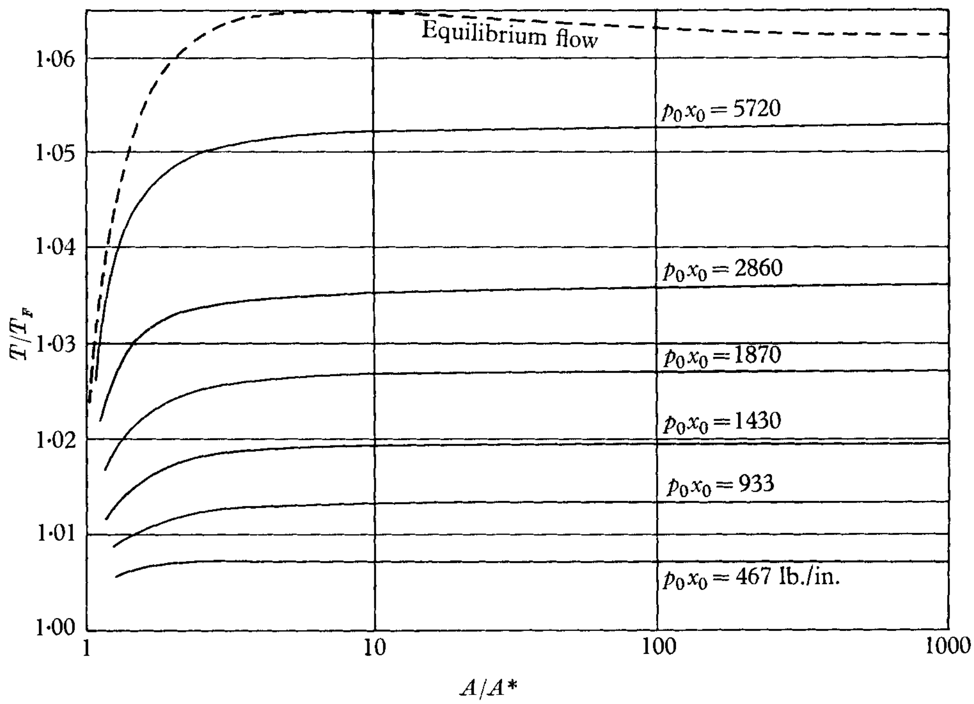

FIGURE 5. Variation of temperature in non-equilibrium flow, exact solution, $T_0 = 1000$ °K.

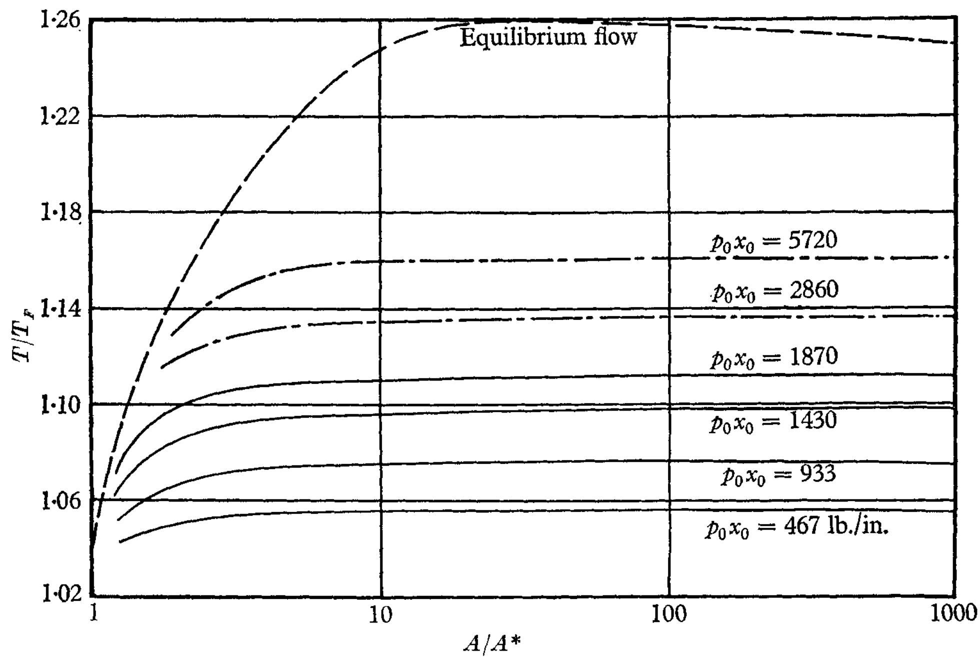

FIGURE 6. Variation of temperature in non-equilibrium flow, exact solution, $T_0 = 2000$ °K.

paper Blythe (1963) considers one-dimensional nozzle flows in which the vibrational energy is small. He integrates the linear form of the rate equation, which may be written non-dimensionally as

$$d\sigma'/d\xi = (\bar{\sigma}' - \sigma')/L', \tag{17}$$

and shows that a criterion indicative of rapid transition from the equilibrium solution is

$$\bar{\sigma}^{-1} d\bar{\sigma}/d\xi = L^{-1} f(x), \quad \text{where} \quad f(x) = pa_0/p_0 u. \tag{18}$$

This is of the same form as the criterion derived by Bray (1959) from qualitative arguments for the case of a dissociating gas.

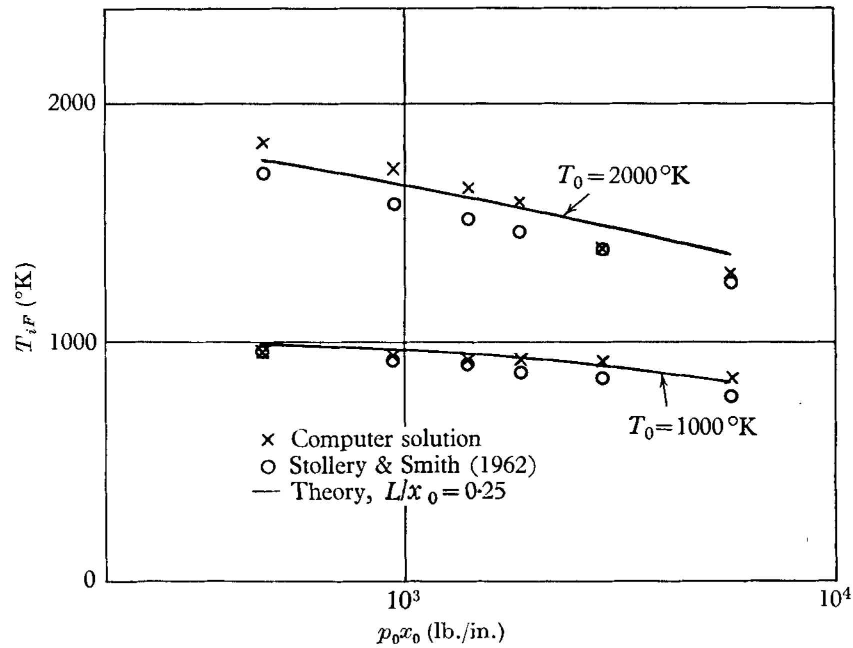

FIGURE 7. Estimates of the frozen vibrational temperature levels.

Blythe also considers the particular example of a hypersonic gas stream, initially in equilibrium, expanding through a divergent conical nozzle and obtains an analytic expression for $\sigma(x)$. In the convergent-divergent nozzle flows examined here freezing is never delayed until hypersonic velocities are reached so that no comparison is possible.

A simpler criterion than (18), one involving much less calculation, is now given. For the nozzle flows considered here, a typical variation of $L'(\xi)$ shows the relaxation length increasing so rapidly along the nozzle that there is a point ξ_1 beyond which $d\sigma'/d\xi$ is sensibly zero (from equation (17)). Therefore, beyond ξ_1, we have $\sigma \simeq$ const., i.e. the flow is frozen. There exists then the possibility of fixing the freezing point (FP) by selecting an approximate value of the relaxation length, L'_{FP} (see figures 8 and 9). A plot was made of the relaxation lengths at the freezing points versus the parameter $p_0 r^*/\tan\theta$ from the computer solutions obtained both here and at the National Research Council in Canada by Campbell & Meyer (to be published). (The freezing point is defined as the position in the perfect gas solution where the temperature equals the frozen vibrational temperature of the non-equilibrium solution, i.e. $T_F = T_{iF}$. The values of v and p used in calculating L' were the perfect gas ones.) The plot showed that despite the non-similarity in nozzle shape (θ-subsonic was not proportional to θ-supersonic), all the values of L'_{FP} fell in the range $0{\cdot}2 < L' < 0{\cdot}6$.

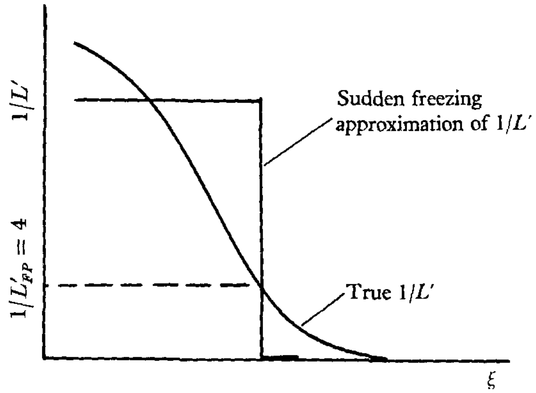

FIGURE 8. Variation of $1/L'$ (not to scale).

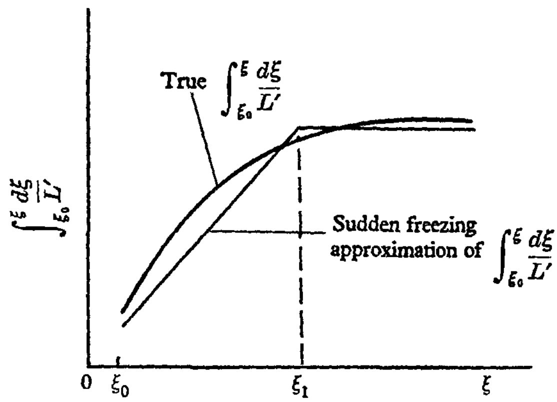

FIGURE 9. Variation of $\int_{\xi_0}^{\xi} \frac{d\xi}{L'}$ (not to scale).

Figure 7 shows that the error incurred by assuming $L'_{FP} = 0{\cdot}25$ when calculating T_{FP} is less than 5 % for the cases considered. The figure also includes for comparison the values of T_{iF} calculated previously (Stollery & Smith 1962), and it may be seen that the agreement with the computer solutions is quite good.

5. Conclusions

There are significant differences between the various equilibrium air flow results already published. The values presented here agree most closely with those given by the Ames Research Staff (1953).

The non-equilibrium real gas effects on static pressure can exceed the equilibrium real gas effects. This result seems to be connected with freezing occurring upstream of the throat.

For all the twelve non-equilibrium cases considered, freezing took place close to the nozzle throat. The Mach numbers at the freezing point ranged from 0·48 to 1·70.

Vibrational real gas effects are significant, particularly in the range

$$3000 \geqslant T_0 \geqslant 2000\,^{\circ}\mathrm{K}.$$

The simple sudden freezing criterion $L' = 0{\cdot}25$ is adequate for the cases considered.

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