THE EFFECTS OF RECOMBINATION IN EXPANDING GAS FLOWS

By R. L. Pope*

[*Manuscript received June* 9, 1969]

Summary

An approximate analysis of the one-dimensional expanding flow of an ideal dissociating gas, which is initially in a frozen state, is presented. The different types of solutions of the equations of the flow, for variations in the rates of expansion and recombination, are discussed. Some numerical results indicating the distances and other dimensions involved are included. The results of the approximate analysis are compared with some numerical solutions and are found to be valid for all cases in which the analysis can be expected to apply.

I. Introduction

In this paper an investigation is made of the phenomena which may occur when a flow, in which the process of recombination of the gas from a dissociated state has been arrested, is allowed to expand through a nozzle with a variation in area of the form

$$A' = A'_0(1+x'/x'_0)^\nu\,, \tag{1}$$

where $\nu > 0$. It is assumed that the flow has undergone a rapid expansion process, such as may occur in the conical nozzle of a shock tunnel, where the flow starts in a region of stagnation at a very high temperature and is consequently almost completely dissociated in this region. Due to the expansion which takes place in the gas as it flows down the conical nozzle, the rate of recombination of the gas is insufficient to maintain equilibrium in the flow and the amount of dissociation becomes frozen. The Mach number of the flow is assumed to be large, as is the case in the expansion of a gas from a region of stagnation at a very high temperature.

The region of particular interest in the flow through the nozzle, described by equation (1), is that where the apparent increase in entropy due to the recombination becomes appreciable. This increase in pseudo-entropy, defined as

$$\int \frac{\theta_{\mathrm{d}}\,\mathrm{d}\alpha}{(1+\alpha)T}$$

in dimensionless variables, is equivalent to the increase in entropy which would occur if an amount of heat equivalent to that released to the other degrees of freedom by the recombination of the gas were added to the flow. Blythe (1967) has outlined a series of asymptotic expansions for relaxation of the vibrational mode in an expanding flow through a nozzle of the type given by equation (1). He has indicated that a similar solution for the region where the increase in pseudo-entropy due to recombination is important can be obtained by a suitable redefinition of variables for flows in which the amount of dissociation is frozen. The length of such a region in relation

* Research School of Physical Sciences, Australian National University, P.O. Box 4, Canberra, A.C.T. 2600.

to the dimensions of experimental apparatus could be important, since it would provide a means of producing equilibrium in the flow in a shock tunnel if the length is sufficiently small.

Since the initial conditions for the problem are the same as those which occur at the exit point of a nozzle in a shock tunnel, the parameters A'_0 and x'_0 can be determined by matching the nozzle described by equation (1) to the nozzle of the shock tunnel to maintain the continuity of A' and $\mathrm{d}A'/\mathrm{d}x'$. Also, because the nozzles used are generally of limited divergence so that the flow will remain uniform, it is possible to consider the flow as being one-dimensional.

II. Flow Equations

The dependence on temperature of the constant in the equation for the rate of recombination, following Freeman (1958), is assumed to have the form

$$k_{\mathrm{r}} = A_{\mathrm{r}} T^{\delta},$$

where δ is taken to be completely arbitrary for the purposes of the present discussion. Then, from Lighthill (1957), the equations for the one-dimensional flow of an ideal dissociating gas are

$$\rho u A = u_0, \tag{2}$$

$$\frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}x} - \frac{3}{1+\alpha}\frac{1}{T}\frac{\mathrm{d}T}{\mathrm{d}x} = \frac{\theta_{\mathrm{d}}}{(1+\alpha)T}\frac{\mathrm{d}\alpha}{\mathrm{d}x}, \tag{3}$$

$$(4+\alpha)T + \theta_{\mathrm{d}}\alpha + \tfrac{1}{2}u^2 = 4+\alpha_0+\theta_{\mathrm{d}}\alpha_0 + \tfrac{1}{2}u_0^2, \tag{4}$$

$$\frac{\mathrm{d}\alpha}{\mathrm{d}x} = \frac{\Lambda \rho^2 T^{\delta}}{u}\Big((1-\alpha)(\rho_{\mathrm{d}}/\rho)\exp(-\theta_{\mathrm{d}}/T) - \alpha^2\Big), \tag{5}$$

and

$$p = \{(1+\alpha)/(1+\alpha_0)\}\rho T. \tag{6}$$

The dimensionless variables p, ρ, T, u, and α denote pressure, density, temperature, velocity, and the fraction of dissociation respectively, while θ_{d} and ρ_{d} are the characteristic temperature and density of the ideal dissociating gas. The dimensionless variables are defined as

$$\left.\begin{array}{llll} \rho = \rho'/\rho'_0, & T = T'/T'_0, & p = p'/p'_0, & \theta_{\mathrm{d}} = \theta'_{\mathrm{d}}/T'_0, \\ \rho_{\mathrm{d}} = \rho'_{\mathrm{d}}/\rho'_0, & A = A'/A'_0, & x = x'/x'_0, & u = u'(RT'_0/W_2)^{-\frac{1}{2}}, \\ \text{and} & \multicolumn{3}{l}{\Lambda = 4(1+\alpha_0)x'_0\, k'_{r0}\, \rho_0'^2 (RT'_0/W_2)^{-\frac{1}{2}} W_2^{-2},} \end{array}\right\} \tag{7}$$

where R is the universal gas constant, W_2 denotes the molecular weight of the gas, the subscript 0 indicates conditions at the entry to the nozzle, and the primes denote dimensional quantities.

It is assumed that the flow is frozen at $x = 0$, so that the dissociation term in equation (5)

$$(1-\alpha)(\rho_{\mathrm{d}}/\rho)\exp(-\theta_{\mathrm{d}}/T) = \{(1-\alpha)/(1-\alpha_{\mathrm{e}})\}\alpha_{\mathrm{e}}^2,$$

where α_e is the value of the fraction of dissociation at equilibrium, can be neglected. It is also assumed that $u \approx u_0$, since the flow resulting from the high temperatures in the stagnation region, which are necessary to produce an appreciable degree of dissociation, will have a high Mach number. Lastly it is assumed that $\alpha \approx \alpha_0$, since initial densities are generally sufficiently small to make Λ small.

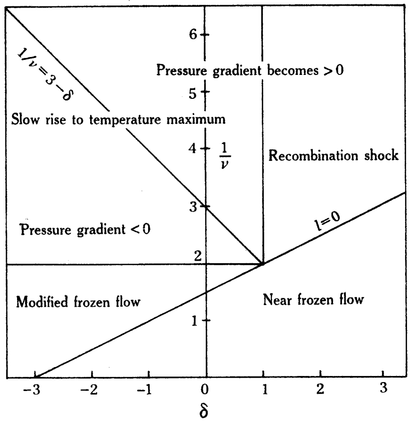

Fig. 1.—Domains in the $(\delta, 1/\nu)$ plane showing the types of solutions for $\alpha_0 = 0\cdot 5$: Modified frozen flow region
$T \underset{x\to\infty}{\sim} x^{(1+2\nu)/(1-\delta)}$
Near frozen flow region
$T \underset{x\to\infty}{\sim} x^{-\frac{1}{3}(1+\alpha_0)\nu}$.

Applying these assumptions in equations (2)–(6), equation (3) can be rewritten as

$$\frac{\nu}{1+x}+\frac{3}{1+\alpha_0}\frac{1}{T}\frac{\mathrm{d}T}{\mathrm{d}x}=\frac{\Lambda\,\theta_{\mathrm{d}}\,\alpha_0^2}{u_0(1+\alpha_0)}(1+x)^{-2\nu}T^{\delta-1}\,,$$

and this equation can be integrated to give the results,

$$\delta\neq 1,\quad l\neq 0 \qquad T^{1-\delta}=(1+x)^{-\frac{1}{3}(1+\alpha_0)(1-\delta)\nu}\left\{1+\frac{B(1-\delta)}{l}\Big((1+x)^l-1\Big)\right\}; \tag{8a}$$

$$\delta=1,\quad l\neq 0 \qquad T=(1+x)^{-\frac{1}{3}(1+\alpha_0)\nu}\exp\left\{\frac{B}{l}\Big((1+x)^l-1\Big)\right\}; \tag{8b}$$

$$\delta\neq 1,\quad l=0 \qquad T^{1-\delta}=(1+x)^{-\frac{1}{3}(1+\alpha_0)(1-\delta)\nu}\{1+B(1-\delta)\log(1+x)\}; \tag{8c}$$

$$\delta=1,\quad l=0 \qquad T=(1+x)^{B-\frac{1}{3}(1+\alpha_0)}; \tag{8d}$$

where $B = \Lambda\theta_{\mathrm{d}}\,\alpha_0^2/3u_0$ and $l = 1-\nu\{2+\frac{1}{3}(1+\alpha_0)(\delta-1)\}$.

The behaviour of these solutions can best be appreciated by considering them in terms of certain domains in the $(\delta, 1/\nu)$ plane, shown in Figure 1, which is modelled on similar figures presented by Blythe (1967) and Cheng and Lee (1968). Before doing so, it is of interest to consider the following expression for the pressure gradient, obtained from equations (2)–(6), with substitution of the solution for the temperature from equations (8), that is,

$$l\neq 0,\qquad F(x)\frac{\mathrm{d}p}{\mathrm{d}x}=-\frac{\nu\left\{1-\dfrac{B(1-\delta)}{l}+B\left(\dfrac{1-\delta}{l}-\dfrac{3}{(4+\alpha_0)\nu}\right)(1+x)^l\right\}}{(1+x)\left\{1+\dfrac{B(1-\delta)}{l}\Big((1+x)^l-1\Big)\right\}}; \tag{9a}$$

$$l = 0, \qquad F(x)\frac{\mathrm{d}p}{\mathrm{d}x} = -\frac{\nu\left\{1-\dfrac{3B}{(4+\alpha_0)\nu}+B(1-\delta)\log(1+x)\right\}}{(1+x)\{1+B(1-\delta)\log(1+x)\}}; \tag{9b}$$

where

$$F(x) = \{M_f^2(x)-1\}/\rho(x)\,u^2(x) > 0$$

and M_f^2 is the frozen Mach number.

TABLE 1

DISTANCE x_s OF RECOMBINATION SHOCK DOWNSTREAM FROM ORIGIN FOR NITROGEN

$x_0' = 114$, $u_0' = 7\times10^5$ cm sec^{-1}, $k_r(300°\mathrm{K}) = 7\times10^{14}$ cm^6 mole^{-2} sec^{-1}, $\alpha_0 = 0\cdot5$, and $\nu = 0\cdot2$, $\delta = 2$

ρ_0' (g cm^{-3})	x_s (cm) for $T_0' = 100$	250	500	750	1000	2000°K
10^{-3}	0·012	0·0050	0·0025	0·0017	0·0012	0·00062
10^{-4}	1·3	0·51	0·25	0·17	0·13	0·062
10^{-5}	250	79	34	21	15	7·0
10^{-6}	$1\cdot1\times10^5$	$3\cdot3\times10^4$	$1\cdot3\times10^4$	$7\cdot6\times10^3$	$5\cdot2\times10^3$	$2\cdot0\times10^3$

If $\delta > 1$ and $l \geqslant 0$, then the temperature becomes unbounded at

$$\begin{aligned} x = x_s &= \{B(\delta-1)/l\}^{1/l}-1, \qquad l > 0, \\ &= \exp\{1/B(\delta-1)\}-1, \qquad l = 0. \end{aligned}$$

This singularity defines the position of the recombination shock which is characterized by a sharp increase in temperature and pressure as a consequence of which the flow returns to equilibrium. Although the assumption $\alpha \approx \alpha_0$, which was made earlier, becomes invalid for large values of B, the predicted position of the recombination shock is still accurate to within a few per cent when compared with numerical solutions, although the error in the temperature may be very large. An indication of the dimensions of the recombination shock can be obtained by consideration of the values of x_s which are tabulated in Table 1, and also from equations (9), which show that the pressure begins to increase at

$$\begin{aligned} x &= \left\{\left(\frac{1}{B}+\frac{\delta-1}{l}\right)\Big/\left(\frac{\delta-1}{l}-\frac{3}{(4+\alpha_0)\nu}\right)\right\}^{1/l}-1, \qquad l \neq 0, \\ &= \exp\left\{\left(\frac{1}{B}-\frac{3}{(4+\alpha_0)\nu}\right)\Big/(\delta-1)\right\}-1, \qquad l = 0. \end{aligned}$$

If $\delta \leqslant 1$ and $\nu < \frac{1}{2}$, then for x sufficiently great

$$T \sim x^{(1-2\nu)/(1-\delta)}$$

so that the temperature again becomes unbounded as $x \to \infty$. Thus a maximum in the temperature will eventually occur. However, in this case the rise in temperature will be much slower and will occur over a distance of much greater magnitude as can be seen by inspection of Tables 2 and 3. The order of magnitude of the distance which is necessary for the flow to approach equilibrium can be estimated in the following manner. Since for most of the diatomic gases the heat of recombination is large compared with the specific heat of the gas, very little recombination is necessary for the temperature to rise sufficiently to establish equilibrium in the flow. Hence let

$$T_e = \theta_d[\log\{\rho_d(1-\alpha_0)/\rho\alpha_0^2\}]^{-1},$$

so that x_e can be estimated from the relation

$$\theta_d^{1-\delta}\left\{\log\left(\frac{\rho_d(1-\alpha_0)}{\alpha_0^2}(1+x_e)^\nu\right)\right\}^{\delta-1} = (1+x_e)^{-\frac{1}{2}(1+\alpha_0)(1-\delta)\nu}\left\{1+\frac{B(1-\delta)}{l}\left((1+x)^l-1\right)\right\}.$$

TABLE 2

ESTIMATED DISTANCE x_e DOWNSTREAM FROM ORIGIN FOR EQUILIBRIUM UNDER CONDITIONS OF TABLE 1 WITH $\delta = \frac{1}{2}$

ρ_0'	x_e (cm) for					
(g cm^{-3})	$T_0' = 100$	250	500	750	1000	2000°K
10^{-3}	0·041	0·038	0·035	0·033	0·031	0·024
10^{-4}	4·0	3·7	3·3	3·1	2·8	2·2
10^{-5}	760	690	620	560	520	370
10^{-6}	$2\cdot2\times10^5$	$2\cdot0\times10^5$	$1\cdot8\times10^5$	$1\cdot6\times10^5$	$1\cdot5\times10^5$	$1\cdot1\times10^5$

TABLE 3

ESTIMATED DISTANCE x_e DOWNSTREAM FROM ORIGIN FOR EQUILIBRIUM FLOW UNDER CONDITIONS OF TABLE 1 WITH $\rho_0' = 10^{-4}$ g cm^{-3} AND $T_0' = 1000$°K

δ	x_e (cm) for					
	$1/\nu = 3$	5	10	50	100	1000
0	11·3	11·0	10·7	9·9	9·6	9·3
-1	1400	430	250	157	146	135
-2	$2\cdot4\times10^6$	$3\cdot9\times10^4$	$8\cdot1\times10^3$	$3\cdot0\times10^3$	$2\cdot7\times10^3$	$2\cdot3\times10^3$
-3	$3\cdot3\times10^9$	$3\cdot8\times10^6$	$2\cdot9\times10^5$	$6\cdot4\times10^4$	$5\cdot4\times10^4$	$4\cdot5\times10^4$

It is worth noting that equations (9) show that for $\delta < 1$ the pressure gradient becomes positive only if

$$3-\delta < 1/\nu.$$

If $l \geqslant 0$ and $\nu \leqslant \frac{1}{2}$, then for x sufficiently great

$$T \sim x^{(1-2\nu)/(1-\delta)},$$

and the approximation remains valid for all values of x, since $T \to 0$ as $x \to \infty$, although the temperature decrease is not as rapid as for the case when $l < 0$, since the recombination does have some effect on the flow.

If $l < 0$, then for x sufficiently great

$$T \sim x^{-\frac{1}{2}(1+\alpha_0)\nu},$$

which is the asymptotic form for a completely frozen flow, so that the recombination of the gas has no effect at all on the flow to a first approximation. However, it is worth noting that if δ is sufficiently large for $B(1-\delta)/l$ to be greater than unity, even though Λ may be small, there will be a recombination shock at

$$x_s = \{1+l/B(\delta-1)\}^{1/l}-1\,.$$

Such a recombination shock is generally much steeper than that which occurs when $l>0$, and the position given by the above relation compares exceedingly well with numerical results.

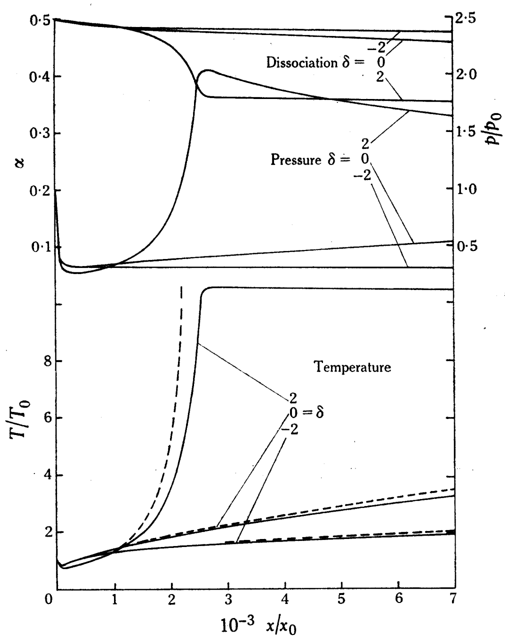

Fig. 2.—Numerical solutions for the pressure p, dissociation α, and temperature T compared with the estimated temperature (dashed curves) for $\nu = \frac{1}{2}$, $\Lambda = 0\cdot01$, $\alpha_0 = 0\cdot5$, and $T_0' = 500°K$ in nitrogen.

III. Discussion

The numerical solution for a typical problem is compared in Figure 2 with the approximation described above. Although the value of Λ used is small the integrated effects of the error in the assumption $\alpha \approx \alpha_0$ produce quite large errors in the temperature far downstream. In fact, for larger values of Λ, the error is generally much smaller, because equilibrium is reached much sooner, and the error does not have time to grow to significant proportions.

Tables 2 and 3 give an indication of the orders of distances involved in the slow rise to a maximum in the temperature, where the flow returns to equilibrium. It appears that the initial densities would have to be at least of the order of atmospheric density, if any appreciable increase in temperature is to be achieved within the limits imposed on the flow by experimental apparatus. Table 1 shows that in the case of a recombination shock the distance necessary to reach equilibrium is much less than in the case when $\delta < 1$, when the temperature rises to a maximum value much more slowly. In addition the length of the nozzle required to reach equilibrium varies considerably with the initial temperature. However, if $\delta > 1$, it would be possible to produce the sharp rise in temperature, which characterizes the recombination shock, within the order of experimental distances, provided that the initial density is at least of the order of 10^{-5} g cm^{-3}.

At present, however, although experiment indicates that δ is negative, estimates of both variation with temperature and absolute value of the rate of recombination vary over large ranges and more definite information is required before it can be decided whether the distances required for the flow to regain equilibrium are compatible with the dimensions of experimental apparatus.

IV. References

Blythe, P. A. (1967).—*Phil. Trans. R. Soc.* A **262,** 203.
Cheng, H. K., and Lee, R. S. (1968).—*AIAA Jl* **6,** 823.
Freeman, N. C. (1958).—*J. Fluid Mech.* **4,** 407.
Lighthill, M. J. (1957).—*J. Fluid Mech.* **2,** 1.