J. Fluid Mech. (1973), *vol.* 58, *part* 1, *pp.* 187–196
Printed in Great Britain

Vibrational relaxation effects in weak shock waves in air and the structure of sonic bangs

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(Received 11 December 1972)

Vibrational relaxation of oxygen and nitrogen is shown to be important in determining the structure of weak shock waves in air. Of particular interest are waves with pressure jumps of 100 Pa† or less which are present in the atmosphere as sonic bangs. It is found that the structure of the waves depends on shock strength, ambient pressure, temperature and humidity.

1. Introduction

It has been established by Hodgson & Johannesen (1971) that the shock waves of sonic bangs are so weak that the small vibrational specific-heat contribution of atmospheric oxygen may be sufficient to cause them to be fully dispersed.

A detailed study of the relaxing energy modes of the molecular species occurring in the atmosphere indicates that the vibrational mode of nitrogen should also be taken into account. All other molecular relaxation effects may be ignored; either the specific-heat contributions are too small, or the relaxation frequencies so high that departures from equilibrium are negligible.

The contribution of the vibrational mode of nitrogen to the specific heat of atmospheric air is about one fifth of that of the vibrational mode of oxygen. However, the vibrational relaxation frequency of atmospheric oxygen is 50–250 times that of nitrogen. The result is that nitrogen is more important than oxygen if the shock waves are very weak. The relaxation frequencies of both oxygen and nitrogen are critically dependent on the water-vapour concentration, which is therefore a major factor in determining the shock wave structure.

2. Governing equations

For a steady one-dimensional wave with the x axis in the direction of flow the conservation equations may be written in the usual notation as

$$\rho u = \rho_1 u_1, \tag{1}$$

$$p + \rho u^2 = p_1 + \rho_1 u_1^2, \tag{2}$$

$$c_p T + \sigma_{\mathrm{N}} + \sigma_{\mathrm{O}} + \tfrac{1}{2}u^2 = c_p T_1 + \sigma_{\mathrm{N}1} + \sigma_{\mathrm{O}1} + \tfrac{1}{2}u_1^2, \tag{3}$$

where the subscript 1 refers to initial conditions ahead of the wave. c_p is the frozen specific heat at constant pressure and σ_{N} and σ_{O} are the energy contributions of

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† 1 Pa ≡ 1 pascal = 1 N m^{-2}.

the vibrational modes of nitrogen and oxygen to the mixture as a whole. Equation (3) refers to a unit mass of atmospheric air. The well-known equation describing vibrational relaxation becomes, for the two modes in a steady flow,

$$u(d\sigma_N/dx) = \Omega_N(\bar{\sigma}_N - \sigma_N) \tag{4}$$

and

$$u(d\sigma_O/dx) = \Omega_O(\bar{\sigma}_O - \sigma_O), \tag{5}$$

where Ω_N and Ω_O are the relaxation frequencies of the two modes. $\bar{\sigma}_N$ and $\bar{\sigma}_O$ are the local equilibrium values of σ_N and σ_O respectively. If the internal specific-heat contributions for atmospheric air c_N and c_O are assumed constant, equal to their initial values of c_{N1} and c_{O1}, then

$$\bar{\sigma}_N = \bar{\sigma}_{N1} + c_{N1}(T - T_1) \tag{6}$$

and

$$\bar{\sigma}_O = \bar{\sigma}_{O1} + c_{O1}(T - T_1). \tag{7}$$

The equation of state is

$$p = \rho RT, \tag{8}$$

where R is the gas constant for a unit mass of atmospheric air.

The method of solution of the above eight equations has been given by Clarke & Rodgers (1965), assuming that Ω_N and Ω_O are constant through the wave. Elimination of ρ, p, T, $\bar{\sigma}_N$, $\bar{\sigma}_O$, σ_N and σ_O leads to a second-order nonlinear differential equation for u in terms of x, which can be solved numerically.

3. Thermodynamics and gas kinetics

The vibrational specific-heat contributions of oxygen and nitrogen were calculated using the harmonic oscillator approximation with characteristic temperatures of 2228 °K and 3336 °K, respectively. The atmosphere was considered to be a mixture of nitrogen, oxygen and water vapour, nitrogen and oxygen being in the ratio in which they appear in the standard atmosphere.

The relaxation frequencies of the vibrational modes of oxygen and nitrogen are critically dependent on water vapour content. The nonlinear dependence of the vibrational relaxation frequency of oxygen on water vapour concentration has been the subject of controversy amongst acousticians for forty years, and there are a large number of papers in the literature concerned with this subject. The data used for the present investigation are recommended by Monk (1969), and include in the expressions for the relaxation frequency of atmospheric oxygen the effects of collisions with water vapour, nitrogen and other oxygen molecules. The actual formulae used were

$$\Omega_{O1} = 2\pi p_1(135 + 6{\cdot}97 \times 10^5 h + 4{\cdot}23 \times 10^8 h^2)\ \mathrm{s}^{-1}$$

for $h < 0{\cdot}002$, where h is the mole fraction of water vapour, and

$$\Omega_{O1} = 2\pi p_1 h\left[1{\cdot}75 \times 10^5 + 6{\cdot}14 \times 10^6 \frac{0{\cdot}112 + 100h}{1{\cdot}04 + 100h}\right]\ \mathrm{s}^{-1}$$

for $h > 0{\cdot}002$. Inclusion of the pressure p_1 (in atmospheres) assumes that binary collisions govern the relaxation process. Most of the results presented here are for an ambient pressure of one atmosphere, and the pressure dependence is included primarily to determine shock structure under high-altitude atmospheric conditions. The above formulae are based on experimental observations carried out at 22 ± 1·3 °C. The temperature dependence of Ω_{O1} is unknown. The factor 2π is included in all the expressions for the relaxation frequency since the actual formulae given in the appropriate references are for the frequencies of maximum acoustic absorption (Napier frequencies).

The effect of water vapour on the relaxation frequency of nitrogen has not received the same attention as the corresponding phenomenon for oxygen. Indeed, until very recently the vibrational specific heat of nitrogen at room temperature has been considered too small for sound absorption experiments. The formula used here is based on the observations of Evans (1972), who found that for pure nitrogen in mixtures with water vapour

$$\Omega_N = 2\pi \times 2{\cdot}74 \times 10^9 (h/T) \exp[-40{\cdot}8/T^{\frac{1}{3}}]\ \mathrm{s}^{-1}$$

at 1 atm and temperature T. This equation is expected to be accurate over the range 250–500 °K. However, since the temperature dependence of Ω_{O1} is unknown and Ω_N varies by only about 10 % throughout the temperature range of interest here, the expression has been evaluated at 22 °C and the temperature dependence ignored. As $h \to 0$, Ω_N should approach the values for pure nitrogen. According to Henderson (1962), whose experiments were conducted at 203 °C, the frequency of maximum sound absorption in pure nitrogen occurs at about 1 Hz atm^{-1}. At room temperature it is hardly likely to be greater than this figure, which leads to a value of Ω_N which is negligible compared with that derived using Evans's expression for all conditions likely to occur in the atmosphere. To avoid the anomaly of having $\Omega_{N1} \to 0$ as $h \to 0$ the following expression was used to evaluate the relaxation frequency of nitrogen:

$$\Omega_{N1} = 2\pi p_1 (1 + 2{\cdot}04 \times 10^4 h)\ \mathrm{s}^{-1}.$$

If only as an academic exercise, the structure of weak shock waves in perfectly dry air may now be calculated. This expression for Ω_{N1} ignores the effect of oxygen on the relaxation of nitrogen, but owing to the dramatic effect of water vapour this is not important except perhaps under extremely dry conditions.

4. Results

The translational temperature T and the vibrational temperatures of the two relaxing modes T_{vO} and T_{vN} are plotted in terms of distance through a typical weak wave in figure 1. The wave strength is 50 Pa and the initial conditions are $T_1 = 285°$ K, $p_1 = 1$ atm and 50 % relative humidity. It is clear that the local departure from equilibrium $(T - T_v)$ is greater for nitrogen than for oxygen. This is consistent with the fact that $\Omega_N < \Omega_O$. The rapid increase in translational temperature near the front of the wave is due mainly to the relaxation of oxygen. The vibrational temperature of nitrogen changes by only a small amount in this part of the wave. Towards the rear of the wave the translational temperature gradient is smaller and controlled mainly by relaxation of nitrogen since the oxygen is very near to equilibrium. Thus the translational temperature profile may be considered to be composed of two (overlapping) parts each dominated by one of the relaxing energy modes.

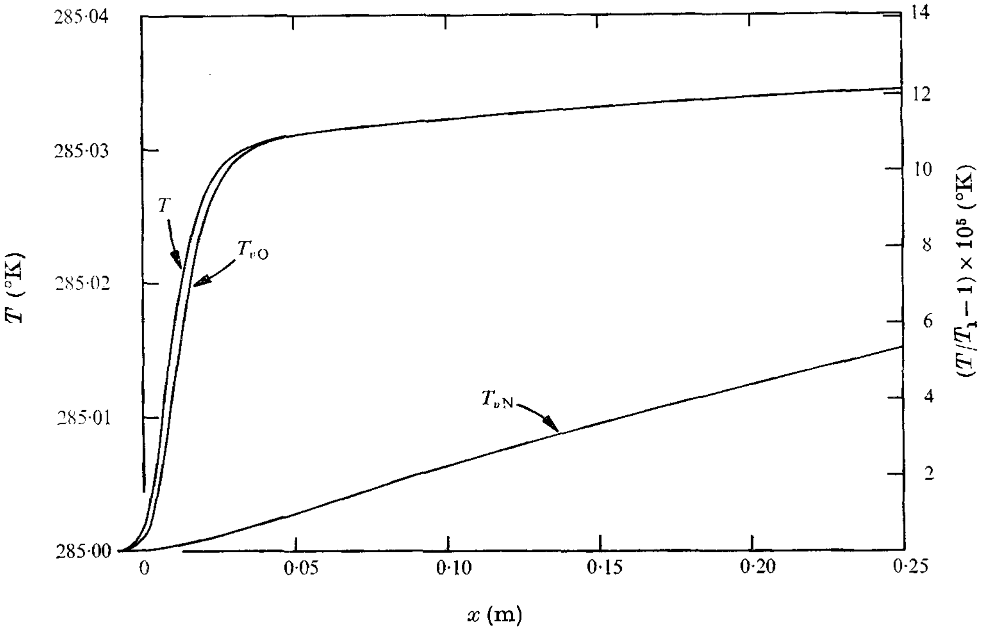

FIGURE 1. Temperature profiles of a wave of strength 50 Pa with initial conditions of 285 °K, 1 atm and 50 % relative humidity.

For a sufficiently large increase in strength a frozen shock occurs at the front of the wave. This third part of the wave appears only if the specific heats of the vibrational modes are insufficient to fully disperse the waves. For the particular initial conditions of figure 1, the total vibrational specific-heat $c_{O1}+c_{N1} = 0{\cdot}0061R$, which is sufficient to fully disperse waves weaker than 82 Pa. In passing it should be pointed out that the real structure of the frozen shock is determined by relaxation of the rotational modes of the molecules. However, since the relaxation frequencies of these modes are very much greater than those of the vibrational modes, the frozen shock is considered here to be a mathematical discontinuity in all quantities except vibrational temperatures and energies. The rotational modes are assumed to be in local equilibrium with the translational modes throughout the wave.

For a sufficiently weak wave the oxygen-dominated part of the wave is absent and the structure is dominated by the relaxation of nitrogen. This situation occurs if the wave is weak enough to be fully dispersed by the vibrational specific heat of nitrogen alone. For the particular initial conditions of figure 1, $c_{N1} = 0{\cdot}00088R$, which is sufficient to fully disperse waves weaker than 12 Pa.

Summarizing the results so far, a particular wave will be entirely dominated by nitrogen relaxation only if the vibrational specific heat of nitrogen is large enough to fully disperse the wave. If it is not large enough then vibrational relaxation of oxygen affects the front part of the wave. If the combined vibrational specific heats are insufficient to fully disperse the wave then a frozen shock appears and the wave is partly dispersed.

In this paper, which is essentially concerned with sonic bangs, only pressure

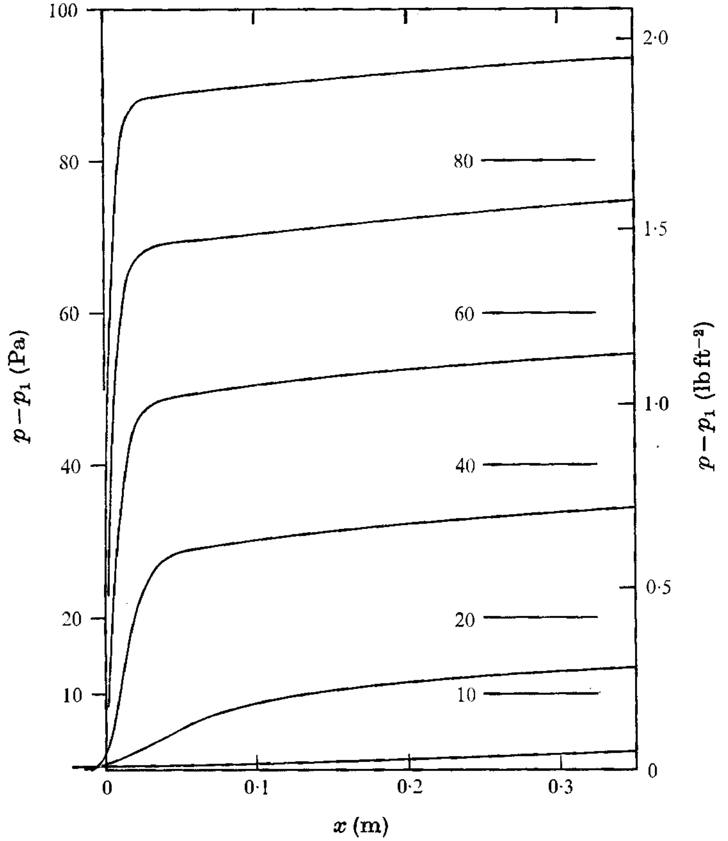

FIGURE 2. Pressure profiles of waves having strengths between 10 Pa and 100 Pa with initial conditions of 285 °K, 1 atm and 50 % relative humidity.

profiles are illustrated in the remaining figures. For the same initial conditions as figure 1, pressure profiles of waves of various strengths are shown in figure 2. As the wave strength increases oxygen relaxation becomes important and then the frozen shock appears. In the case of fully dispersed waves the distance through the wave is measured from the point at which $p-p_1 = 0{\cdot}05\ (p_2-p_1)$. Apart from the absolute shock strength the remaining factors which affect the wave structure are defined by the initial temperature, pressure and humidity. In order to illustrate how each of these affects the wave structure the shock strength and two of the three initial conditions are held constant for the plotting of pressure profiles.

With shock strength, T_1 and p_1 constant, varying the humidity leads to profiles having not only vastly different widths, but different shapes too. In figure 3 the variation in overall width is separated out by dividing the distance through each wave by Δ, the distance to the point where $p-p_1 = 0{\cdot}95\ (p_2-p_1)$. The variation in shape comes about because of the different functional dependences of Ω_{O1} and Ω_{N1} on humidity.

The effect of varying the initial temperature is shown in figures 4 and 5. In figure 4 the shock strength, initial pressure and mole fraction of water vapour are kept constant. The only effect of increasing T_1 is in this case to increase the

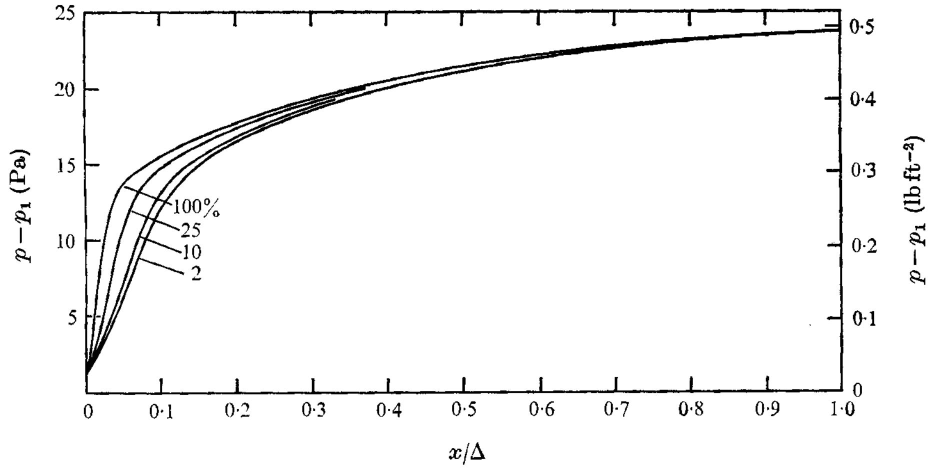

FIGURE 3. The effect of humidity on shape and width of waves of strength 25 Pa with fixed initial temperature (285 °K) and pressure (1 atm).

Relative humidity (%)	2	10	25	100
Δ (m)	27·8	6·25	2·48	0·608

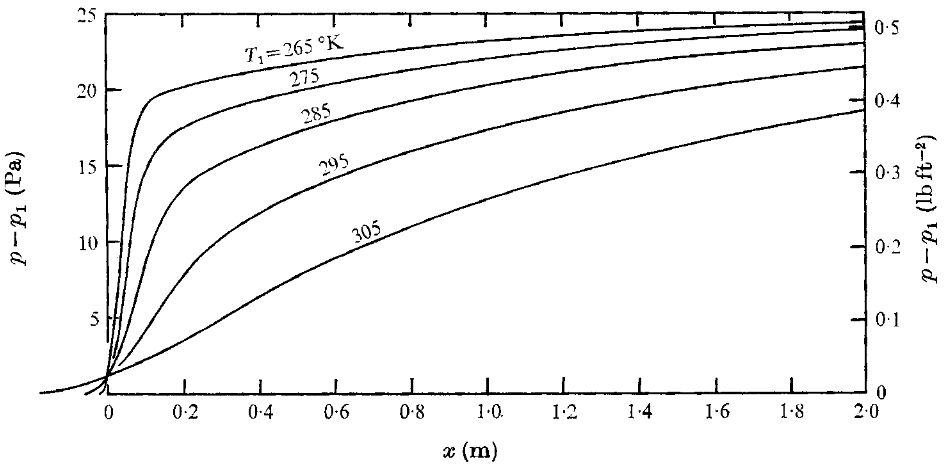

FIGURE 4. Pressure profiles of waves of strength 25 Pa for various initial temperatures but with constant initial pressure (1 atm) and mole fraction of water vapour ($h = 0{\cdot}00329$, corresponding to saturation at 265 °K).

vibrational specific heats. The molecular constitution of the gas and hence Ω_{01} and Ω_{N1} remain unchanged. Under these conditions any wave is more likely to be fully dispersed at higher temperature. It is also, as figure 4 actually illustrates, more likely to be dominated by relaxation of nitrogen. It is probably more pertinent to compare pressure profiles for different values of T_1 but with constant relative humidity. An extra complication arises since the saturated vapour pressure of water is a sensitive function of temperature. The consequences are that Ω_{N1} and Ω_{01} increase as T_1 increases, and the overall width of a wave decreases. This is accompanied by a slight change of shape owing to the different

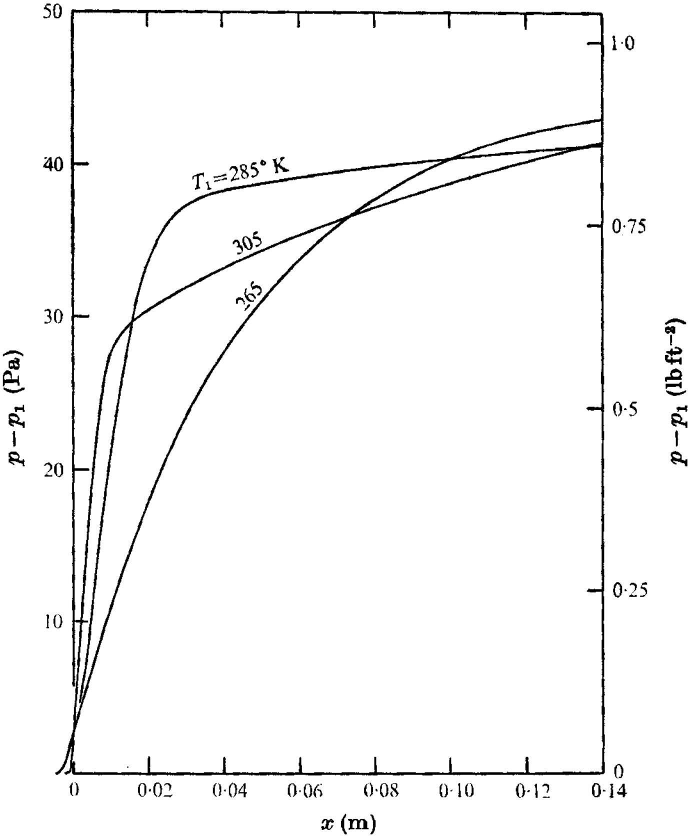

FIGURE 5. Pressure profiles of waves of strength 50 Pa for various initial temperatures with constant initial pressure (1 atm) and relative humidity (50 %).

functional dependences of Ω_{N1} and Ω_{O1} on the mole fraction of water vapour. These effects combine with the fundamental temperature effect on the vibrational specific heats and typically lead to the pressure profiles shown in figure 5.

We now examine what happens if we keep the shock strength, initial temperature and humidity constant while varying the initial pressure. Typical profiles are shown in figure 6. As the pressure decreases from 1 atm it is clear that the relaxation of oxygen becomes more important and eventually a partly dispersed wave occurs. The effect of decreasing p_1 is almost identical to that of increasing p_2-p_1 as far as the thermodynamic structure of the shock is concerned. This is not surprising since the thermodynamics of all waves which have the same value of $(p_2-p_1)/p_1$ and the same specific heats are identical. However, the gas kinetics of the wave structure are somewhat different since the relaxation frequencies depend on the absolute pressure and on the mole fraction of water vapour. For constant humidity the mole fraction of water vapour is inversely proportional to the pressure. It follows that Ω_{N1} is virtually independent of initial pressure for constant humidity. For Ω_{O1} the cancellation of the p_1 dependence is not so dramatic and Ω_{O1} increases as p_1 decreases.

Having examined the way in which the pressure profiles of normal shock waves

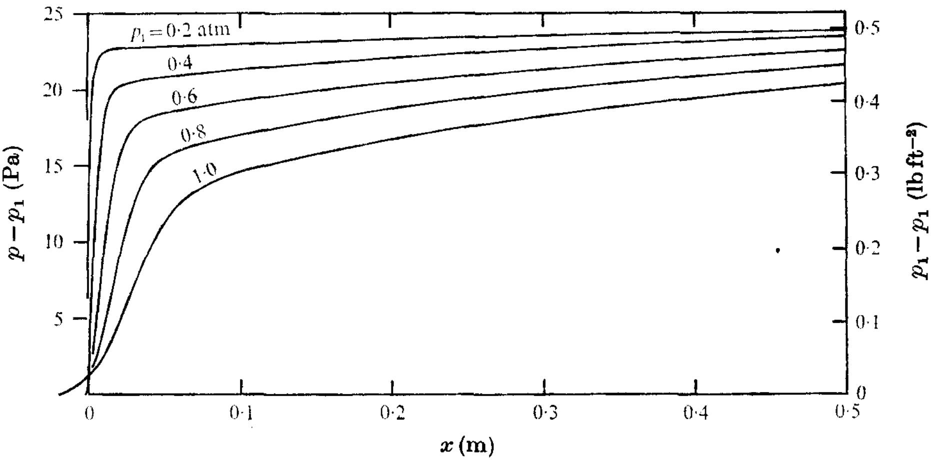

FIGURE 6. Pressure profiles of waves having constant strength (25 Pa), initial temperature (285 °K) and relative humidity (50 %) for various initial pressures.

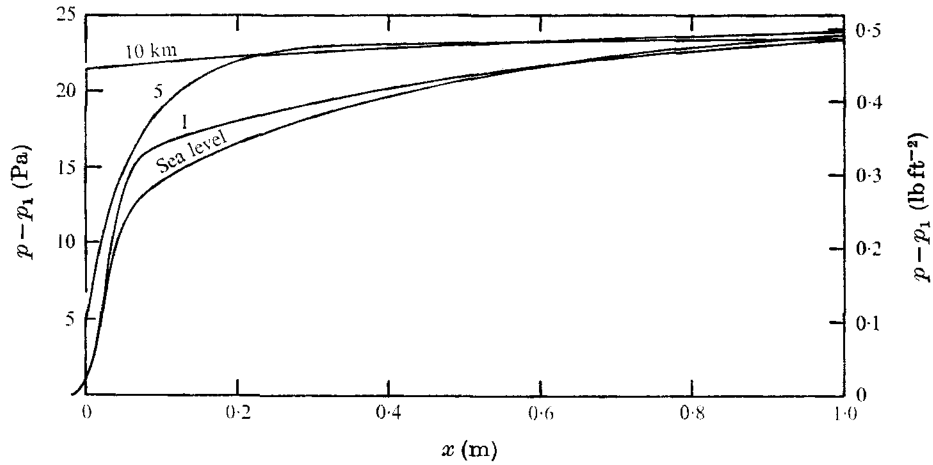

FIGURE 7. The variation of pressure profiles of waves of constant strength (25 Pa) with initial conditions defined by various altitudes of the standard atmosphere with water added to 50 % relative humidity.

Altitude (km)	0	1	5	10
T_1(°K)	288·2	282·2	256·2	223.2
p_1(atm)	1·0	0·887	0·498	0·261

depend on shock strength and the initial conditions, it is interesting to look at one or two special cases. Figure 7 contains profiles of shocks of strength 25 Pa with initial temperatures and pressures defined by the standard atmosphere at various altitudes. The relative humidity has been assumed to be 50 %. Above about 5 km the strength of the frozen shock is significant, whereas at lower altitudes the two parts of the wave dominated by oxygen relaxation and nitrogen relaxation are distinguishable.

Finally, in figure 8 (*a*) are shown pressure profiles of very weak shocks in a cold dry atmosphere and in figure 8 (*b*) profiles of stronger shocks in hot wet conditions.

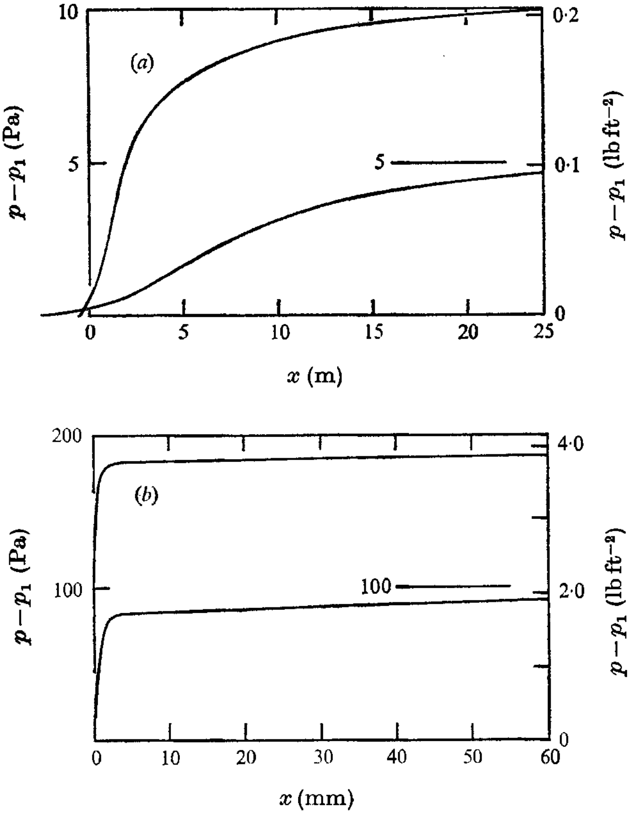

FIGURE 8. (*a*) Pressure profiles of very weak shock waves (5 Pa and 10 Pa) in cold (260 °K), fairly dry (25 % relative humidity) air. The initial pressure is 1 atm. (*b*) Pressure profiles of stronger shock waves in hot (300 °K) saturated air at 1 atm.

These profiles may be considered extreme types and are included here to illustrate the enormous variation in wave shape and overall width. In cold dry conditions weak shock waves may be several metres wide, whereas stronger shock waves in a hot humid atmosphere may be only a few millimetres wide.

5. Conclusion

Vibrational relaxation of both oxygen and nitrogen has been shown to be effective in dispersing weak shock waves in the atmosphere. The effect on pressure profiles of shock strength and the initial conditions of temperature, pressure and relative humidity has been illustrated. The absolute shock strength $p_2 - p_1$ rather than the normalized shock strength $(p_2 - p_1)/p_1$ has been used in this paper to relate the end-points of each wave so that the data may then be more readily interpreted in terms of sonic-bang rise times. Simple geometric transformation of the calculated shock waves leads to favourable comparisons with observed pressure signatures. However since the relative humidity, so vital to the theory, is usually omitted from published pressure measurements precise comparisons have not been possible except in a very few instances. Further, not all observed sonic-bang pressure signatures are free from turbulence effects, which are known to cause sharp spikes in the signatures. Relaxation would cause the dispersal and attenuation of these spikes during further transmission through the atmosphere. Any comparison between this work and sonic bangs must assume fully developed bang profiles. This of course requires changes in atmospheric conditions to be sufficiently gradual for the wave to adjust itself to a steady profile. Finally there remains the possibility of checking the value of the vibrational relaxation frequency of nitrogen including its dependence on oxygen and water vapour using sonic-bang pressure signatures.

The author wishes to thank Professor N. H. Johannesen for many helpful discussions during the course of this work.

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