Analysis of Some Discontinuous Initial-Value Problems for Free-Molecular Gas Mixtures, II

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SUMMARY Some general 'diffusion' relations are used to derive the formulae for the mass average velocity, the pressure tensor and, by implication, the 'hydrodynamic' pressure of a gas mixture formed as the result of the free-molecular free expansion of a spherical gas cloud (initially in equilibrium) being combined with a corresponding 'dissipation' motion of a surrounding gas medium (initially separated from the cloud by a spherical impermeable membrane, and also in equilibrium). A discussion of some typical or specific features of the behaviour of the mixture's density, mass average velocity and pressure is presented, and illustrated by some selected diagrams.

1 INTRODUCTION

This paper is a continuation of and a complement to our earlier paper (East and Glikson, 1974). In that paper, we considered two special subcases of a quite general problem of free-molecular expansion. The problem and the method of its solution can be stated briefly as follows:

An impermeable membrane (or a set of membranes) of fixed shape separates two ideal (in general, distinct) rarefied gases, each of them in equilibrium, i.e., the molecular velocity distribution function of each gas can be taken as absolute Maxwellian. This configuration occupies the whole of the physical space. At a certain moment of time, t = 0 say, the membrane is instantaneously removed without disturbing the gases. The resulting flow is assumed to be free-molecular, and so the problem can be studied adequately on the basis of two Boltzmann equations - one for each gas constituent - with zero collision integrals (more precisely, on the basis of some molecular velocity distribution functions satisfying these 'reduced' Boltzmann equations). All macroscopic quantities for a particular gas constituent are of course defined as corresponding moments of the velocity distribution function of this constituent. Subsequent expressions for mean quantities of the resulting mixture can be given in terms of these moments and/or some initial quantities. (For a purely mathematical statement of the problem and the method of its solution, as well as for some additional comments and a list of related references, see East and Glikson (1974).)

The special cases of boundaries considered in East and Glikson (1974) were (i) two straight infinite parallel membranes, and (ii) a spherical membrane. The corresponding problems were termed respectively the "infinite layer" problem and the "spherical cloud"problem. (For the latter problem to be feasible, the Maxwellian distribution functions involved have to be centred about zero mean velocities.) While the solution of the first problem was considered and discussed in that paper to a reasonably full extent, the solution of the second one contained neither expressions for the components of the pressure tensor, nor were diagrams or detailed observations for this problem included. Also a misinterpretation of a formulae quoted there from Hirshfelder et al (1954) led to an evaluation of

the average of all possible molecular speeds instead of the mass average (radial) velocity of the flow. In the present paper, we complete these points which are not contained in our earlier work on the spherical cloud problem.

The method used below for the derivation of mean gas quantities differs from that of East and Glikson (1974), and relies essentially on the use of certain 'diffusion' relations which are, in some respects, generalizations of those of Narasimha (1962). These generalized relations are presented in Section 2.

Details of calculations, leading to the results of Sections 2 and 3, will be given elsewhere.

NOTATION

The subscript $i \in \{1,2\}$ refers to the ith constituent of the gas mixture. For the gas inside the membrane(s), i=1; for the outer gas, i=2. (An omission of the subscript i refers to the gas mixture as a whole.)

The subscripts j,k \in {1,2,3} refer to corresponding components (elements and/or rows) of a vector or tensor

The superscript 0 refers to the value of a quantity at the initial time t=0.

a - radius of the spherical membrane;

 $h \equiv (2kT/m)^{\frac{1}{2}}$ - most probable random speed of a gas;

k - Boltzmann's constant;

m - mass of a particle of a gas;

n - number density;

p - hydrodynamic pressure;

P - pressure tensor;

 $r\equiv x_1/a$, where x_1 is the distance from the centre of the spherical membrane;

t - time;

T - temperature;

u - mean velocity of a single gas;

ū - mass average velocity of a gas mixture;

 u_1 , \bar{u}_1 - radial components of u and \bar{u} , respectively;

{x_j} - a system of (curvilinear) coordinates in the
 physical space;

$$\mu_1 \equiv \rho_1^0/\rho_2^0;$$

$$v_i \equiv h_i^0/h_2^0;$$

ρ - mass density;

$$\tau \equiv th_2^0/a$$
.

The remaining notation is defined where it appears.

2 FREE MOLECULE DIFFUSION

2.1 The Origin of the Method

For a particular subcase of a general free expansion problem, in which one of the gases is 'replaced' by vacuum, Narasimha (1962) has shown that ρ satisfies a certain diffusion equation if and only if the initial velocity distribution function is isothermal Maxwellian. (As a by-product, this theorem explains the success of the rather heuristic approach of Molmud (1960).) Furthermore, relations were found between ρ , ψ , T, P and the heat flow vector of the gas, which provide a useful method of calculating these quantities after the value of one of them, say ρ , has been found by direct integration.

2.2 Diffusion Relations for Free-Molecular Mixtures

Provided that the Maxwellian distribution functions of the general problem of Section 1 are centred about zero mean velocities, some relations (similar to those mentioned in Subsection 2.1) can be found for such a general case, by using the equations of continuity

$$\frac{\partial \rho_{i}}{\partial t} + \operatorname{div}(\rho_{i} \tilde{u}_{i}) = 0, \tag{1}$$

and a generalization of a certain relation from Narasimha (1962),

$$\rho_{i} = -\frac{1}{2} t(h_{i}^{0})^{2} \text{ grad } \rho_{i}.$$
 (2)

They are as follows:

$$\rho_{\widetilde{u}}^{\overline{u}} = - \operatorname{t} \operatorname{grad}\left(\sum_{i} \frac{1}{2} \rho_{i} \left(h_{i}^{0}\right)^{2}\right); \tag{3}$$

$$T = \sum_{i} \left(n_i + \frac{1}{3} t \frac{\partial n_i}{\partial t} \right) \frac{T_i^0}{n} - \frac{\rho \overline{y}^2}{3kn}; \tag{4}$$

$$P = \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}, \quad p_j \text{ is the } j^{th} \text{ row of } P,$$

where

$$p_{j} = \sum_{i} \left\{ \frac{1}{2} \rho_{i} (h_{i}^{0})^{2} (\delta_{j} - t \operatorname{grad} u_{ij}) + \rho_{i} u_{ij} u_{i} \right\}$$

$$- \rho \overline{u}_{j} \overline{u}_{i}, \qquad (5)$$

 δ_{j} is the jth row of $\left[\delta_{jk}\right]$ = the Kronecker delta.

(A generalization of the diffusion equation mentioned in Subsection 2.1 is obtained by substituting (2) into (1).)

The abovementioned relations, found by Narasimha

(1962) for the case of a single gas and vacuum, are obtained from (1) - (5) when i takes only one value; of course $\bar{\underline{u}}=\underline{u}_{\underline{i}}$ in such a case. (Note that β_0 of (3.24a) of Narasimha's paper should be replaced by $2\beta_0$.) It has to be pointed out, though, that (1) - (5) are applicable in any coordinate system $\{x_{\underline{i}}\}$ in the physical space, whereas Narasimha's relations (especially the one corresponding to (5)) are basically applicable in cartesian coordinate systems. This was found to be important in the present paper, since in Section 3 below spherical polar coordinates are chosen in preference to a cartesian system.

Also, it should be stressed that the relations (2) - (5), as well as the diffusion equation resulting from (1) and (2), are not in general applicable to the infinite layer problem (described in the Introduction), unless the mean velocities of the constituent gases are equal to zero; otherwise additional terms have to be introduced into (2) - (5) and the diffusion equation.

2.2.1 Mixture pressure

The pressure of a component of the considered gas mixture, at a point x and instant t, is given by p = nkT (Hirshfelder et al, 1954). Using (4), it may be readily shown that

$$p = \sum_{i} \left\{ \frac{1}{2} \rho_{i} (h_{i}^{0})^{2} (1 - \frac{1}{3} t \text{ div } \underline{u}_{i}) + \rho_{i} \underline{u}_{i}^{2} \right\} - \rho \overline{\underline{u}}^{2}$$
 (6)

and, as expected, a comparison with (5) yields

$$p = \frac{1}{3}(p_{11} + p_{22} + p_{33}). (7$$

3 COMPLETION OF THE SPHERICAL CLOUD PROBLEM

3.1 Mass Average Velocity

Because of the spherical symmetry of the problem, a natural choice for coordinates in the physical space is a spherical polar system $\{x_1, x_2, x_3\}$ whose origin is located at the centre of the spherical membrane of radius a. In the following, x_1 represents the distance from the centre of the membrane.

Expressions for ${\bf n}_{\tt i},~\rho_{\tt i}$ and ρ for the spherical cloud problem are given in East and Glikson (1974), and show that all these densities are independent of ${\bf x}_2$, ${\bf x}_3$. (The expression for ${\bf n}_{\tt i}$ contains a typographical error, namely, "+" inside the brackets should be replaced by "-".) It follows then from (3), that $\bar{\bf u}$ has only one non-zero component, $\bar{\bf u}_1$ (i.e. the radial one), given by

$$\rho \bar{u}_{1} = \sum_{i} \left\{ \frac{(-1)^{i} h_{i}^{0} \rho_{i}^{0}}{4\sqrt{\pi} r^{2}} \right\} \left\{ (\tau^{2} v_{i}^{2} - 2r) \exp \left[-\left(\frac{1-r}{v_{i}\tau}\right)^{2} \right] - (\tau^{2} v_{i}^{2} + 2r) \exp \left[-\left(\frac{1+r}{v_{i}\tau}\right)^{2} \right] \right\}, \quad (8)$$

where the non-dimensional quantities r, ν_{i} , τ are defined as follows:

$$\mathbf{r} \equiv \mathbf{x_1/a}, \quad \mathbf{v_i} \equiv \mathbf{h_i^0/h_2^0}, \quad \boldsymbol{\tau} \equiv \mathbf{th_2^0/a}.$$

Expression (8) represents the average (evaluated at each (x,t)) of the components in the x₁-direction, of all possible molecular velocities, whereas, in our previous paper, the result found was the average of all possible molecular speeds. It may be verified that for the subcase described in 2.1 and discussed by Narasimha (1962), our expression (8) reduces to Narasimha's result in (3.14), provided his expression is corrected by (i) multiplying the right-hand side by ρ_0 , and (ii) replacing the term τ^2/ξ^2 by $\tau^2/2\xi^2$. (This second omission was pointed out to us, independently of our calculations, by Professor Narasimha.)

3.2 Pressure Tensor of the Mixture

Since both \underline{u}_i and $\overline{\underline{u}}$ have non-zero components only in the x_1 -direction, (5) gives the nine components of P in the spherical polar coordinates as follows:

$$p_{jk} = 0 \quad \text{if} \quad j \neq k, \tag{9}$$

$$p_{22} = p_{33} = \sum_{i} {}^{1}_{2} \rho_{i} (h_{i}^{0})^{2},$$
 (10)

$$p_{11} = \sum_{i} \frac{1}{2} (h_{i}^{0})^{2} \left[\rho_{i} - t \frac{\partial}{\partial x_{1}} (\rho_{i} u_{i1}) \right] - \rho \bar{u}_{1}^{2},$$

or, after evaluating the derivative,

$$\begin{split} \mathbf{p}_{11} &= \sum_{\mathbf{i}} \, ^{1}\!\!\!\!\! \mathbf{p}_{\mathbf{i}} \, (\mathbf{h}_{\mathbf{i}}^{0})^{\,2} \, - \, \rho \, \bar{\mathbf{u}}_{1}^{2} \\ &- \sum_{\mathbf{i}} \! \left\{ \! \frac{ (-1)^{\, \mathbf{i}} \rho_{\, \mathbf{i}}^{\, 0} \, (\mathbf{h}_{\, \mathbf{i}}^{\, 0})^{\, 2} }{ 4 \sqrt{\pi} \, \, \mathbf{r}^{\, 3} \tau \nu_{\, \mathbf{i}} } \right\} \, \left\{ (\mathbf{R}_{\mathbf{i}} \, - \, \mathbf{S}_{\, \mathbf{i}}) \, \mathbf{exp} \left[- \left(\frac{1 \, - \, \mathbf{r}}{\nu_{\, \mathbf{i}} \, \tau} \right)^{\, 2} \right] \, \, (11) \end{split}$$

+
$$(R_i + S_i) \exp \left[-\left(\frac{1+r}{v_i\tau}\right)^2 \right]$$

where

$${\bf R}_{\bf i} \equiv ({\bf r}^2 + {\bf v}_{\bf i}^2 {\bf \tau}^2) \, 2{\bf r}, \quad {\bf S}_{\bf i} \equiv 2{\bf r}^2 + ({\bf r}^2 + {\bf v}_{\bf i}^2 {\bf \tau}^2) \, {\bf \tau}^2 {\bf v}_{\bf i}^2 \, .$$

3.3 Diagrams

We complete Section 3 by presenting a number of diagrams selected to illustrate graphically some typical and/or specific features of the evolution in time and space of the mixture density ρ (Figures 1-3), mass average velocity \bar{u}_1 (Figures 4-6) and mixture pressure p (Figures 7, 8). In the diagrams, these mean quantities are scaled with respect to the corresponding initial quantities of the outer gas, that is, with respect to ρ_2^0 , h_2^0 and $\rho_2^0 = \frac{1}{2}\rho_2^0(h_2^0)^2$. (The importance of the dimensionless parameters ν_1 and $\mu_1 \equiv \rho_1^0/\rho_2^0$ should be noticed.) Recall that ρ is basically given by the formulae of Subsection III(ii) (a) of our earlier paper (East and Glikson, 1974) with an amendment mentioned in 3.1 above; \bar{u}_1 is given by (8); the expression for p follows from (7), (10) and (11).

In all figures the numbers assigned to the curves represent the values of the dimensionless time variable τ .

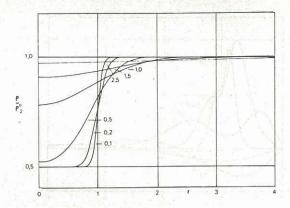


Figure 1 Mixture density; $\mu_1 = \frac{1}{2}$, $\nu_1 = 1$

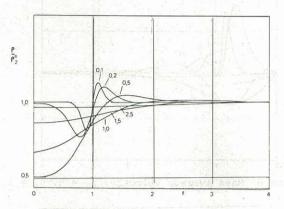


Figure 2 Mixture density; μ_1 = 1, ν_1 = 2

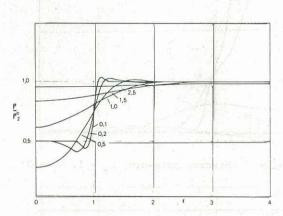


Figure 3 Mixture density; $\mu_1 = \frac{1}{2}$, $\nu_1 = 2$

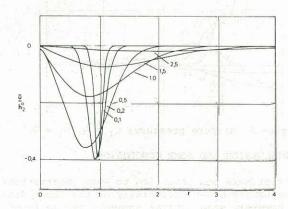


Figure 4 Mass average velocity; $\mu_1 = \frac{1}{2}$, $\nu_1 = 1$

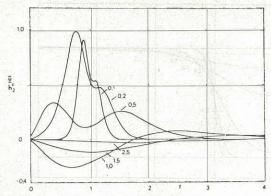


Figure 5 Mass average velocity; $\mu_1 = 1$, $\nu_1 = 2$

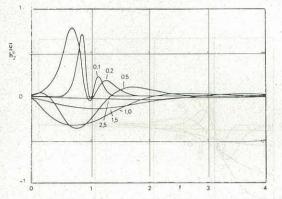


Figure 6 Mass average velocity; $\mu_1 = \frac{1}{2}$, $\nu_1 = 2$

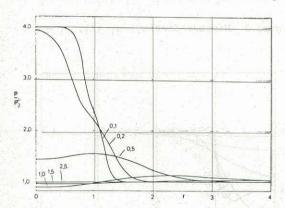


Figure 7 Mixture pressure; $\mu_1 = 1$, $\nu_1 = 2$

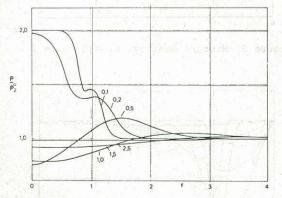


Figure 8 Mixture pressure; $\mu_1 = \frac{1}{2}$, $\nu_1 = 2$

DISCUSSION AND SOME CONCLUSIONS

We restrict here our attention to some observations and conclusions based essentially on the above diagrams, however, some general comments may be found in Section IV of our earlier paper. It may also be noted here that, since (1)-(5) are valid under the general restriction that the gases be initially isothermal, the stronger restriction of Section 1

(i.e., that the gases are initially in absolute equilibrium) could be appropriately weakened.

A detailed analytical discussion of the results of Sections 2 and 3 is postponed to a subsequent paper, where, in particular, we draw a parallel to an analysis, carried out by Narasimha (1962), of the progression of the 'shock' wave front in the problem briefly described in Subsection 2.1. (Narasimha concludes that after a certain 'long' period of time, $\tau \gg 1$, the 'shock' wave travels at a speed equal to the initial isothermal speed of sound in the gas. A somewhat different situation is expected, however, for the case $\mu_1 = 1$, $\nu_1 \neq 1$ discussed below, if a similar analysis were carried out.)

Setting ν_1 = 1 with $\mu_1 \neq 1$ produces a case similar to that of 2.1. This has been discussed elsewhere (Kornowski, 1959), (Molmud, 1960), (Narasimha, 1962), and graphs similar to Figures 1 and 4 may be found in the two latter papers. The diagram of the mixture 'hydrodynamic' pressure, for this case, is not presented here because of space limitations. It indicates a continuous smoothing out of the initial pressure difference, in an almost identical manner to that exhibited in Figure 1.

To gain a better understanding of the case where simultaneously $\mu_1 \neq 1$ and $\nu_1 \neq 1$, it seems reasonable and useful to also consider the case $\mu_1 = 1$ and $v_1 \neq 1$. Figures 2, 5, 7 show a typical example of the situation for such a case if $v_1 > 1$. A 'shock' wave is evidently moving (initially) outward from the position of the initial membrane, r = 1, with a corresponding trough moving toward r = 0. In our previous paper (East and Glikson, 1974), it was pointed out that h; represent statistically the deviation from the mean of the initial molecular velocities (for the spherical cloud problem, $u_i^0 = 0$). Initially, therefore, the gas with the larger h; value is in a higher state of thermal excitation, and consequently, having a higher pressure (see Figure 7), it diffuses more rapidly in the initial stages. A 'similar' pattern is exhibited for the case when v_1 < 1. Then the 'shock' wave moves toward r = 0, while the trough moves outward from r = 1.

The abovementioned features of the restrictions ν_1 = 1 and μ_1 = 1 are seen to be combined in the examples shown in Figures 3, 6 and 8 where no such restrictions are placed on ν_1 and μ_1 . A complete discussion of this case, however, will require an analysis of the 'shock' wave progression.

5 REFERENCES

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