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GENERALIZED DISSOCIATING GAS FLOW

By Paul D. Arthur* and Allen J. Schwalb**

ABSTRACT

A generalized approach to the one-dimensional flow of a dissociated gas is presented. The flow is characterized by the flow parameters F , G , H , and I , and the degree of dissociation, which are defined. The equation of state and the equations for the dynamic and thermodynamic properties of the gas are presented for the dissociating gas. Equations are presented which give the aerothermodynamic flow properties as a function of the degree of dissociation α , the frozen flow Mach number M_F , and the initial values of G , H , and I for any arbitrary given flight condition. These equations are solved for the limiting subsonic and hypersonic solutions for the flow variables as the frozen flow Mach number M_F tends towards zero and infinity, respectively. Several aspects of the physical significance of these results are discussed from the point of view of atmospheric planetary entry of an aerospace vehicle. The generalized nondimensional flow function F is defined in terms of the flow parameters G , H , and I , and is also given as a function of M_F , H , and α , in general. This functional relationship is displayed in graphical form which is useful for determining various aspects of the resulting flow, and providing further insight into the flow process under consideration. Specifically, several flow regimes are delineated.

Introduction

During atmospheric entry the energy induced into the gas surrounding a vehicle, due to the vehicle's high kinetic energy, is large enough to dissociate gaseous molecules into atoms. Therefore, dissociation of the gas must be taken into account when predicting aerodynamic (performance), thermodynamic (heat transfer), or electromagnetic (communications) effects. This phenomenon occurs primarily in the plasma sheath surrounding the vehicle during entry into the atmosphere.

In order to understand and take these dissociation effects into account, a generalized approach to the analysis of the one-dimensional flow of a dissociating (chemically reacting) gas was considered. This flow is analogous to the classical one-dimensional Rayleigh flow (flow with heat addition), Fanno flow (flow with friction), and shock wave flow.

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Analysis

Basic Equations

In general, one-dimensional flow is characterized by the flow parameters G , H , and I : the mass flow, total enthalpy, and stream thrust, respectively. These parameters are equivalent to the parameters, m , H_n , and P of Reference 1. In general, i.e., for a perfect (ideal) or real (dissociating) gas, the equations defining these parameters are the usual hydrodynamic conservation equations (for example see Reference 1):

$$\text{Mass flow:} \quad G = \rho v \quad (1)$$

$$\text{Total enthalpy:} \quad H = h + v^2/2 \quad (2)$$

$$\text{Stream thrust:} \quad I = p + \rho v^2 \quad (3)$$

where p , ρ , h , and v are the gas pressure, density, enthalpy, and velocity, respectively.

For ideal or dissociating Rayleigh flow with no mass addition, G and I are constant throughout the flow field, however H varies. Similarly for ideal or dissociating Fanno flow with no mass additions, G and H are constant throughout the flow field, however I varies. For ideal or dissociating shock wave flow with no mass addition, G , H , and I are all constant throughout the flow field (across the shock). Thus, this type of flow is more amenable to analysis.

Gas Model - Ideal Dissociating Gas

The basic assumption of the gas model utilized, namely the ideal dissociating gas, is that one-half of the vibrational energy of the diatomic gas is excited. The gas considered is a binary mixture of diatomic molecules (of mass m_m) and atoms (of mass m_a).

The equation of state for the Lighthill ideal dissociating gas (see References 2-5) is:

$$p = \rho RT (1 + \alpha) \quad (4)$$

where p and ρ were defined previously, R is the undissociated specific gas constant, and T is the gas temperature.

The degree of dissociation α is defined as the mass fraction of the dissociated gas $m_a / (m_m + m_a)$, i.e., the ratio of the mass of the dissociated atoms (m_a) to the total mass of the gas (References 2-5). The value of α can vary from zero (undissociated gas) to unity (completely dissociated gas). The variation of α in the flow causes variations in all of the thermodynamic and dynamic variables in the flow field. Therefore it is advantageous to derive a set of equations which

gives the flow properties directly as a function of the degree of dissociation α , the frozen flow Mach number M_F , and the flow parameters G, H, and I. These equations are presented in the following section and are based upon two further definitions and equations for the thermodynamic properties for the ideal dissociating gas (i.e., enthalpy and sound speed as follows (Reference 3)):

The static enthalpy (per unit mass) is given by the equation:

$$h = (4 + \alpha) RT + \alpha D, \quad (5)$$

where D is the dissociation energy of the specific gas.

The sound speed (frozen) is given by the equation:

$$a_f = \left[(4 + \alpha) (1 + \alpha) RT/3 \right]^{1/2}. \quad (6)$$

Basic Equations for the Present Gas Model

Using Equations (1)-(6) and the definition of the frozen Mach number, $M_F = v/a_f$, the following equations were developed which give the aerothermodynamic flow variables p, ρ , T, v, a_f , and h, as a function of α , M_F , and the initial values G, H, and I for any given flight condition:

$$p = \frac{I}{A}, \quad \rho = \frac{G^2 A}{I B}, \quad T = \frac{I^2 B}{G^2 A^2 R (1 + \alpha)} \quad (7)$$

$$v = \frac{I B}{G A}, \quad a_f = \frac{I B}{G A M_F}, \quad h = H - \frac{1}{2} \frac{I^2 B^2}{G^2 A^2}$$

where:

$$A = 1 + \frac{4 + \alpha}{3} M_F^2 \quad (8)$$

$$B = \frac{4 + \alpha}{3} M_F^2.$$

(Note: $B = A - 1$.)

Limiting Conditions and Solutions

An analysis of these equations was carried out for hypersonic ($M \gg 1$) and subsonic ($M_F < 1$) Mach numbers. The resulting equations for the subsonic case become simply the set of equations (7) where A is set identically equal to one. Therefore, for example, at very low Mach numbers (subsonic), the pressure p is simply equal to the value of I. For hypersonic Mach numbers, the set of equations (7) can be expanded in a series. Using these two sets of resulting equations, limiting values for the aerothermodynamic flow variables were determined in the limit of subsonic Mach numbers ($M \rightarrow 0$) and hypersonic Mach numbers ($M \rightarrow \infty$). These results are shown in Table I.

TABLE I

Subsonic and Hypersonic Limiting Values

Variable	Subsonic Flow ($M \rightarrow 0$)	Hypersonic Flow ($M \rightarrow \infty$)
p	I	0
ρ	∞	$\frac{G^2}{I}$
T	0	0
v	0	$\frac{I}{G}$
a	0	0
h	H	$H - \frac{1}{2} \left(\frac{I^2}{G^2} \right)$
α	H/D	$H/D \left(1 - \frac{I^2}{2 G^2 H} \right)$

These limiting values are useful for defining the extremes of Mollier charts for dissociating gases more clearly, and, for predicting numerical results at these limits.

In order to determine the limiting value of α associated with (consistent with) the limiting values of the thermodynamic variables presented in Table I, the concept of the generalized flow function F was utilized (Reference 6). The generalized nondimensional flow function F is defined as a function of the mass flow parameter G, the total enthalpy H, and the stream thrust (impulse) I, by the equation:

$$F = \frac{G^2}{I^2} H \quad (9)$$

which represents the only possible nondimensional grouping of G, H, and I (Reference 6). This flow function F also can be presented as a function of the frozen Mach number M_F , the degree of dissociation of the gas α , and the ratio of the total enthalpy of the gas H to the dissociation energy of the gas D (i.e., H/D). This relationship is easily derived by straightforward application (continuous direct substitution) of Equations (1)-(6) presented previously. The desired result is:

$$F = \frac{(4 + \alpha)^2 M_F^2 (1 + \alpha M_F^2)}{3 (1 + \alpha) \left(1 - \frac{\alpha}{H/D} \right) \left(1 + \frac{E M_F^2}{F} \right)^2} \quad (10)$$

where:

$$C = (1 + \alpha)/6 \quad (11)$$

$$E = (4 + \alpha)/3.$$

To determine the limiting value of α for (1) the limiting subsonic case and (2) the limiting hypersonic case, the following approach was used. The corresponding values of M_F , zero and infinity, respectively, were substituted into Equation (10) above. For case (1) where M_F approaches zero, α must be equal to H/D , as indicated in Table I, to ensure that F will remain finite (although indeterminate from Equation (10)). For case (2), where M_F approaches infinity, α is found to be equal to $H/D(1 - 1/2F)$, which, using Equation (9), yields the value $H/D(1 - I^2/2G^2H)$, as indicated in Table I. It is interesting to note that in both cases the limiting value of α is simply h/D (the ratio of the static enthalpy of the gas to the dissociation energy of the gas). This can be seen easily from the definition of h , $h = (4 + \alpha)RT + \alpha D$, since in both limiting cases the static temperature T is zero (i.e., $T = 0$ in both the subsonic and hypersonic limit).

The physical interpretation and significance of these two cases (or sets of conditions) is as follows. For the shock wave flow considered here, the limiting hypersonic case represents the free-stream conditions in front of the shock wave (hypersonic flight), and the limiting subsonic case represents the corresponding flow conditions behind the shock wave.

It is also interesting to note that for highly hypersonic flight conditions through a partially dissociated gas (such as is found in the atmosphere above 150,000 feet), the gas will (in this limit) dissociate to a greater degree behind the shock wave (in the vicinity of the aerospace vehicle) by a factor of $(1 - 1/2F)$.

General Case

For the general case (other than the two limiting cases presented above), i.e., for any arbitrary free-stream (flight) Mach number, Equation (10) is useful for determining the entire flow process in terms of M_F and α as described below. This functional relationship is displayed by useful curves of F as a function of M_F for several values of α and H/D (Figures 1-5). These curves provide insight into the flow processes under consideration here. Specifically, several special flow regimes are delineated.

For example, in Figure 1, for an initial value of $H/D = 100$, the flow cannot exist in the Mach number and α regimes indicated, i.e., above the highest curve ($\alpha = 0$) or below the lowest curve ($\alpha = 1$). Also, for any particular value of the flow function F (which is constant throughout the flow), the curves define the Mach number and degree of dissociation ranges for the flow.

Discussion of Results

A numerical example will now be given to illustrate the utility of such a diagram. For a flight Mach number of 3.5, a free-stream degree of dissociation α of 0.5, and an H/D of 100, the

point can be located on the graph of $H/D = 100$ (see Figure 1). This condition represents the free-stream conditions in front of the shock wave. Then since the flow function, F , equal to 0.6, is constant throughout the flow field, one moves horizontally across the graph in the direction of decreasing Mach number (to the left) until the desired α curve is located in the subsonic ($M < 1$) flow regime. For the case given here it is assumed that the flow was frozen*, and thus the final α is equal to 0.5 (i.e., α does not change across the shock wave). Therefore, one can locate the resulting point on the graph (at $\alpha = 0.5$ and $F = 0.6$), on the subsonic side of the graph, representing the flow properties behind the shock wave. The value of the Mach number at this point can then be read on the abscissa. For the present case the Mach number is found to be 0.5.

Once M_F and α have been determined using either the preprepared curves or Equation (10), the other aerothermochemical properties of the flow field can be obtained easily using the set of equations (7), which give these properties as a function of M_F and α .

Note, that in moving to the left, α was increasing, i.e., the gas was dissociating until $\alpha = 1.0$. At that point the shock wave was encountered and a jump was made from a supersonic to a subsonic Mach number which is characteristic of a shock wave. In the subsonic region, the gas recombines back to the final degree of dissociation as determined by the type of chemical reaction (frozen, nonequilibrium or equilibrium). In this case $\alpha = 0.5$. This is a consequence of the fact that F is inversely proportional to α . However, this is not always the case, since at lower values of H/D the curves of constant α cross and reverse their order. As the value of H/D is decreased, this crossover occurs at lower Mach numbers as shown in Figures 2 and 3. In fact, at values of H/D less than or equal to one (i.e., $H/D \leq 1.0$), F is directly proportional to α . Therefore, for this situation, the gas recombines to $\alpha = 0$, and then the gas dissociates to the final value of α .

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*Equilibrium flow is treated in a subsequent paper.

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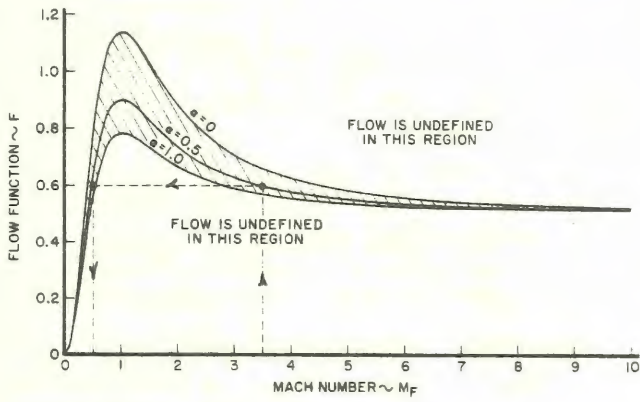


Figure 1. - F vs. M_F for $H/D = 100$

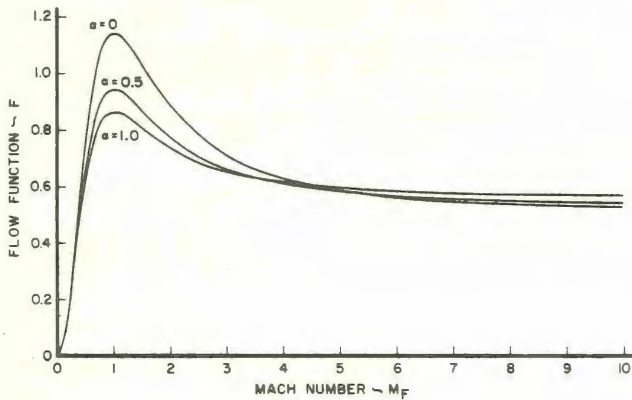


Figure 2. - F vs. M_F for $H/D = 10$

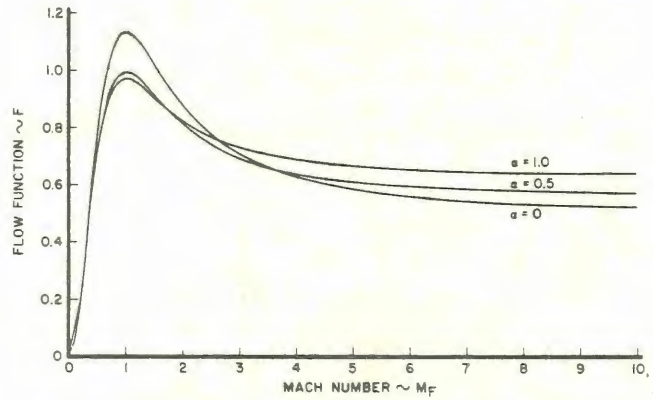


Figure 3. - F vs. M_F for $H/D = 5$

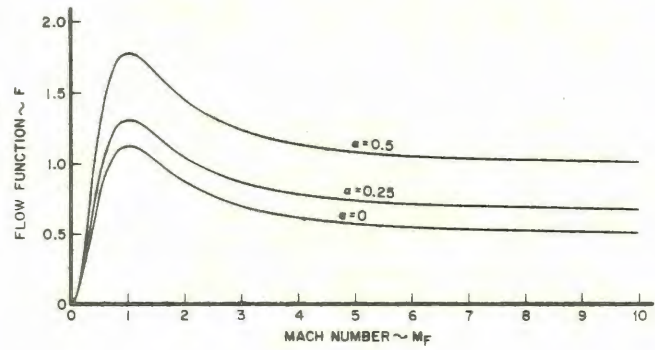


Figure 4. - F vs. M_F for $H/D = 1$

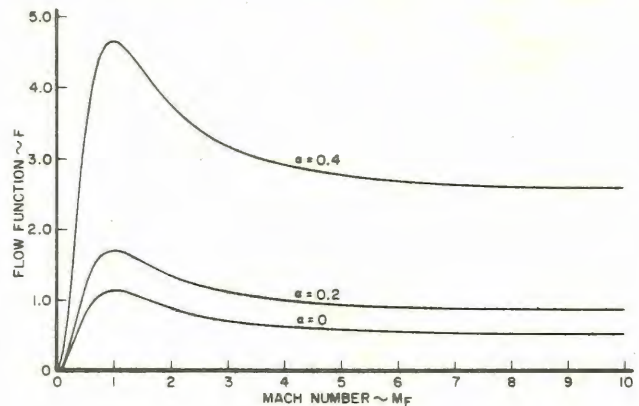


Figure 5. - F vs. M_F for $H/D = .5$