

# SIMILAR SOLUTIONS IN NONEQUILIBRIUM NOZZLE FLOWS

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## ABSTRACT

*A method of obtaining similar solutions for pseudo-one-dimensional, non-equilibrium nozzle flows is discussed. A diatomic gas undergoing simultaneous relaxation of both vibrational and dissociational modes including coupling among them is considered. Similar solutions for oxygen and nitrogen, with nonequilibrium effects starting from the nozzle reservoir are presented. General correlating parameters have been deduced from the transformed governing equations. It is shown that all the approximate correlating parameters that have been hitherto formulated using approximate methods can be deduced from the present general correlating parameters as special cases. With the present similar solutions the flow quantities in the nozzle can be readily obtained from the charts for any given initial conditions in the nozzle.*

Key words: Nozzle flows, nonequilibrium effects.

## 1. INTRODUCTION

Nonequilibrium effects in nozzle flows have long been of interest in the propulsion field because of the thrust loss resulting from chemical freezing (recombination lag) occurring in nozzle expansion process. In recent years the problem of chemical freezing in nozzles has assumed greater importance with the development of high performance chemical rockets using hydrogenfluorine system and the interest in development of advanced hypersonic ram jet engine. Nozzle flow nonequilibrium is also of much concern in connection with hypersonic wind tunnel testing. The current test devices such as jets and shock tunnels utilize nozzle expansions of air from initial high temperature conditions where a major portion of the air may be dissociated. Usually some degree of freezing occurs in the nozzle expansion, which produces a test air flow not in an equilibrium state.

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Hence, the actual physical and chemical state of the test gas in a hypersonic facility is essential for successful wind tunnel testing.

The present state-of-the-art for analysing nonequilibrium nozzle flows requires complex computer programmes<sup>1</sup> with which the flow variables are determined by numerical integration for any given initial and boundary conditions. These conditions usually are the reservoir temperature and pressure, nozzle shape and a specified gas. Because of many variables involved, the numerical solutions do not provide suitable theoretical comparisons for use by an experimentalist. Several approximate analyses have been proposed to correlate at least the frozen enthalpy in the nozzle. Bray<sup>2</sup>, while introducing 'sudden freeze' analysis, found that the frozen mass fraction in the nozzle, for a certain range of reservoir conditions and a particular nozzle geometry, depends on the reservoir entropy alone. This was later used by Lordi and Mates<sup>3</sup> and Harris and Warren<sup>4</sup> to correlate the frozen enthalpy in air. Harney<sup>5</sup> improved on the entropy correlation by including the nozzle scale parameter. However, these correlations do not include the effects of variations in the total enthalpy and do not correlate all quantities of interest. Ring and Johnson<sup>6</sup> used a correlation based on the reservoir entropy and a time  $\tau_c$  characterising the flow expansion rate for the nonequilibrium flow parameters. It should be emphasized that all these methods were not based on any rational analysis but their success or otherwise was solely judged by correlating the numerically computed nozzle flow quantities in a rather restricted range of reservoir conditions.

From the preceding discussion it is obvious that suitable similar solutions to this problem are highly desirable. Such similar solutions would not only eliminate the need for repeated computations using complex computer programmes but also provide, for the experimentalist, the badly needed general correlating parameters. The present work discusses a method of obtaining similar solutions for pseudo-one-dimensional, inviscid, adiabatic, nonequilibrium nozzle flows. The case of a single diatomic gas undergoing either vibrational relaxation or dissociational relaxation has been already considered by Reddy and Daum<sup>7</sup>. Similar solutions for the case of oxygen, considering only the dissociational nonequilibrium effects, have been presented in ref. 8. But in the real problem a diatomic gas undergoes both these relaxations simultaneously with coupling between them. In the present work a realistic model for a single diatomic gas like oxygen or nitrogen undergoing simultaneous vibrational and dissociational relaxation is considered. A cut-off harmonic oscillator model is used for describing the vibrational rate process. The coupling between vibrational and

dissociational modes is also taken into account. The assumption of equilibrium flow upstream of the nozzle throat made by Reddy and Daum<sup>7</sup> has been avoided and the present analysis is capable of handling the non-equilibrium situation throughout the nozzle beginning from the nozzle reservoir.

General correlating parameters have been deduced from the transformed governing equations. It is shown that all the approximate correlating parameters that have been hitherto formulated can be deduced from the present general correlating parameters as special cases. The similar solutions for oxygen are presented in the form of graphs. With the present similar solutions the flow quantities in the nozzle can be easily read off from the charts for any given initial conditions in the nozzle reservoir. Similar solutions for nitrogen can be found in ref. 9.

## 2. GOVERNING EQUATIONS

The governing equations (in nondimensional form) for a steady state, pseudo-one-dimensional, adiabatic, inviscid flow are given below. A detailed derivation is given in ref. 9.

$$\text{Conservation of Mass ; } \rho u A = \rho_* u_* = \text{constant} \quad (1)$$

$$\text{Conservation of Momentum : } u du + dp/\rho = 0 \quad (2)$$

$$\text{Conservation of energy : } h + \frac{u^2}{2} = H_0 = \text{constant} \quad (3)$$

where

$$h = \left( \frac{7}{2} + \frac{3\alpha}{2} \right) T_t + (1 - \alpha) \epsilon + \alpha$$

and

$$\bullet = \theta_v / (e^\phi - 1) - (N \theta_v / e^{N\phi} - 1)$$

for a cut-off-harmonic oscillator approximation;  $N$  is the maximum number of vibrational levels.

$$\text{Equation of state : } p = \rho T (1 + \alpha) \quad (4)$$

Dissociational rate equation

$$\frac{d\alpha}{dx} = \frac{I k_{r1} T \bar{a}^s \rho \bar{a}^2 \alpha^2 (1 - \alpha)}{m \bar{a}^2 u \bar{a}} (\theta_v)^s [V (\theta_v / \psi)^s \\ \times e^{-\psi / \theta_v} (\theta_v / \psi)^3 (1 - \alpha) \alpha^{-2} (1 - e^{-\psi}) (1 - e^{-N\psi})^{-1} - 1] \quad (5)$$

where

$$k_r = k_{r1} T_t^s.$$

Vibrational rate equation :

$$\frac{d\epsilon}{dx} = [\epsilon(\infty) - \epsilon] \delta - (\bar{E} - \epsilon) VL' I/u(1 - \alpha) + (\bar{G} - \epsilon) I/u(1 - \alpha) \quad (6)$$

where

$$\begin{aligned} \delta &= \theta'_{v1} \rho_d u_d \rho (1 + \alpha) e^{-C_2 \psi^{11/3}} / u C_1 \psi \\ I &= lk_{r1} T_d^s \rho_d^2 T_t^s \rho^2 (1 - \alpha) \alpha^2 / m \alpha^2 u_d. \end{aligned}$$

The preceding six equations are sufficient to determine the six unknowns  $p$ ,  $\rho$ ,  $T_t$ ,  $u$ ,  $\epsilon$  and  $\alpha$ .

### 3. TRANSFORMATION OF GOVERNING EQUATIONS

An independent variable  $\eta$  is defined as  $\eta = \log_e \rho$ . Then the governing equations can be written in terms of this new variable as :

$$\text{Conservation of mass : } \eta = \log_e (uA/\rho_* u_*) \quad (7)$$

$$\text{Conservation of momentum : } udu + e^\eta dp = 0 \quad (8)$$

Conservation of energy :

$$u^2/2 + (7 + 3\alpha) \theta_v/2\psi + (1 - \alpha) \epsilon + \alpha = H_0 \quad (9)$$

$$\text{Equation of state : } p = e^{-\eta} \theta_v (1 + \alpha)/\psi \quad (10)$$

Dissociational rate equation :

$$\begin{aligned} \frac{d\alpha}{dx} &= \frac{lk_{r1} T_d^s \rho_d^2 e^{-2\eta} \alpha^2 (1 - \alpha)}{m \alpha^2 u u_d} (\theta_v/\psi)^s [V e^{-(\eta + \theta_v/\psi)} \\ &\times (\theta_v/\psi)^{\frac{1}{2}} (1 - \alpha) \alpha^{-2} (1 - e^{-\psi}) (1 - e^{-N\psi})^{-1} - 1]. \end{aligned} \quad (11)$$

The vibrational rate equation can be written in terms of vibrational temperature function  $\phi$  with a cut-off-harmonic oscillator approximation as

$$\begin{aligned} \frac{d\phi}{dx} &= \delta (e^\phi - 1) (e^\psi - e^\phi) (1 - f_2)/e^\phi (e^\psi - 1) (1 - f_1) \\ &\quad - VLI (e^\phi - 1) (1 - e^\psi) (f_2 - f_1)/u (1 - \alpha) (e^\psi - e^\phi) f_2 (1 - f_1) \\ &\quad + [I(1 - e^\phi)/2u(1 - \alpha) e^\phi (e^N - 1) (1 - f_1)] [(N-1)(e^\phi e^{N\phi} - 1) \\ &\quad + (N+1)(e^\phi - e^{N\phi})] \end{aligned} \quad (12)$$

where the function  $f_1$  and  $f_2$  are functions of temperature and are given in ref. 9.

In a one-dimensional nozzle flow with an area distribution given by  $A = (1 + x^2)^{\frac{1}{2}}$ , it can be easily shown<sup>7</sup> that,

$$\frac{da}{d\eta} = (\rho_* u_* e^\eta)^{1/ij} \frac{da}{dx} / ij (N_s)_2 \quad (13)$$

where the function  $(N_s)_2$  is given by

$$(N_s)_2 = \left( \frac{M^2}{M^2 - 1} \right) (1 - A^{-1/i})^{(j-1)/j} u^{(1+1/ij)}.$$

The velocity term in the function  $(N_s)_2$  has been nondimensionalised by  $u_d$ . This will be changed in the following manner for reasons that will be explained later

$$u = \frac{u'}{u_d} = \frac{u'}{(p'_0/\rho'_0)^{\frac{1}{2}}} \times \frac{(p'_0/\rho'_0)^{\frac{1}{2}}}{u_d} = u_r \frac{(p'_0/\rho'_0)^{\frac{1}{2}}}{u_d} \quad (14)$$

where suffix 0 refers to the nozzle reservoir conditions. With eqns. (13) and (14), the dissociational rate equation [eq. (11)] can be written as:

$$\begin{aligned} \frac{da}{d\eta} = & \exp[\lambda_d - \eta(2 - 1/ij)] (\theta_v/\psi)^s (1 - a) a^2 [V \exp(-\eta - \theta_v/\psi) \\ & \times (1 - a) a^{-2} (1 - e^{-\psi}) (1 - e^{-N\psi})^{-1} - 1] / (N_s)_1 \end{aligned} \quad (15)$$

where

$$(N_s)_1 = \left( \frac{M^2}{M^2 - 1} \right) (1 - A^{-1/i})^{(j-1)/j} u_r^{(1+1/ij)}$$

and

$$\lambda_d = \log_e [Ik_{r1} T_d^s \rho_d^2 (ijm_a^2 u_d)^{-1} (\rho_* u_*)^{1/ij} (u_d/u'_0)^{(1+1/ij)}]$$

where

$$u'_0 = (p'_0/\rho'_0)^{\frac{1}{2}}$$

Proceeding in the same way and arranging the terms, as in the previous case, the vibrational rate equation (eq. 12) can be written as

$$\begin{aligned} \frac{d\phi}{d\eta} = & \frac{1}{(N_s)_1} \left[ \exp\{\lambda_v + \eta(1 - 1/ij) - C_2 \psi^{1/3} - \phi\} \right. \\ & \times \left. \left\{ \frac{(1 + a)(e^\phi - 1)(e^\psi - e^\phi)(1 - f_1)}{\psi(e^\psi - 1)(1 - f_2)} \right\} \right. \\ & \left. - VL \exp\{\lambda_d - \eta(2 - 1/ij)\} \right] \end{aligned}$$

$$\begin{aligned} & \times (\theta_v/\psi)^s \alpha^2 \left\{ \frac{(e^\phi - 1)(1 - e^{-\psi})(f_2 - f_1)}{(e^\phi - e^\psi)(1 - f_1)f_2} \right\} \\ & + \exp\{\lambda_d - \eta(2 - 1/ij) - \phi\} (\theta_v/\psi)^s \alpha^2 (1 - e^\phi) \\ & \times \left\{ \frac{(N - 1)(e^\phi e^{N\phi} - 1) + (N + 1)(e^\phi - e^{N\phi})}{2(1 - f_1)(e^{N\phi} - 1)} \right\} \end{aligned} \quad (16)$$

where

$$\lambda_v = \log_e [(\rho_* u_*)^{1/ij} \theta_v \rho_d u_d (u_d/u'_0)^{(1+1/ij)/ij} C_1] \\ (N_s)_1 \text{ and } \lambda_d \text{ are the same as in eq. (15).}$$

By using the differential form of conservation of energy and equation of state, the conservation of momentum (eq. 8) can be expressed as

$$\begin{aligned} & [(e^\phi - 1)^{-1} - N(e^{N\phi} - 1) - (2\psi)^{-1} - \theta_v^{-1}] da + \left(\frac{5 + \alpha}{2}\right) \psi^{-2} d\psi \\ & + [e^\phi(1 - \alpha)(1 - f_1)(e^\phi - 1)^{-2}] d\psi - (1 + \alpha)\psi^{-1} d\eta = 0. \end{aligned} \quad (17)$$

It is clearly seen that the problem under consideration has been reduced to solving three differential eqs. (15) (16) and (17) for three unknowns  $\alpha$ ,  $\phi$  and  $\psi$  with  $\eta$  as the independent variable. The other unknowns namely  $p$ ,  $\rho$  and  $u$  are obtained from the other governing equations which are simple algebraic equations.

The main motivation in expressing the rate equations for the dissociational and vibrational mode in the form given in eqs. (15) and (16) is to combine all the parameters of the problem into two parameters  $\lambda_d$  and  $\lambda_v$ . It can be easily shown that, for a given gas, the parameter  $\lambda_v$  is a constant multiple of  $\lambda_d$ . So one can write  $\lambda_v = Q\lambda_d$  where  $Q = \log_e [k_{r1} T_d^s C_1 \rho_d / m_d^2 u_d^2 \theta_v]$ . So it is obvious that a single parameter  $\lambda_d$  is sufficient to define the problem. However, the similar governing equations contain additional parameters  $C_2$ ,  $s$  and  $ij$ . The parameters  $C_2$  and  $s$  are also fixed for a given gas and are usually obtained from experimental measurements. The parameter  $ij$  is the nozzle shape parameter and a given value of  $ij$  covers a family of nozzle shapes. Fortunately, for the commonly used nozzle shapes of conical and hyperbolic type the value of  $ij = 2$ . The governing equations also contain a rather undesirable term  $(N_s)_1$  which is different for different reservoir conditions and also varies along the nozzle length. If the function  $(N_s)_1$  could be expressed in terms of only the independent variable  $\eta$ , then similar solutions for translational and vibrational temperature functions  $\psi$  and  $\phi$  as well as for atom mass fraction  $\alpha$  can be obtained

with  $\eta$  as the independent variable. The parameters to be specified are  $\lambda_d$  and  $ij$  since the other parameter  $\lambda_p$  is related to  $\lambda_d$  and the parameters  $C_s$  and  $s$  are constants for a given gas. A method to express  $(N_s)_1$  in terms of  $\eta$  is given in the following section.

#### 4. FUNCTION $N_s$

The expression for  $(N_s)_2$  given in eq. (13) is a function of  $M$ ,  $u$  and  $A$ . Hence it will have different values for different reservoir conditions and it also varies along the nozzle axis. The significant variable is the velocity  $u$  since it is nondimensionalised by  $u_d$  which is independent of reservoir conditions. It was observed from a number of nozzle computations that the velocity, when nondimensionalized with a velocity  $u'_0 = (p'_0/p'_0)^{1/2}$ , did not change very much for different reservoir conditions. That is why the expression for  $(N_s)_2$  was re-written earlier in terms of  $u_r$  and the resulting constant was included in  $\lambda_d$  and  $\lambda_p$ . A typical variation of  $(N_s)_1$  with nozzle area ratio is shown in Fig. 1. It is noted that moving upstream from nozzle throat  $(N_s)_1$  rapidly tends to zero since  $M$  and  $u_r$  both tend to zero. At the geometric throat, since the rate of change of area with  $x$  goes to zero, the function  $(N_s)_1$  has an indeterminate form since  $M$  also becomes unity at the nozzle throat. However, it can be shown<sup>10</sup> that the function  $(N_s)_1$  tends to a definite limit at the throat.

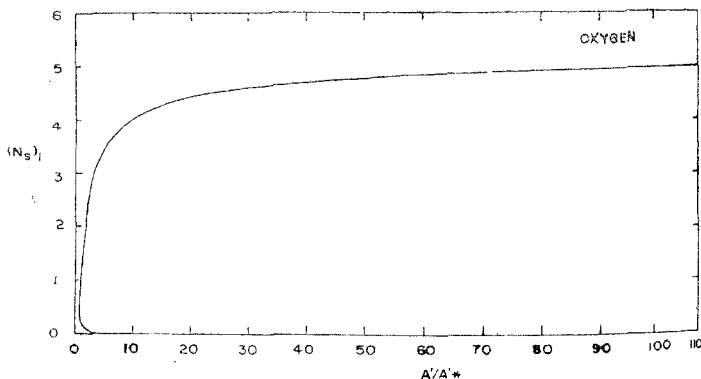


FIG. 1. Typical variation of function  $(N_s)_1$  with area ratio for oxygen.

The exact nozzle flow quantities were computed for oxygen with a number of nozzle reservoir conditions by using the computer programme given by Tung Chen and Eschenroeder<sup>1</sup>. The function  $(N_s)_1$  was also computed for several reservoir conditions and are plotted in Fig. 2 with a new independent variable  $\xi$  defined as  $\xi = (S_0 - \eta)$  where  $S_0$  is the entropy of gas in the nozzle reservoir. The purpose of introducing  $\xi$  is explained in the following sections. It is apparent from Fig. 2 that there is still a significant effect of the reservoir conditions (temperature and pressure) on  $(N_s)_1$ , more so towards the end of the nozzle. In an effort to obtain a better correlation, the  $(N_s)_1$  values were multiplied by a factor  $(mp'_0/T'_0)^n$  where  $m$  and  $n$  were found to be 4.15 and  $-0.037$  respectively in the case of oxygen. The constants  $n$  and  $m$  were determined by equating the maximum and minimum values of  $(N_s)_1$  at a value of  $(\xi_0/\xi) = 1.15$ . This procedure is somewhat arbitrary but seems to be effective in obtaining a better correlation for the function  $N_s$ , which can now be written as

$$N_s = (N_s)_1 (4.15 p'_0/T'_0)^{-0.037} \tag{18}$$

The  $N_s$  values computed from eq. (18) are shown in Fig. 3 for the same reservoir conditions given in Fig. 2. All the values for different reservoir conditions correlate well and can be represented by a mean curve as shown

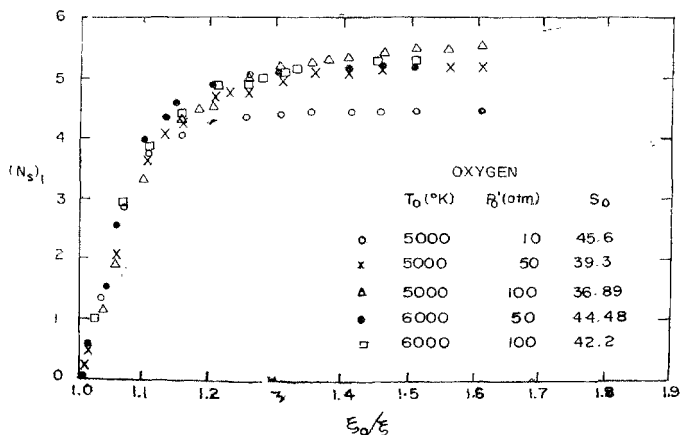


FIG. 2. Variation of  $(N_s)_1$  with parameter  $(\xi_0/\xi)$  for oxygen.



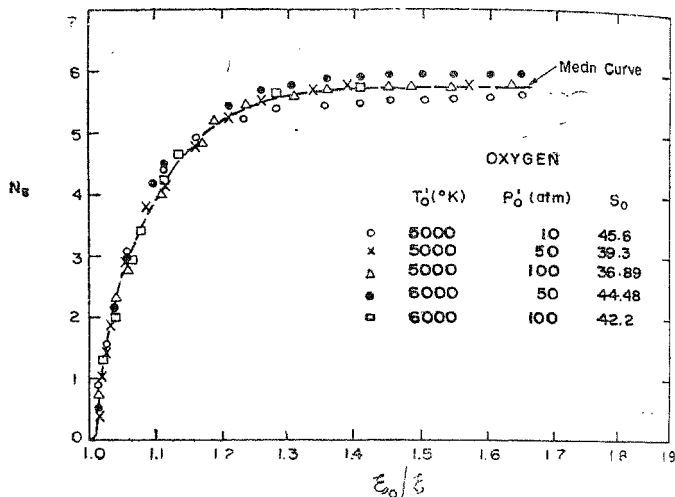


FIG. 3. Correlation of  $N_s$  with the parameter  $(\xi_0/\xi)$  for oxygen.

by the dotted line. The actual values correlated in this way are within  $\pm 5$  per cent of the mean curve. In the present analysis the success of correlation of the function  $N_s$  is crucial for obtaining similar solutions. Hence, use of a mean curve for  $N_s$  given in Fig. 3 has to be justified quantitatively. Towards this end the following procedure was adopted. Apart from using a mean curve to represent the  $N_s$  values, two more curves were fitted corresponding to the extreme values in the scatter. A few cases were tested using all the three values of  $N_s$  in the governing equations. For a particular case, the species mass fraction values obtained with all the three categories of  $N_s$  are plotted in Fig. 4. It is clear that the difference in  $\alpha$  values is negligible. This is expected since the  $\alpha$  values will not be too sensitive to small changes in  $N_s$  towards the end of nozzle where the flow is almost frozen. However, small changes in  $N_s$  can cause significant changes in  $\alpha$  in the early expansion region in the nozzle where the flow is rapidly changing from equilibrium to nonequilibrium state. Fortunately, the  $N_s$  values do not seem to vary very much in this region. Therefore, fairly accurate similar solutions can be obtained with a single mean curve to represent the function  $N_s$  for all

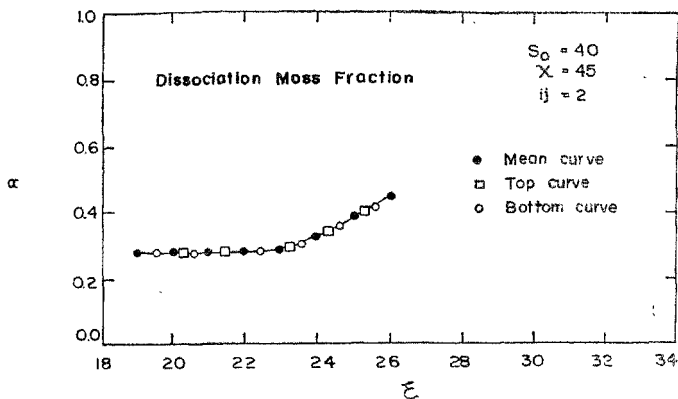


FIG. 4. Effect of using different ( $N_s$ ) curves on similar solutions.

the reservoir conditions. The mean curve for  $N_s$  can be expressed in a simple analytical form as:

$$\begin{aligned}
 N_s &= 715(1 - \xi_0/\xi)^2 - 60(1 - \xi_0/\xi) \text{ for } 1.01 \geq (\xi_0/\xi) \geq 1.0 \\
 &= 5.7 - 5.125(2.0 - \xi_0/\xi)^{1/2} \text{ for } 2.0 \geq (\xi_0/\xi) \geq 1.01 \\
 &= 5.7 \text{ for } (\xi_0/\xi) > 2.0.
 \end{aligned}$$

It is important to note here that the  $N_s$  values have been correlated starting from the nozzle reservoir. Hence, one need not assume equilibrium flow up to the nozzle throat as was done by Reddy and Daum<sup>7,10</sup>. In order to estimate the effect of different nozzle shapes on the function  $N_s$ , its values were obtained with different conical nozzle shapes ( $l = 1.0$  to 3.0 cm) as well as hyperbolic nozzle shapes ( $l = 0.5$  to 2.0 cm). It was found that the differences in the  $N_s$  values were within the accuracy of  $N_s$  correlation shown in Fig. 3. The additional factor  $(4.15 p'_0/T'_0)^{-0.087}$  was also included in the expressions for  $\lambda_d$  and  $\lambda_v$  so that its effect is properly taken into consideration.

## 5. INITIAL VALUE PROBLEM

After having obtained a universal correlation for the function  $N_s$  in terms of the independent variable, similar solutions can be obtained by a simultaneous solution of the transformed governing equations given by

eqs. (15), (16) and (17). As this is a well-known initial value problem, starting values of  $\phi$ ,  $\psi$ ,  $\alpha$  corresponding to a given value of  $\eta$  have to be specified. The stagnant gas in the nozzle reservoir will be in chemical and thermodynamic equilibrium and it departs from this equilibrium state as it expands in the nozzle. Hence, for the specification of initial values, a relation between  $\psi$ ,  $\phi$ ,  $\alpha$  and  $\eta$  for equilibrium state is required. This relation can be easily obtained as a limiting case from the general transformed governing equations.

This limiting case is achieved when the vibrational mode is fully excited and dissociational reactions occur at an infinite rate. This means that the vibrational relaxation time  $\tau_v$  and the recombination rate constant  $K_r$  separately tend to zero and hence the parameters  $\lambda_d$  and  $\lambda_v$  each tend to  $\infty$ . With this situation, the equality of translational and vibrational temperature functions  $\phi = \psi$  can be inferred from the vibrational rate eq. (16). With  $\phi = \psi$ , the generalized momentum eq. (17) can be integrated and given as

$$\begin{aligned} (3\alpha/2) + (1 + \alpha)(\psi/\theta_v) - \psi(N - 1) + \psi(e^\psi - \alpha)(e^\psi - 1) \\ - N\psi(e^{N\psi} - \alpha)/(e^\psi - 1) + 2 \log_e [\alpha/(1 - \alpha)] + 2 \log_e \\ \times [(e^{N\psi} - 1)/(e^\psi - 1)] = \text{constant}. \end{aligned} \quad (20)$$

The preceding equation is also the expression for the change in entropy in an equilibrium flow<sup>11</sup>, and it also shows that entropy is conserved which is expected in an equilibrium flow. The constant in eq. (20) can be written as  $(S_0 - S_T)$ , where  $S_0 = (S'_0/R)$  is the nondimensional entropy of gas in the nozzle reservoir,  $S_T$  is the nondimensional reference entropy and  $R$  is the gas constant. With  $\lambda_d \rightarrow \infty$ , the equilibrium law of mass action can be inferred from the rate eq. (15) and is given as

$$(\eta - \psi/\theta_v) = \log_e \{(\psi/\theta_v)^2 [\alpha e^2/(1 - \alpha e)] [(1 - e^{N\psi})/(1 - e^\psi)]\} \quad (21)$$

where the coupling factor  $V$  is taken as unity in equilibrium flow. It may be noted that the equilibrium flow does not depend on the nozzle shape, as it should be.

The equilibrium solution given in eqs. (20) and (21) could be used to obtain the initial values required for the nonequilibrium solutions. For any given value of  $\eta$ , the corresponding values of  $\psi$  and  $\alpha$  can be obtained from eqs. (20) and (21) by using an iteration procedure. But it introduces an additional parameter namely the reservoir entropy  $S_0$  through the constant given in eq. (20). Hence the nonequilibrium similar solutions would depend on two parameters  $S_0$  and  $\lambda_d$ , for a given gas and nozzle

shape parameter  $ij$ . The two parametric dependence can be reduced to a single parameter<sup>7,10</sup> by using the following transformations:

$$\begin{aligned}\xi &= (S_0 - \eta); & \beta &= (S_0 - \psi/\theta_v); \\ \gamma &= (S_0 - \phi/\theta_v) & \text{and } \alpha & \text{remains the same.}\end{aligned}$$

The equilibrium and nonequilibrium governing equations can be rewritten in terms of the new variables  $\xi$ ,  $\beta$ ,  $\gamma$  and  $\alpha$ . These equations are not given here since they are essentially similar in nature compared to eqs. (20), (21), (15), (16) and (17) and besides, are too lengthy<sup>9</sup>. The significant aspect that arises out of this transformation is that the governing equations are controlled by a new parameter  $\chi_d = [(2 - 1/ij) S_0 - \lambda_d]$  with  $\xi$ , instead of  $\eta$ , as the independent variable. There is another parameter  $\chi_v = [(2 - 1/ij) S_0 - \lambda_v]$  which also appears in the governing equations but it is not independent of  $\chi_d$  since  $\lambda_v$  is related to  $\lambda_d$  for a given gas. The governing equations written with  $\xi$  as the independent variable contain also  $S_0$  separately. But it was shown in ref. 10 that its influence on similar solutions is negligible. This fact is also apparent from the similar solutions presented elsewhere in this report. It should be noted that the general correlating parameter  $\chi_d$  is a combination of two parameters  $S_0$  and  $\lambda_d$ , the former arises out of initial value problem and the latter out of nondimensionalising the governing equations.

## 6. SIMILAR SOLUTIONS

### 6.1. Method of Solution

The equilibrium solutions for  $\alpha$  and  $\beta$  were obtained from eqs. (20) and (21) for given values of  $\xi$  and  $S_0$  by Newton Raphson iteration procedure. These equilibrium solutions were used as the initial starting values for the nonequilibrium solutions which were obtained from eqs. (15), (16) and (17) with  $\chi_d$  as parameter. The well-known fourth order Runge-Kutta method was used for solving these nonlinear rate equations. The usual method of finding the correct step size by trial and error consumes much computing time. Hence, in the present computation the correct step size was obtained by using Richardson's extrapolation.

### 6.2. Similar Solutions for Oxygen

The mass fraction  $\alpha$  and temperature  $T_t$  and  $T_v$  corresponding to a particular case ( $p'_0 = 50$  atm.,  $T'_0 = 5000^\circ$  K,  $S_0 = 39.3$ ,  $q = -2.5$ ) obtained from the present similar solutions have been compared in Figs. 5 and 6 with the values obtained by the exact numerical computations of Tung Chen and Eschenroeder<sup>1</sup>. The agreement is quite good. The

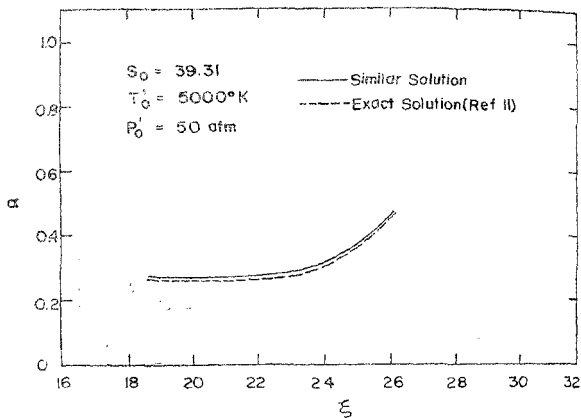


FIG. 5. Comparison of dissociation mass fractions for oxygen.

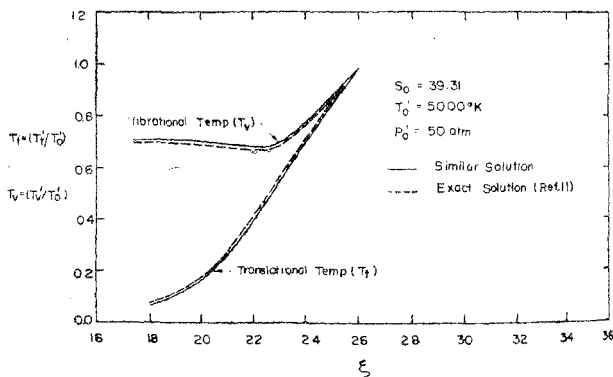


FIG. 6. Comparison of vibrational and translational temperatures for oxygen.

nonequilibrium similar solutions of  $\alpha$ ,  $\beta$  and  $\gamma$  for oxygen for various  $S_0$  and  $\chi\alpha$  values are given in Figs. 7, 8 and 9. The corresponding equilibrium solutions with ( $ij = 2$ ) are also shown.

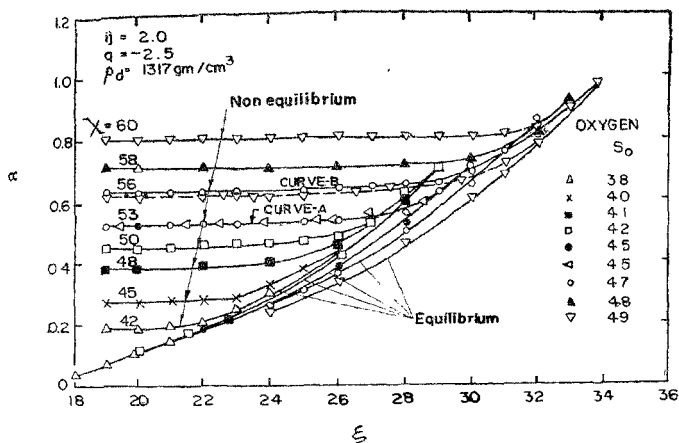
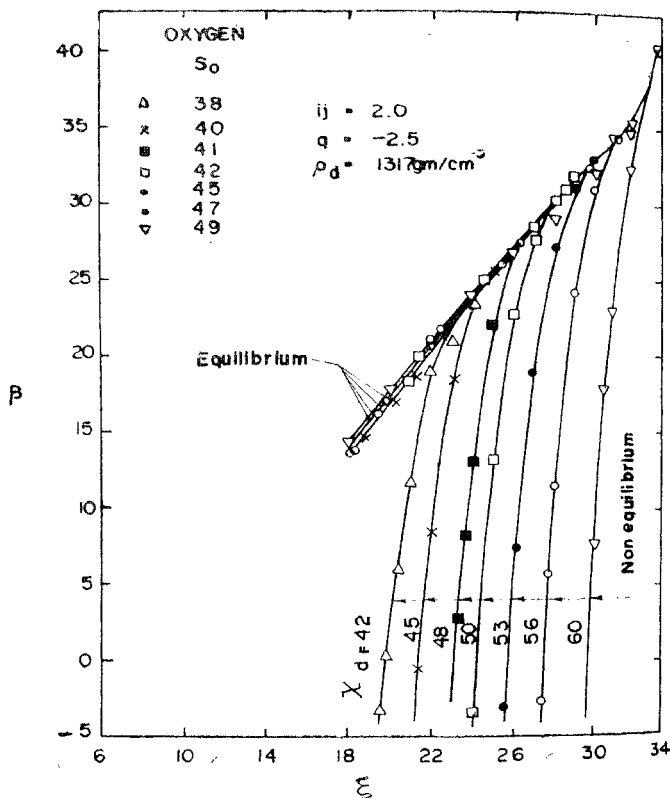


FIG. 7. Species concentration variation with parameter  $\xi$  for oxygen.

### 6.3. Discussion of Similar Solutions

It can be seen from Fig. 7 that all the equilibrium solutions do not collapse on to a single curve since the transformed equations with  $\xi$  as the independent variable still contain the reservoir entropy  $S_0$ . The separation between the different solutions of  $\alpha$  increases towards the higher values of  $S_0$ . The spread between the different equilibrium solutions of  $\beta$  (Fig. 8) is not as pronounced as it is in  $\alpha$ . The vibrational temperature function  $\gamma$  (Fig. 9) increases slightly before it freezes. This behaviour is possible since the vibrational de-excitation along the nozzle axis might become negligible because of rapid decrease in temperature and pressure, whereas the net recombination would contribute significantly to the vibrational energy for a longer distance along the nozzle<sup>12</sup>. The nonequilibrium solutions with the same  $S_0$  and  $\chi_d$  but different  $P'_0$  and  $T'_0$  are identical as shown by curve A in Fig. 7. The  $\alpha$  values with the same  $\chi_d$  but slightly different  $S_0$  start with the corresponding equilibrium values but tend to the same frozen limit as indicated by the curve B in Fig. 7. This suggests that the reservoir entropy  $S_0$ , which appears as a separate parameter in the transformed equations with  $\xi$  as independent variable does not effect the solutions to any significant extent.

FIG. 8. Translational temperature function variation with  $\xi$  for oxygen.

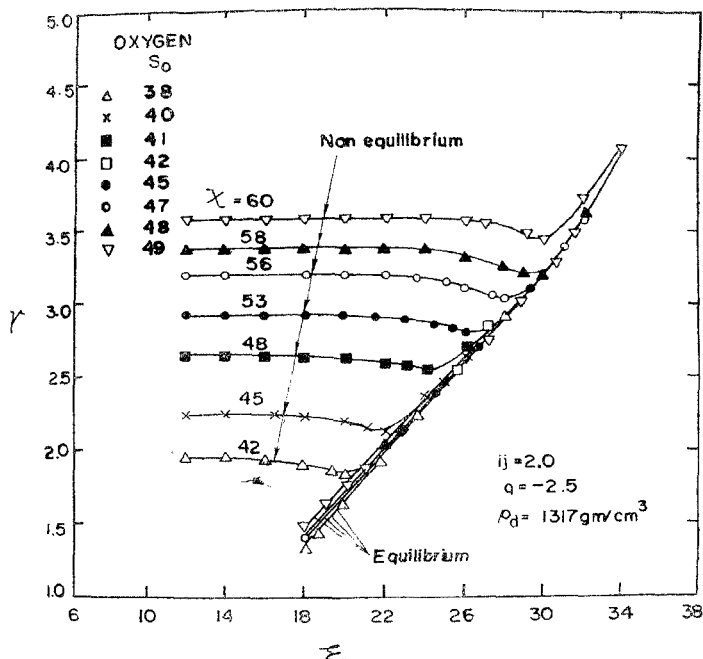


Fig. 9. Vibrational temperature function variation with  $\xi$  for oxygen.

The variation of frozen mass fraction  $a_f$ , which is a function of  $\chi d$  only is shown in Fig. 10. Another important feature of the present analysis is that the function  $N_s$  has been correlated starting from the nozzle reservoir. Hence an assumption of equilibrium flow in the subsonic region of the nozzle is not necessary and in the present analysis the nonequilibrium solutions were obtained starting from the nozzle reservoir unlike in the analysis of Reddy and Daum<sup>10</sup>.



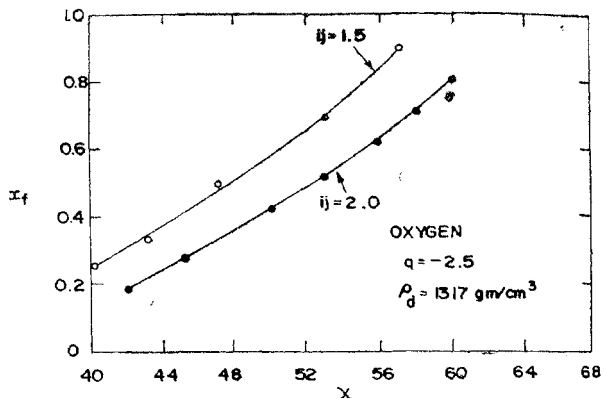


FIG. 10. Frozen species concentration with the parameter  $\chi_d$  for oxygen.

## 7. UNIVERSAL CORRELATING PARAMETERS $\xi$ AND $\chi_d$

### 7.1. Parameter $\xi$

The similarity parameter  $\xi$  is already defined as  $\xi = (S_0 - \eta) = [S_0 - \log_e (uA/\rho_* u_*)]$ . This parameter is not only a function of the reservoir and nozzle throat conditions but also a function of velocity. Therefore, the velocity ratio  $(u'/u'_*) \equiv (u/u_*)$  was computed for several reservoir conditions for oxygen. It was observed that this type of correlation still results in a significant amount of reservoir pressure and temperature effects which is similar to that noticed in  $N_s$  correlation. In order to obtain a better correlation, each velocity ratio was multiplied by the corresponding reservoir function as given below:

$$\left(\frac{u'}{u'_*}\right)_1 = \left(\frac{u'}{u'_*}\right) (4.15 p'_0/T'_0)^{-0.04} \quad (22)$$

where the constant factor  $-0.04$  was obtained by using considerations similar to those used previously in the correlations of  $N_s$ . This modified velocity ratio  $(u/u_*)_1$  was replotted for all the reservoir conditions as shown in Fig. 11 for oxygen. All the values now correlate fairly well and a mean curve can be taken to represent the velocity ratio for all the reservoir

conditions. This mean curve for oxygen can be represented by a simple expression of the type.

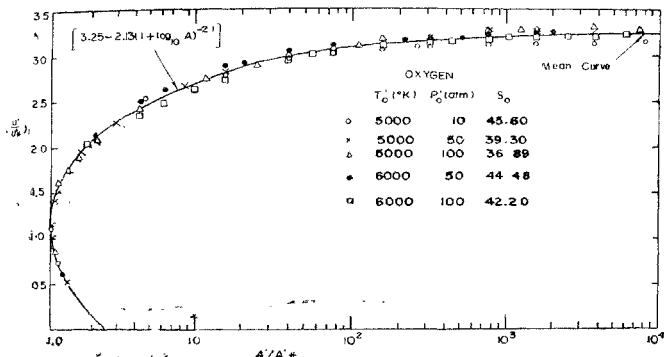


FIG. 11. Velocity correlation with area ratio for oxygen.

Upstream of the nozzle throat:

$$\frac{u'}{u_*} = (4.15 p'_0/T'_0)^{-0.04} [-1.01 + 2.13 (1 + \log_{10} A)^{-2.1}] \quad (23)$$

Downstream of the nozzle throat:

$$\frac{u'}{u_*} = (4.15 p'_0/T'_0)^{-0.04} [3.25 - 2.13 (1 + \log_{10} A)^{-2.1}] \quad (24)$$

It is shown by Reddy and Daum<sup>10</sup> that a correlation for the density at the throat can be obtained for oxygen as

$$\rho'_* = \rho'_0 (0.529 + 9 \times 10^{-6} T'_0 \text{ } ^\circ K). \quad (25)$$

With eqs. (24) and (25), the expression for  $\xi$  in the downstream portion of the nozzle for oxygen can be given as

$$\xi = S_0 - \log_e [(4.15 p'_0/T'_0)^{-0.04} (A'/A'_*) \{3.25 - 2.13 \times (1 + \log_{10} (A'/A'_*))^{-2.1}\} (\rho_d/\rho'_0) \times (0.529 + 9 \times 10^{-6} T'_0 \text{ } ^\circ K)^{-1}]. \quad (26)$$

7.2. *Parameter  $\chi_d$* 

The parameter  $\chi_d$  has been defined as  $\chi_d = [S_0(2 - 1/ij) - \lambda_d]$  where  $\lambda_d$  is given by eq. (15). Since the function  $\lambda_d$  contains the mass flow term  $\rho_* u_*$ , their values for several reservoir conditions have been correlated by Reddy and Daum<sup>10</sup> and can be written for oxygen as,

$$(\rho'_* u'_*) = \rho'_0 u'_0 (0.585 + 1.33 \times 10^{-5} T'_0 \text{ } ^\circ\text{K}). \quad (27)$$

Then the expression  $\chi_d$  for oxygen can be written as

$$\begin{aligned} \chi_d = S_0(2 - 1/ij) - \log_e [(0.95/ij) C_4^{1/ij} IK_{r1} T_d \rho_d^{(2-1/ij)} \\ \times m_d^{-2} (\rho'_0)^{-0.54} \rho'_0^{(0.5+1/ij)} (T'_0)^{0.037}] \end{aligned} \quad (28)$$

where

$$C_4 = (0.585 + 1.33 \times 10^{-5} T'_0 \text{ } ^\circ\text{K}).$$

The parameters  $\xi$  and  $\chi_d$  are now expressed in terms of the initial and boundary values only and hence can be readily computed for any given reservoir conditions and nozzle shape.

7.3. *Discussion of General Correlating Parameters  $\xi$  and  $\chi_d$* 

It has been mentioned earlier that Bray<sup>2</sup> has shown that the frozen mass fraction, for a given nozzle and gas, correlates very well with reservoir entropy alone. Bray concluded this by correlating a number of values of  $\alpha_f$  computed for different reservoir conditions using 'sudden freeze' analysis. From the present analysis, it is shown formally that the frozen mass fraction depends on only one parameter  $\chi_d$  and for a given gas and nozzle shape  $\chi_d$  can be written as

$$\begin{aligned} \chi_d = S_0(2 - 1/ij) - \log_e [(\rho'_0)^{-0.54} \rho'_0^{(0.5+1/ij)} (T'_0)^{0.037} \\ + \text{constant} \end{aligned} \quad (29)$$

From eq. (29) it is obvious that the major controlling parameter is the reservoir entropy  $S_0$  and for a certain combination of reservoir conditions the logarithmic term in eq. (29) could be small so that  $\chi_d$  depends on  $S_0$  only. Thus, the frozen mass fraction  $\alpha_f$  may not correlate with  $S_0$  only for all possible combinations of reservoir conditions. Again by using a number of computed values of  $\alpha_f$  for different nozzles, Harney<sup>5</sup> added another term like  $\log_e(l)$  to the entropy to obtain the necessary correlation. It is noted that in the present general correlating parameter  $\chi_d$ , the type of expression deduced by Harney appears formally and Harney's parameter is not complete

in the sense that the general correlating parameter should contain additional reservoir parameters as given in eq. (28). Ring and Johnson<sup>6</sup> used a correlation based on two independent parameters, namely  $S_0$  and a non-dimensional time  $\tau_c$  characterising the flow expansion rate. It can be shown formally that their parameter  $\tau_c$  is a part of the function  $N_s$  which controls the behaviour of the rate equation and hence the extent of non-equilibrium flow in the nozzle. It should be emphasized that all these preceding procedures adopted for correlation were thought of on an *ad-hoc* basis. In contrast the present analysis is based on formally treating the complete governing equations and it is evident that the general correlating parameter  $\chi_d$  consists of two parts namely  $\lambda_d$  and  $S_0$ , the former arises from the nondimensionalization of governing equations and the latter (a significant part) arises from the 'initial value problem' consideration.

### 8. CONCLUSIONS

Based on the present analysis the following conclusions are noted:

1. Similar solutions have been obtained for nonequilibrium nozzle flows of oxygen undergoing simultaneous vibrational and dissociational relaxation by using a new similarity parameter  $\xi$ .
2. The similar solutions presented can be used over a wide range of initial conditions and nozzle scale parameters.
3. The equilibrium solutions depend on only one parameter  $\xi$  and the nonequilibrium solutions depend on two parameters  $\xi$  and  $\chi_d$ . The frozen species concentration depends on  $\chi_d$  only.
4. The parameters  $\xi$  and  $\chi_d$  would serve as universal correlating parameters since they contain all the physical quantities of the problem. The hitherto used approximate correlating parameters can be deduced from the present general correlating parameter  $\chi_d$ .
5. For any given initial conditions the nozzle flow quantities can be read off from the graphs without resorting to complex computer programmes.

## NOMENCLATURE

$A$	area ratio ( $A = A'/A'_*$ )
$C_1$ and $C_2$	constants in $\tau_v p' = C_1 e^{+c_2\psi^{1/3}}$
$E$	defined in ref. 9
$\bar{G}$	defined in ref. 9
$h$	static enthalpy ( $h = h'/RT'_0$ )
$H$	total enthalpy ( $H = H'/RT'_0$ )
$k_r$	recombination rate constant ( $k_r = kr_1 T_t^{-8}$ )
$l$	nozzle scale length ( $l = r'_*/\tan \theta$ )
$L$	defined in ref. 9
$m_a$	atomic weight
$M$	Mach number
$N$	Maximum number of vibrational levels in a cut-off-harmonic oscillator
$p$	pressure ( $p' = p'/p_d$ )
$s$	entropy
$u$	velocity ( $u = u'/\sqrt{RT'_0}$ )
$V$	coupling factor (ref. 9)
$x$	distance along the nozzle
$\alpha$	dissociation mass fraction
$\epsilon$	vibrational energy ( $\epsilon = \epsilon'/RT'_0$ )
$\theta_v$	characteristic vibrational temperature
$\phi$	vibrational temperature function ( $\phi = \theta_v/T_v$ )
$\rho$	density ( $\rho = \rho'/\rho_d$ )
$\eta$	defined in eq. (7)

- $\psi$  translational temperature function ( $\psi = \theta_v/T_t$ )  
 $\xi$  defined as  $\xi = (S_0 - \eta)$

## Subscripts

- \* conditions at the nozzle throat  
 o reservoir conditions  
 t translational temperature  
 v vibrational temperature  
 d characteristic dissociation values

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