

SIMILITUDE FOR NORMAL SHOCK WAVES IN NON-EQUILIBRIUM FLOWS

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FOREWORD

This report(Interim Technical Report No. 5, RF Project 1580) was prepared by the Aerodynamic Laboratory for The Ohio State University Research Foundation on Contract AF 33(657)-10416, "Research on Similarity Parameters Relating Model Tests in High-Enthalpy Hypersonic Wind Tunnels to Corresponding Full-Scale Flight Conditions." The work reported herein was performed on Project 1426, "Experimental Simulation of Flight Mechanisms," Task 142604, "Theory of Dynamic Simulation of Flight Environments." The project was monitored by Mr. F. J. A. Huber of the Air Force Flight Dynamics Laboratory, Research and Technology Division.

Manuscript was released by the authors in February, 1965, for publication as an RTD technical report

This technical report has been reviewed and is approved.

for Philip P. Antonatos

Chief, Flight Mechanics Division Air Force Flight Dynamics Laboratory



ABSTRACT

Similarity parameters are developed which govern the length of non-equilibrium zones behind normal shock waves. Non-equilibrium effects produced by both vibrational relaxation and dissociation are considered. The parameters can also account for arbitrary levels of free-stream vibrational energy or dissociation level.

The validity of the parameters is examined using numerical computations of the properties of the non-equilibrium fields. These computations are made with the aid of experimentally based rate expressions.

The parameters, when written in a form describing the variation of non-equilibrium zone length with Mach number, are shown to have acceptable accuracy.

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Contrails SYMBOLS

		Units
A	constant, equation (45)	ft
Aı	constant, equation (78)	ft ^{2 O} R/sec ²
В	constant, equation (45)	
Bı	constant, equation (78)	ft ² /sec ²
C	constant of intergration	
Cı	constant, equation (78)	ft ² /sec ² -OR
$C_{\mathtt{p}}$	specific heat at constant pressure	BTU/lb _m
Da	constant, equation (78)	$ft^2/sec^2-(^OR)^2$
Eı	constant, equation (79)	ft ² OR/sec ²
EΑ	activation energy	
\mathtt{E}_{D}	dissociation energy, per molecule	
$\mathtt{E}_{\boldsymbol{V}}$	vibrational energy, per unit mass	ft ² /sec ²
E(K)	error level	
$e_{\mathbb{D}}$	dissociation energy, per unit mass	ft ² /sec ²
F_{1}	constant, equation (79)	ft^2/sec^2
Gı	constant, equation (79)	ft ² /sec ² -OR
Hı	constant, equation (79)	$ft^2/sec^2-(^OR)^2$
$\mathbf{H}_{\mathbf{f}}$	heat of formation, per unit mass	ft ² /sec ²
h	enthalpy, per unit mass	ft ² /sec ²
K	numerical integration index	
K1,K2	constants	variable
k	Boltzmann constant	ft-lb/OR
L	length of non-equilibrium zone	feet
M	Mach number	
M *	arbitrary particle designation	
m	molecular weight	slugs



	SYMBOLS (Continued)	
		Units
$N_{\mathbf{A}}$	Avogadro's number	
p	pressure	lb _f /ft ²
q	dynamic pressure	lb _f /ft ²
R	gas constant	ft ² /sec ² - ⁰ R
S	temperature exponent	
T	temperature	o Rankine
t	time	seconds
u	velocity, x-direction	ft/sec
v	velocity, y-direction	ft/sec
x	distance perpendicular to shock front	feet
У	distance perpendicular to x-axis	feet
Greek		
α	fraction dissociated	
γ	ratio of specific heats	
ρ	density	slugs/ft ³
τ	relaxation time, vibrational mode	sec
θ	characteristic temperature	^O Rankine
ω	temperature exponent	
Subscript	<u>s</u>	
A	flight condition	
a	location behind shock front, active modes in equilibrium	
В	test facility condition	
D	dissociation	
eq	equilibrium	
	vii	



SYMBOLS (Continued)

Subscripts (continued)

L left side of interval

local local condition

R right side of interval

rot rotation

l location just upstream of shock wave

Superscript

* active modes



I. INTRODUCTION

The role of similarity parameters in aerodynamic testing has long been recognized. They have been used both to assure that aerodynamic phenomena are properly simulated in laboratory test facilities and to judge the effect of non-simulation of flight conditions. In addition, such parameters frequently allow an incisive analysis of test data to determine the dominant factors in associated theoretical expressions, leading, in some cases, to simplifications which can produce results of adequate accuracy.

For most aerodynamic test facilities, the usual similarity parameters (Mach number, Reynold's number, ratio of specific heats, and Prandtl number) are adequate for the analysis of results obtained in a non-reacting steady stream which is in thermodynamic equilibrium. These parameters can be obtained from the usual compressible flow equations by the methods of dimensional analysis or the linear relation method.

Advanced testing facilities currently in use may produce conditions in the test media which depart from the flight condition in such ways and to such degrees that the above set of similarity parameters becomes inadequate. Processes may occur in the facility which are not described by the "usual" energy equation, and hence, the parameters derived from this relation are too limited. Therefore, it is necessary to establish the additional similarity laws and to evaluate their validity. This task is the objective of this study.

It is convenient to attack the problem of aerodynamic similitude in a high enthalpy stream in two steps. In the first step the factors involved in scaling in an equilibrium stream are used to evolve similarity relations which are generally those listed above.

The second step of the problem, which represents the main objective of this study, includes the scaling of non-equilibrium effects. It is necessary to be able to scale the regions of a body flow field which are affected by chemical and thermodynamic non-equilibrium processes for the following reason: Consider a shock wave produced by a body moving in free flight at hypersonic speeds through air and assume that the wave strength is such that non-equilibrium effects occur over a distance of five feet downstream from the wave. If the body is ten feet long, then non-equilibrium phenomena occur over the forward fifty per cent of the body. In attempting to simulate these flight conditions in laboratory experiments, suppose that a geometrically similar body, ten inches long, is to be tested and the flow fields are to be duplicated. For proper scaling, the non-equilibrium effects should occur over the forward five inches of the model. Therefore, the factors affecting the rate processes are of primary importance in scaling the two flow fields.

One might logically question the practical importance of scaling the non-equilibrium fields. If the effect of the rate processes on the pressure and temperature distributions over the vehicle is low, say less



than one per cent, the effect on the general aerodynamic performance of the vehicle can be expected to be small. In such a circumstance one could use frozen flow theory for the analysis of at least the inviscid portion of the flow field and a test facility which provides frozen flow results could be employed.

The magnitude of the non-equilibrium effects is illustrated in the work of Sedney, South, and Gerber and Hsu and Anderson. In the former study, the effect of vibrational non-equilibrium in the inviscid flow over a wedge was computed with the method of characteristics. An interesting result for this wedge flow is that far from the leading edge, the equilibrium state near the body is not the same as that behind an equilibrium oblique shock wave. Although the pressure is the same, the temperature is higher in the non-equilibrium case, indicating the existence of an entropy layer near the wedge surface. Typical variations of the pressure and temperature along the wedge surface for a pure diatomic gas are reproduced from Reference 3 in Fig. 1. The results shown in Fig. 1 are presented with p and T made non-dimensional using the free stream values. The distance along the wedge surface is non-dimensionalized with $\tau_{\rm a}q_{\rm l}$. The variations of pressure and temperature shown in Fig. 1 indicate that the effects of vibrational non-equilibrium can be significant.

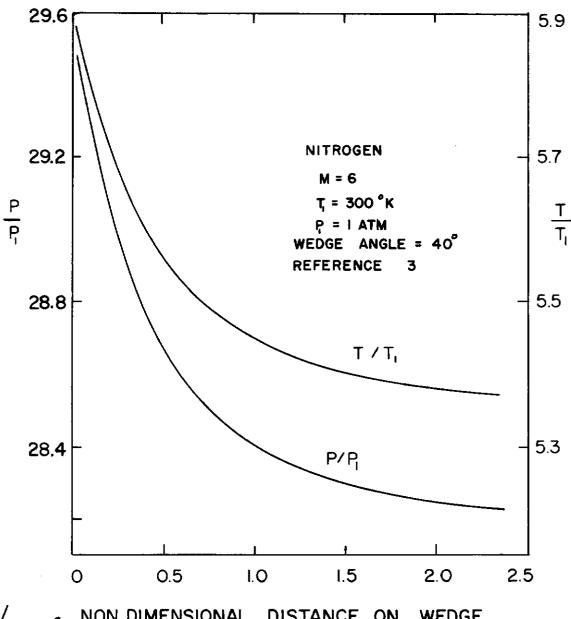
The study by Hsu and Anderson⁴ treats the non-equilibrium dissociating flow of a simple diatomic gas over a cusped body that supports a plane oblique shock wave. Numerical results are presented for N_2 at an altitude of 250,000 feet with Mach number as a parameter varying from 13 to 26 and a shock angle of 80° . Typical results are shown in Figure 2 where the variations of pressure and temperature along a streamline are given. It can be seen that the effects of chemical non-equilibrium can be important in body flow fields.

The usual similarity parameters governing compressible viscous and inviscid flows can be found in many places, e.g., in the works of Schlicting, Pai, Shapiro, and Leipman and Roshko. Specialization of these concepts to equilibrium hypersonic flows were accomplished by Tsien, Cheng, and Lees and Kubota. Viscous and equilibrium real gas effects have been considered by Cheng and Pallone and Sakurai.

Pearce, Samet, and Whalen¹² provide a comprehensive review of the theoretically developed similarity parameters for hypersonic flow together with available experimental evidence and they verify the boundary layer interaction parameters for various types of configurations and test gases. In addition, they discuss non-equilibrium flow concepts but do not develop the associated similarity parameters.

Inger¹³ has developed most of the scaling parameters based on the hypersonic small disturbance theory, but left them in a form which possesses little utility and which is unduly restrictive on test conditions.





L/20 NON DIMENSIONAL DISTANCE ON WEDGE

FIGURE I

EFFECT OF VIBRATIONAL NON-EQUILIBRIUM

ON INVISCID WEDGE FLOW



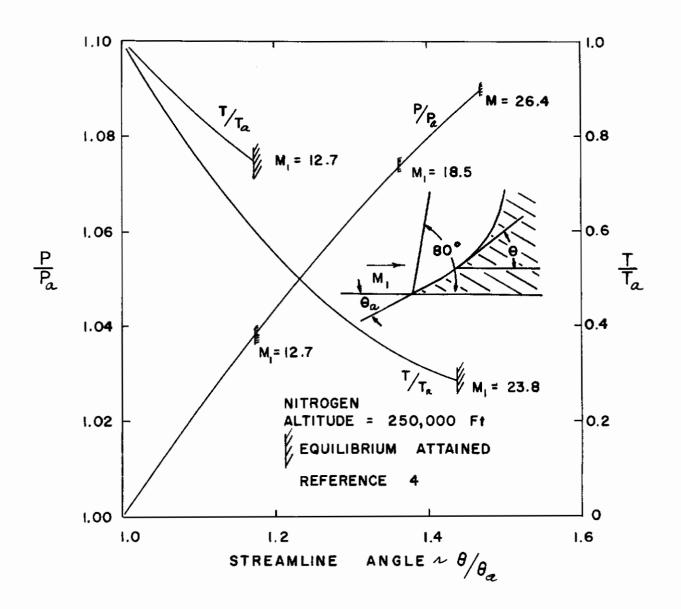


FIGURE 2

EFFECT OF DISSOCIATION NON-EQUILIBRIUM

ON CUSPED BODY FLOW



One of the more important contributions to non-equilibrium similitude is the concept of binary scaling as presented by the members of the staff of the Cornell Aeronautical Laboratory, expecially Gibson and Sowyrda. According to binary scaling, if the test velocity matches that of the flight condition, then the flow fields may be scaled by adjusting the density. This leads to the simple similarity relation

$$\rho_1 L = constant$$
 (1)

The above relation is useful for scaling flow fields involving vibrational as well as dissociation non-equilibrium processes. This point is discussed later.

The general features of non-equilibrium flow fields have been known for some time. One views the modes of energy storage of a diatomic molecule as being active or inert, i.e., fast or slow. For most flows the rotational mode is considered active, thus inducing a non-equilibrium region of negligible size. Usually it is assumed that the translational and rotational modes are active and reach equilibrium quickly while vibrational energy transfer and dissociation generally require much longer times.

There is a surprising lack of information regarding electronic relaxation. If one adopts the Landau-Teller¹⁵ viewpoint of the probability of energy transfer during a collision, one must conclude that electronic energy transfer requires a considerable time. Their view is that if a given mode undergoes a large number of oscillations during a collision, then the transfer of energy is less likely than if the collision time is of the order of the period of the appropriate internal motion. Since the period of electronic motion is much less than the average time for intermolecular collisions, the energy transfer probability is low and the relaxation time is long.

Electronic relaxation will not be considered in the present work, not because it is unimportant, but because there are no expressions for electronic relaxation time which might be used to develop similarity parameters. This is clearly an area where work needs to be done.

In general, the importance of non-equilibrium processes in the nozzle of a test facility has not been recognized. The characteristics of the free-stream flow can play a vital role in the non-equilibrium processes downstream of a model shock wave. Based on recent test data which indicates that the gas may be frozen vibrationally near the nozzle throat, it is not unrealistic to conceive a situation where the gas approaching the shock wave has nearly the vibrational energy required at equilibrium behind the wave, thus eliminating any requirement for vibrational excitation.

Further, in the view of Bauer and Tsang¹⁶ the dissociation process depends heavily on the vibrational excitation process, i.e., on the repopulation rate of the upper vibrational levels. This becomes especially important when one considers that in testing in a high-temperature stream,



the gas may arrive at the shock wave in a highly excited vibrational state. Thus, the gas has, in effect, already climbed a portion of the activation barrier which must be overcome to produce dissociation. The result is a decrease in the region of dissociation non-equilibrium.

The rate expressions for the vibrational relaxation and dissociation generally are developed with the assumption that energy transfer in a gas is accomplished only by collisions. Further, the transfer of vibrational energy and the dissociation of molecules is due to bimolecular collisions, while the recombination of two atoms requires a three-body collision.

The vibrational relaxation equation given by Landau and Teller 15 is

$$\dot{\mathbf{E}}_{\mathbf{v}} = \frac{1}{\tau} \left[\mathbf{E}_{\mathbf{veq}} - \mathbf{E}_{\mathbf{v}} \right] \tag{2}$$

In the above expression, $E_{\rm v}$ is the local vibrational energy and $E_{\rm veq}$ is the vibrational energy the gas would have if it were in equilibrium. τ is the vibrational relaxation time which is a function of the pressure and temperature of the gas. According to Blackman¹⁷ the theoretical expression for the relaxation time is

$$\tau = K_3 T^{\omega} p^{-1} \{ 1 - e^{-\theta/T} \}^{-1} e^{K_4/T^{1/3}}$$
(3)

The dissociation of a molecular species is expressed by the reaction

$$N_2 + M' = 2N + M'$$
, (4)

where M' is another particle. The rate expression for the above reaction is generally written as

$$\frac{d\alpha}{dt} = K_1 (1 - \alpha) T^{-s} (\frac{p}{RT}) e^{-E_D / kT} - K_2 \frac{\alpha^2}{(1+\alpha)} (\frac{p}{RT})^2 T^{-s}$$
(5)

where α is the mass fraction of particles dissociated, R is the specific gas constant of the molecules, E_D is the dissociation energy per molecule, and s is taken to be half the number of degrees of freedom which contribute energy to the dissociation during a collision.

It is probably more correct to adopt the Eyring 18 viewpoint and put E_A , the activation energy, into the exponential factor in place of the dissociation energy. Empirically, the difference between the two can be handled to a degree by altering the pre-exponential factor.



Much effort has been spent in determining the importance of the recombination process in the non-equilibrium flow considerations. Hammitt¹⁹ has reviewed the situation and concludes that except near equilibrium the dissociation effect is more important than the recombination effect. This is caused by the relative scarcity of the three-body collisions necessary for the energy distribution during recombination.

The process of scaling non-equilibrium flow fields is accomplished by examining the relationships between energy transfer rates and the stream velocity. The distance covered by the non-equilibrium zone can be increased by either lowering the rate or increasing the gas velocity. Thus, all the factors affecting these items are important to the scaling process. Binary scaling provides the simplest relationship between energy transfer rate and velocity. When the flight velocities, and thus the temperatures downstream of the shock wave, are duplicated, then the rates in the dissociation zone will be a function principally of density. The density dependency results because the rates are governed by the frequency of two-body collisions.

It is worthwhile to consider the use of binary scaling in facilities which are not of the high-enthalpy type, i.e., facilities such as the conventional hypersonic tunnels having maximum stagnation temperatures in the range from 3000 to 4000°R. In such facilities the primary non-equilibrium effect involves the exchange of vibrational energy. Since the excitation or de-excitation of the vibrational mode depends on two-body collisions, it should be possible to develop scaling laws based on the binary concept. It is interesting to note that in the lower temperature facility the flow-field velocities will, in general, not duplicate those obtained during flight so that Eq. (1) does not apply directly.

Summarizing, it can be stated that it appears feasible to construct scaling laws which can be used to scale non-equilibrium effects produced by pure vibrational effects and dissociation induced non-equilibrium processes. It will be assumed that the vibrational and dissociation processes are uncoupled. Results of calculations described herein provide justification of this assumption.

In the work which follows, the appropriate similarity parameters governing vibrational and dissociational relaxation downstream of normal shock waves are derived. Based on evaluation of these parameters immediately behind the wave, the parameters are written in terms of stream conditions by using approximate normal shock wave relations. The validity of these expressions is then examined with the results of exact calculations for the non-equilibrium zones. These calculations are performed with empirically determined rate expressions.



II. SIMILARITY PARAMETERS FOR FLOWS WITH VIBRATIONAL NON-EQUILIBRIUM

The most widely quoted source of vibrational excitation rates for N_2 and O_2 is Reference 17 where the results of interferometric measurements of density variations downstream of normal shock waves are reported. The linear relaxation equation was employed to relate the density changes to the absorption of energy by the vibrating molecules. The trends of the data in Reference 17 were expressed in the form of Eq. 3 by the present authors as

$$\tau_{O_2} = 3.54 \times 10^{-8} \frac{\sqrt{T}}{p} e^{132.8/T^{1/3}}$$
 (6)

$$\tau_{\text{N}_{2}} = 3.12 \times 10^{-8} \frac{\sqrt{T}}{p} e^{187 \cdot 3/T^{1/3}}$$
 (7)

where τ is in seconds, p is in pounds per square feet, and T is in degrees Rankine.

Since Eqs. (6) and (7) are used in the derivation of the vibrational similarity parameter, it is worthwhile to keep in mind some of the limitations imposed in Reference 17.

- 1. The velocity downstream of the wave is assumed constant.
- 2. The temperature which appears in Eqs. (6) and (7) is actually the average translational temperature downstream of the wave.
- 3. The excitation of the electronic energy mode is included with the vibrational excitation. This may be important at high temperatures.
- 4. The gas ahead of the shock is assumed to have a low temperature, therefore, the data may not account for vibrational non-equilibrium effects in the gas upstream of the shock, a condition which may exist in the flow delivered by a nozzle.
- 5. The τ given by Eqs. (6) and (7) is not the total relaxation time, but rather is the time required for the vibrational mode to reach (1 1/e) of the equilibrium energy. (See Appendix I.)

For simplicity, normal shock waves in diatomic gases are considered initially. It is relatively simple to compute the temperature, pressure, and density changes across the wave based on the assumed equilibration of translational and rotational modes. Downstream of the wave the usual differential equations which describe the flow field are:

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = 0 \qquad , \tag{8}$$

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} , \qquad (9)$$

$$u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial y}$$
, and (10)

$$\frac{D}{Dt}\left(h + \frac{u^2}{2}\right) - \frac{1}{\rho}\frac{\partial p}{\partial t} = 0 \qquad , \tag{11}$$

Restricting the consideration to the distribution of static pressures in the non-equilibrium zone, the scaling laws should come from the energy relation since it is the absorption of energy by the vibrational mode which produces the static pressure change. The energy relation in the non-equilibrium field is

$$\rho(Dh/Dt) - (Dp/Dt) = 0 , (12)$$

which for a one-dimensional steady-state situation (but with vibrational relaxation and chemical reactions) becomes

$$\rho \left[\frac{\partial h^*}{\partial x} + \frac{1}{u} \frac{dE_V}{dt} \right] = \frac{dp}{dx} \qquad (13)$$

Since the relation is applied downstream of the wave, the various terms such as u, dE_V/dx , etc., must be evaluated there. However, it is desirable for scaling to include the stream conditions ahead of the wave and the wave strength. Variation of these parameters results in alteration of the u and dE_V/dt terms, which then changes the pressure distribution in the non-equilibrium zone.



Suppose that the temperature variation in the relaxation region is such that the specific heat of the active modes can be considered constant. Then the relaxation equation can be written in the form

$$C_{p}*\frac{dT}{dx} + \frac{1}{u}\frac{dE_{V}}{dt} = \frac{1}{\rho}\frac{dp}{dx} \qquad (14)$$

Some rather interesting similarity considerations can be developed with this equation. If two relaxation processes are related by the following linear expressions:

the similarity parameter which results is

$$E_V L/uT = constant$$
 . (16)

Since $\check{\mathbf{E}}_{\mathbf{y}}$, u, and T vary in the non-equilibrium zone, the question naturally arises as to where in the zone these elements should be evaluated. Clearly, for greatest utility they should be evaluated at the start of the zone, i.e., just behind the shock wave. One might then be able to express them in terms of the stream conditions and the shock wave relations, thereby introducing Mach number and stream non-equilibrium effects. Therefore, the form of the parameter to be considered is

$$\frac{\dot{E}_{V_a}L}{u_aT_a} \tag{17}$$

Now, E $_{Va}$ is expressed in the form of Eq. (2) with the relaxation time as given by the empirical relationships of Eqs. (6) and (7). For N2,

$$\dot{E}_{V_{a}} = \frac{\left(E_{V_{e_{q}}} - E_{V_{a}}\right)}{3.12 \times 10^{-8} T_{a}^{1/2} p_{a}^{-1} e^{187.3/T_{a}^{1/3}}}$$
(18)

The conditions immediately behind the shock wave (subscript "a") can be related to those upstream of the wave with the normal shock relationships assuming that only translation and rotation of the molecules occur. Hence, the static temperature ratio across the shock is given by

$$\frac{T_a}{T_1} = \frac{(7M_1^2 - 1)(M_1^2 + 5)}{36 M_1^2} , \qquad (19)$$

which for hypersonic Mach numbers can be approximated by

$$T_a = 0.2 M_1^2 T_1$$
 (20)

The static pressure ratio across the wave is given by

$$\frac{p_a}{p_1} = \frac{7M_1^2 - 1}{6} \qquad , \tag{21}$$

which for hypersonic Mach numbers can be approximated by

$$p_a = 1.1 M_1^2 p_1$$
 (22)

Further, immediately behind the wave, the vibrational energy is the same as that in the free-stream. Hence,

$$E_{V_a} = E_{V_1} \tag{23}$$



Finally, it is convenient to approximate \mathbf{E}_{Veq} by

$$E_{Ve_{Q}} = C_{VIB_{Q}} T_{Q}$$
 (24)

This approximation is justified by the relatively small variation of c_{VIB} through the temperature range of interest. The actual variation of c_{VIB} is shown in Fig. 3. Combining Eqs. (18), (20), (22), (23), and (24) gives

$$\dot{E}_{V_{a}} = K_{7}M_{1}^{3}T_{1}^{1/2}p_{1} e^{-(K_{8}M_{1}^{-2/3}T_{1}^{-1/3})}$$

$$- K_{9}EV_{1}M_{1} T_{1}^{-1/2}p_{1} e^{-(K_{8}M_{1}^{-2/3}T_{1}^{-1/3})}$$
(25)

To express the similarity parameter (Eq. 17) in terms of conditions in the free stream, the velocity u_a is written as

$$u_{a} = \frac{(\gamma + 1)M_{1}^{2}}{(\gamma - 1)M_{1}^{2} + 2} u_{1}$$
 (26)

which, for hypersonic Mach numbers becomes

$$u_{a} = (\gamma R)^{1/2} \left(\frac{\gamma + 1}{\gamma - 1}\right) \Gamma_{1}^{1/2} M_{1}$$
(27)

Combining equations (20) and (27) gives

$$u_aT_a = (constant) M_1^3T_1^{3/2}$$
 (28)

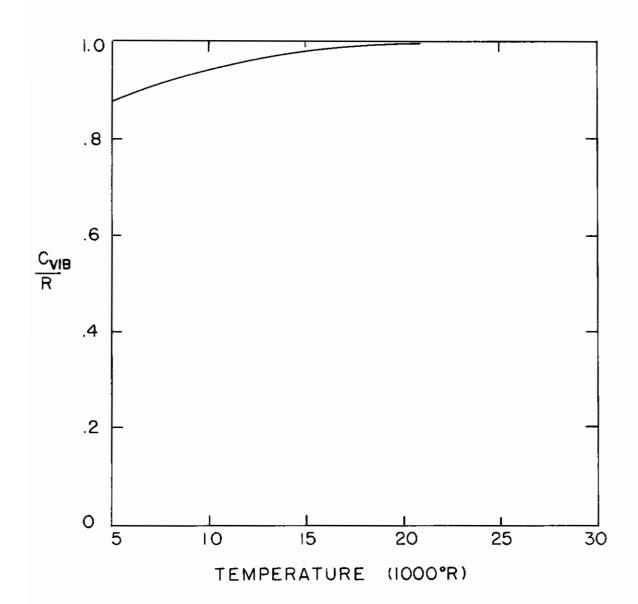


FIGURE 3

VARIATION OF VIBRATIONAL
SPECIFIC HEAT WITH TEMPERATURE



With Eqs. (17), (25), and (28), the vibrational similarity parameter becomes

$$\frac{E_{V_a}L}{u_{aT_a}} = K_{10}T_1^{-1}p_1Le^{-(K_0M_1^{-2/3}T_1^{-1/3})}$$

$$- K_{11}E_{V_{1}}M_{1}^{-2}T_{1}^{-2}p_{1}Le^{-(K_{8}M_{1}^{-2}/3}T_{1}^{-1/3})$$
 (29)

Hence, scaling of a vibrational relaxation zone is accomplished with the relationship

$$\left[\frac{K_{10}}{T_{1}} - K_{11} \frac{E_{V_{1}}}{(M_{1}T_{1})^{2}}\right] p_{1} L e^{-(K_{0}M_{1}^{-2/3}T_{1}^{-1/3})} = constant$$
 (30)

Notice that when a shock wave moves into a gas which is not excited vibrationally, then E_{V_1} = 0 and Eq. (30) becomes

$$\frac{p_1 L}{T_1} e^{-(K_0 M_1^{-2/3} T_1^{-1/3})} = constant$$
 (31)

Rewriting Eq. (31) as

$$\rho_1 \text{Le}^{-K_{1,2} u_1^{-2/3}} = \text{constant}$$
 (32)

shows that if the velocity u_1 is constant then the simple binary scaling expression is obtained.

With constant free-stream conditions, the variation of the length of the relaxation zone with Mach number can be determined from Eq. (31) as

$$lnL = K_{13} + K_{14}M_{1}^{-2/3}$$
 (33)



To check the utility of the parameters developed above, the characteristics of the non-equilibrium zones caused by vibrational relaxation behind normal shock waves have been computed. The equations and procedures employed in the "exact" calculations are summarized in Appendix II. The results of the computations are given in Figs. 4 and 5. Notice in particular the order of magnitude of the length of the relaxation zone. In Section III a comparison will be made between the vibrational relaxation and dissociation zones showing that the separate analysis of the two effects is permissible.

The scaling parameter given by Eq. (30) indicates that the influence of vibrational excitation in the free-stream becomes less pronounced as the Mach number is increased; this effect is illustrated in the curves of Figs. 4 and 5.

To examine the applicability of the scaling parameters, Eq. (33) was employed to produce curves which describe the variation of the length of relaxation zone with Mach number at a fixed altitude and with no free-stream vibrational excitation. These curves are compared with the results of the exact calculations in Figs. 6 and 7. The circled points are taken from Figs. 4 and 5 to eliminate confusion because of the close agreement of the curves developed with Eq. (33) and those obtained from the exact calculations. Considering the approximation inherent in the similarity parameters, the accuracy of the parameters in describing the length of the relaxation zone is surprisingly good.

The calculations indicate that for the conditions examined in this study Eqs. (31) and (33) scale the non-equilibrium zones as long as the free-stream vibrational energy does not exceed 10 percent of the equilibrium vibrational energy behind the shock wave.

Summarizing, in this section, relations governing the length of non-equilibrium zones have been derived. These relations allow scaling of vibrational zones for any combination of pressure, temperature, Mach number, and stream vibrational energy level. If a nozzle can be operated at equilibrium, and at temperatures and pressures duplicating flight, Eq. (33) shows that the Mach number must be increased in order to shorten the relaxation zone. Equation (30) indicates that if the flight situation has negligible stream vibrational energy and the test situation involves freezing of the vibrational energy at some point in the nozzle, the only way in which the relaxation zone can be duplicated is to test at higher Mach numbers, higher temperatures, or both.

III. SIMILARITY PARAMETERS FOR CHEMICAL NON-EQUILIBRIUM FIELDS

The results presented in this section illustrate that the length of the zone of chemical non-equilibrium behind a normal shock wave is much greater than that for the zone of vibrational non-equilibrium. This supports the conclusion reached by Scala, Talbot, and Cary²⁰ that separate (uncoupled)

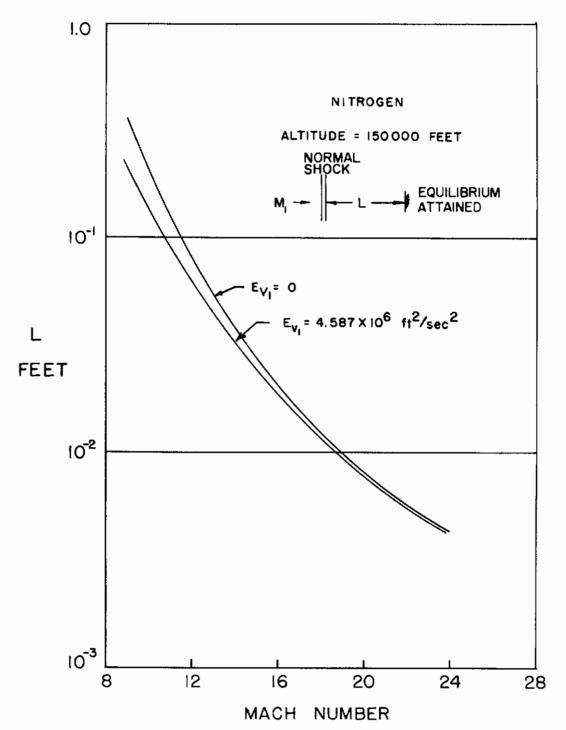
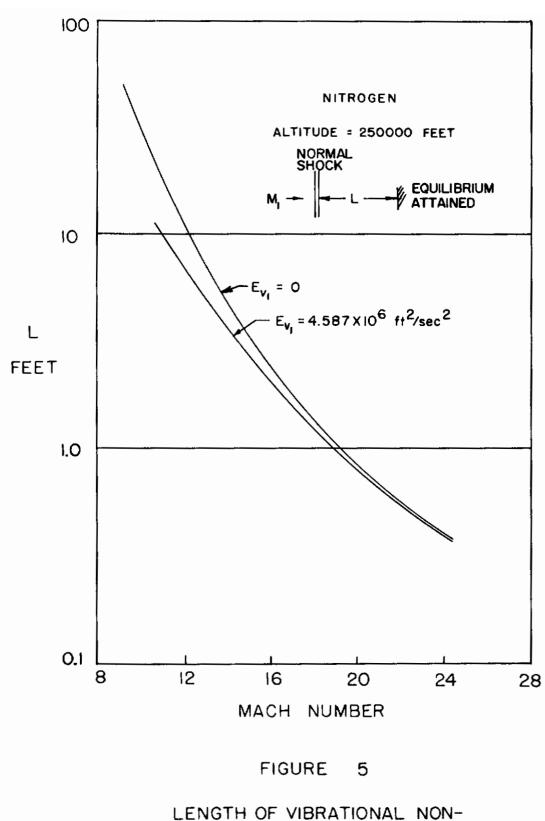


FIGURE 4

LENGTH OF VIBRATIONAL NONEQUILIBRIUM ZONE VERSUS MACH NUMBER





LENGTH OF VIBRATIONAL NON-EQUILIBRIUM ZONE VERSUS MACH NUMBER

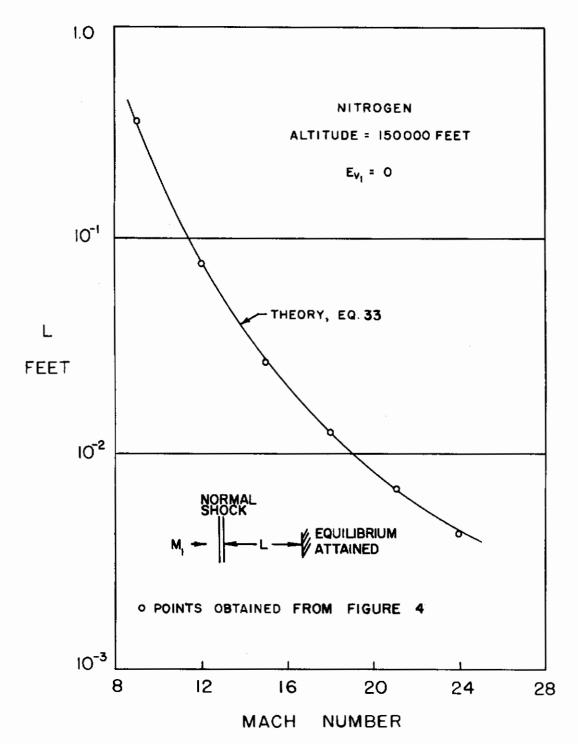


FIGURE 6

EVALUATION OF VIBRATIONAL

SIMILARITY PARAMETER



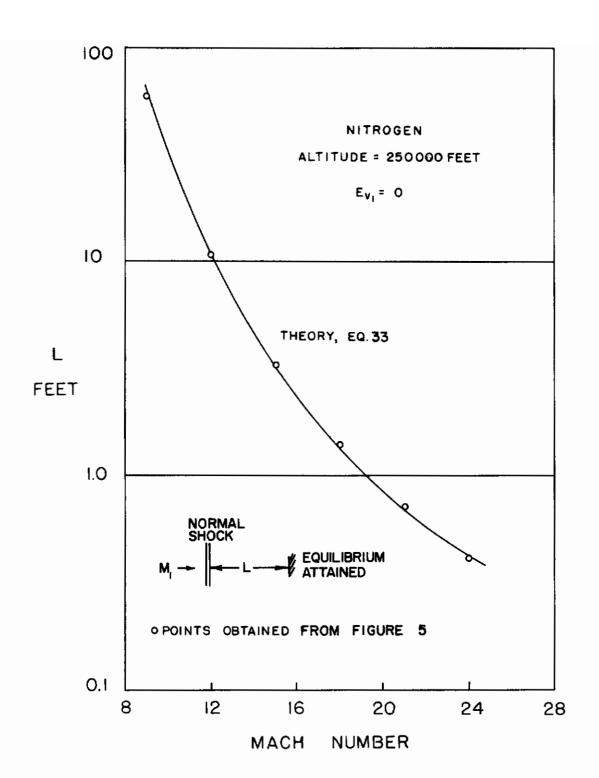


FIGURE 7

EVALUATION OF VIBRATIONAL

SIMILARITY PARAMETER



analysis of the two zones is reasonable. Since the vibrational zone is much shorter than the dissociation zone, consideration of coupling effects would seem to be a needless complication. Accordingly, such coupling will not be considered here.

It should be kept in mind, however, that the presence of dissociated components in the stream approaching the model can sizably affect the rates in both non-equilibrium zones. Such a circumstance is likely to occur in the nozzle of an arc-heated wind tunnel. The rates of energy exchange of both zones will be affected not only by stream dissociation but also by stream vibrational energy.

It is likely that the effect of stream vibrational excitation would be confined largely to the vibrational relaxation zone. Therefore, it could be concluded that, since the two relaxation zones are effectively independent, the dissociation process starts from a condition of near vibrational equilibrium. Accepting this, then, allows one to forego the study of the effect of vibrational non-equilibrium on the dissociation process and confine attention to the modifications caused by stream dissociation.

The dissociation rate expression, Eq. (5), has been arranged to conform to the accepted form for a bimolecular process coupled with a recombination term proportional to the frequency of three-body collisions. The constants have been evaluated by fitting the expression to experimentally determined rates produced in shock tubes.

Although the concept of simple bimolecular and three-body processes yields an expression which agrees with experimental results, it is certain that such a simple expression does not represent all facets of the problem. Bauer and Tsang point out that the dissociation rate depends greatly on the rate at which the upper vibrational levels can be repopulated after being depleted by dissociation.

It can be said further that the dissociation rate is affected by any process which stretches the intermolecular bond. Therefore, although the rate expression doesn't specifically reflect it, dissociation through rotation must exist to some degree. Thus, the ability to replenish the upper rotational levels should also enter the picture.

The combined energy and momentum equations can be used to describe the relaxation produced by dissociation. For one-dimensional flow

$$\rho \left[\frac{dh^*}{dx} + \frac{1}{u} \frac{de}{dt} \right] = \frac{dp}{dx} , \qquad (34)$$

where h* includes all contributions to enthalpy other than dissociation. These are assumed to be in equilibrium with the dissociation process since the latter is relatively slow. This assumption is probably weakest in regard to electronic relaxation, as discussed earlier.



The energy absorbed and released by the dissociation and recombination processes can be expressed in terms of the respective rates and the dissociation energy. The complete rate equation for N_2 is 19

$$\frac{d\alpha}{dt} = K_1(1 - \alpha) T^{-2.5} pe^{-(E_A/kT)} - K_2 \frac{\alpha^2}{(1 + \alpha)} T^{-3.5} p^2 .$$
 (35)

This type of equation is used in the computations described in Appendix III; however, since the scaling laws will be most useful when their components are expressed in terms of stream conditions and Mach number, only the first term of the above equation will be used. That is, the utility of the scaling laws is greatest when they are most easily applied. In the case of a normal shock wave, the conditions just downstream from the shock wave can be computed in terms of the stream conditions. Since this information is usually available, the similarity parameters should be arranged accordingly.

Therefore in the work which follows the properties of the forward part of the non-equilibrium zone are most important. Since the effects of the recombination term are negligible in this area, it will be removed from the similarity considerations. Thus,

$$d\alpha/dt = K_1(1 - \alpha)T^{-2.5}pe^{-(E_A/KT)} \qquad (36)$$

The rate of absorption of energy by the dissociation process is simply the product of the dissociation rate and the dissociation energy. The combined momentum and energy equations then provide

$$\rho \left[\frac{dh^*}{dx} - \frac{N_A E_D}{mu} \quad \frac{d\alpha}{dt} \right] = \frac{dp}{dx} \qquad , \tag{37}$$

where \overline{m} is the molecular weight of the diatomic species.

If the modes other than dissociation are taken to be in equilibrium, then the first term can be written in terms of the local temperature gradient. In the second term the various constant terms can be combined, leading to

$$\rho c_p * \frac{dT}{dx} + K_{L5} \frac{\rho}{u} \frac{d\alpha}{dt} = \frac{dp}{dx}$$
 (38)



The similarity parameters are produced in the usual fashion, with linear relations between two flow situations:

$$T_{B} = \overline{K}_{1} T_{A} ,$$

$$\rho_{B} = \overline{K}_{2} \rho_{A} ,$$

$$X_{B} = \overline{K}_{3} X_{A} ,$$

$$\alpha_{B} = \overline{K}_{4} \alpha_{A} ,$$

$$\alpha_{B} = \overline{K}_{5} u_{A} ,$$

Substitution of Eq. (39) into (38) results in the following scaling parameter:

 $p_B = \overline{K}_6 p_A$

$$\frac{\alpha L}{Tu} = constant$$
 (40)

Application of this parameter is accomplished most readily if it is evaluated immediately behind the shock wave. Hence, Eq. (40) is written as

$$\frac{\alpha_{a}L}{T_{a}u_{a}} = constant$$
 (41)

Substitution of the rate expression, Eq. (36), into Eq. (41) yields

$$\frac{(1 - \alpha_1) p_a Le^{-E_A/kT_a}}{T_a^{3.5} u_a} = constant$$
 (42)



As in the previous section of this report, the conditions immediately behind the shock wave can be related to those in the free-stream with the hypersonic approximations to the normal shock relationships. Since the region of vibrational relaxation generally is much shorter than the region of chemical non-equilibrium, the normal shock relationships probably should be based on a ratio of specific heats different than 1.4. However, as a first approximation, Eqs. (20), (22), and (28) will be employed without modifications for the possible difference in γ . With these normal shock relationships, the dissociation scaling parameter becomes

$$\frac{(1 - \alpha_1) p_1 L e^{-K_{16}/M_1^2 T_1}}{M_1^6 T_1^4} = constant$$
 (43)

Notice that if the stream dissociation is zero, then

$$\alpha_{L} = 0$$
 , (44)

and a somewhat simpler expression results. However, in considering the non-equilibrium processes in the nozzle of an arc-heated test facility it is most desirable that the scaling factor account for a non-zero α_1 . Equation (43) appears to do this.

For fixed free-stream conditions, the length of the zone of chemical non-equilibrium can be correlated in the form

$$L = AM_1^6 e^{B/M_1^2}$$
 (45)

To examine the applicability of the above dissociation similitude parameters, the characteristics of the zones of chemical non-equilibrium downstream of normal shock waves were computed for several combinations of Mach number and altitude with the procedures outlined in Appendix III. The results of these exact calculations are given in Figs. 8 and 9.

The utility of the scaling parameter on the form given by Eq. (45) is illustrated by the comparisons shown in Figs. 8 and 9. The similarity parameter curve labeled "theory" in Figs. 8 and 9 appears to scale the length of the non-equilibrium zone with reasonable accuracy over most of the Mach number range.

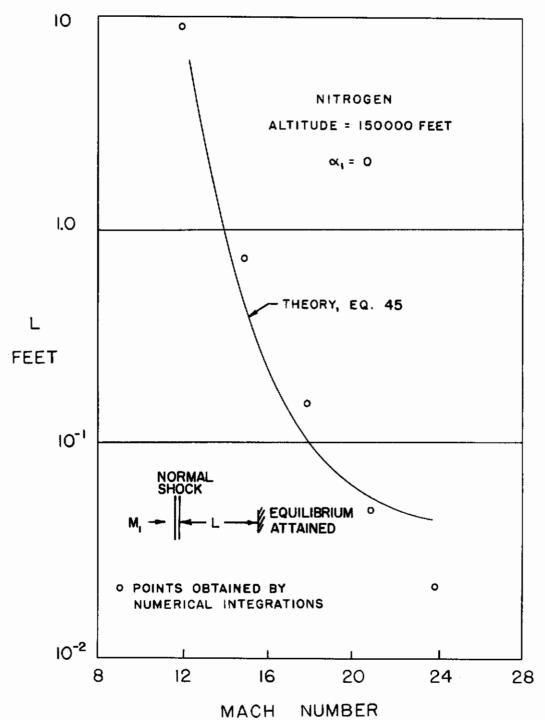


FIGURE 8

EVALUATION OF DISSOCIATION

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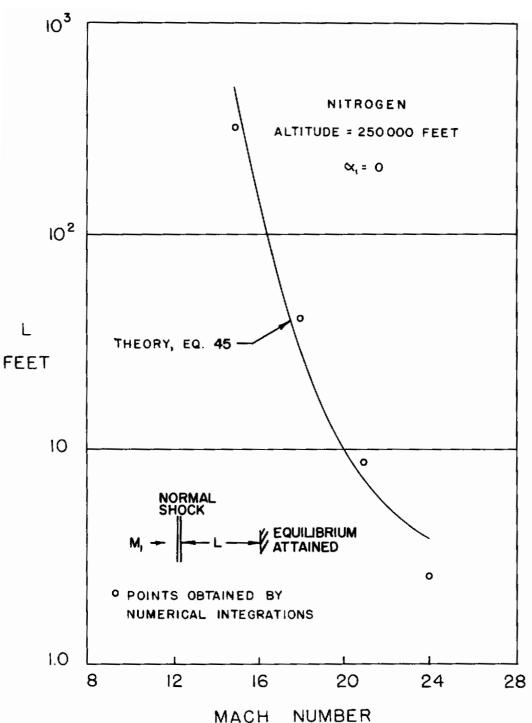


FIGURE 9

EVALUATION OF DISSOCIATION

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Comparisons of the results given in Figs. (6) through (9) show that the length of the zone of chemical non-equilibrium generally is an order of magnitude larger than that for vibrational non-equilibrium. This comparison is the basis for the assumption made here that the two zones can be treated separately.

IV. EXTENSION TO OBLIQUE SHOCK WAVES

At first glance the extension to oblique shock waves would seem to follow in the usual fashion; namely, the parameters are used as they are but are based on the Mach number normal to the oblique shock wave. Such a procedure would adequately handle the temperature and pressure effects but not the velocity effects.

By considering the two fundamental similarity parameters,

$$\frac{E_{V}L}{uT}$$
 = constant , and (46)

$$\frac{\alpha L}{uT} = constant \qquad , \tag{47}$$

it can be seen that the velocity u has great importance. With an oblique shock wave, then, the use of the normal Mach number accounts only for the change in the normal component of velocity but does not include the effect of the tangential component which will certainly be quite important in stretching out the non-equilibrium zone.

It may be most convenient to convert the temperature and pressure elements in terms of normal Mach number and stream conditions and allow the velocity to remain unchanged. The two revised similarity parameters are

$$(K_5M_1 - K_7E_{V_1}M_1^{-1})L u_a^{-1} T_1^{1/2} p_1 e^{-(K_6/M_1 e^{2/3}T_1^{1/3})} = constant$$
 (48)

and.



$$\frac{(1 - \alpha_1) p_1 L_e^{-(K_{11}/T_1 M_1^2)}}{M_1^5 T_1^{3 \cdot 5} u_a} = constant$$
 (49)

One can use the above similarity parameters by calculating the total velocity behind the oblique shock wave and inserting it in the parameter.

V. CONCLUSIONS

A study has been made of the factors affecting simulation and scaling of non-equilibrium flow fields. The flow fields examined included those produced by both vibrational excitation and dissociation of diatomic molecules. As an aid in evaluating the similarity parameters, the characteristics of both types of flow fields were computed for normal shock waves occuring in nitrogen at various Mach numbers, stream pressures, and stream densities.

As a result of this study the following conclusions can be stated:

- 1. The vibrationally induced non-equilibrium fields are much smaller than the fields produced by dissociation at the same Mach number, pressure, and density. It is, therefore, reasonable to analyze the two fields assuming no coupling, i.e., as though they were independent and sequential with the dissociation field following the vibrational field.
- 2. The parameter which can be used to scale vibrational non-equilibrium zones is

$$K_{10}T_{1}^{-1}p_{1}Le^{-(K_{8}/M_{1}^{2/3}T_{1}^{1/3})} - K_{11}E_{V_{1}}M_{1}^{-2}p_{1}T_{1}^{-2}Le^{-(K_{8}/M_{1}^{2/3}T_{1}^{1/3})} = constant. (50)$$

This parameter is valid for inviscid flows at hypersonic (M > 9) Mach numbers for any level of vibrational energy in the stream approaching the shock wave.

3. If the approaching stream is in vibrational equilibrium, the parameter becomes

$$(p_1L/T_1) e^{-(K_8/M_1^2/3T_1^{1/3})} = constant;$$
 (51)



and if stream pressure and temperature duplicate those of flight, the Mach number can be used to scale the flow field according to

$$\ln L = K_{1}s + (K_{1}4/M_{1}^{2/3}) . (52)$$

4. For inviscid flow, the hypersonic Mach number parameter for scaling dissociation fields is

$$\frac{(1 - \alpha_1) p_1 L e^{-(K_{16}/T_1 M_1^2)}}{T_1^4 M_1^6} = constant . (53)$$

when the stream approaching the wave is undissociated, the parameter becomes

$$\frac{p_1 \text{ L e}^{-(K_{16}/T_1M_1^2)}}{T_1^4 M_1^6} = \text{constant} ;$$
 (54)

and if pressures and temperatures duplicate flight conditions, the Mach number scales according to

$$M_1^2 \ln (L/M_1^6) = constant$$
 (55)

Contrails

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APPENDIX I

THE PHYSICAL SIGNIFICANCE OF VIBRATIONAL RELAXATION TIME, τ

In the literature numerous situations are found in which the vibrational relaxation time τ is misunderstood and misused. Generally, in these situations, τ is taken to be the total relaxation time, that is, the time to come arbitrarily close to equilibrium. That τ is not the full relaxation time is the subject of the following elementary considerations.

The equation which defines τ is

$$dE_{V}/dt = \left(E_{V_{eq}} - E_{V_{local}}\right)/\tau \qquad ; \tag{56}$$

then

$$dE_V / (E_{V_{eq}} - E_{V_{local}}) = dt/\tau$$
,

and

$$\ln \left(E_{V_{eq}} - E_{V_{local}} \right) = -t/\tau + \ln c$$
; (57)

or

$$E_{V_{eq}} - E_{V_{local}} = C e^{-t/\tau}$$
 .

If one denotes the condition behind the wave by $()_a$ and specifies that t=0 at that point, then the following boundary condition can be written:

$$t = 0$$
, $E_{Vlocal} = E_{Va}$ (58)



Applying this yields

$$C = E_{V_{eq}} - E_{V_a}$$
 ,

and Eq. (57) becomes

$$E_{\text{Veq}} - E_{\text{Vlocal}} = \left(E_{\text{Veq}} - E_{\text{Va}}\right) e^{-t/\tau} \qquad (59)$$

But when $t = \tau$,

$$E_{V_{eq}} - E_{V_{local}} = \left(E_{V_{eq}} - E_{V_{a}}\right) e^{-1} = 0.368 \left(E_{V_{eq}} - E_{V_{a}}\right)$$
(60)

or

$$E_{V_{local}} - E_{V_a} = .632 \left(E_{V_{eq}} - E_{V_a} \right)$$
 (61)

Therefore, τ is the time required for the vibrational mode to travel through 63.2 per cent of the range through which it would travel if allowed to come to equilibrium.



APPENDIX II

COMPUTATIONAL PROCEDURE FOR VIBRATIONAL NON-EQUILIBRIUM DOWNSTREAM OF NORMAL SHOCK WAVES

Calculation of the properties of vibrational non-equilibrium fields downstream of normal shock waves in nitrogen was completed with the IBM 7094 computer at The Ohio State University Numerical Computation Laboratory. The computations were made for six Mach numbers, two altitudes, and two stream vibrational energy levels.

ALTITUDE, FT.	$^{\mathrm{E}}$ V1			MACH 1	TUMBERS		
150,000	0	9	12	15	18	21	24
150,000	$4.6 \times 10^6 \text{ ft}^2/\text{sec}^2$	9	12	15	18	21	24
250,000	0	9	12	15	18	21	24
250,000	$4.6 \times 10^6 \text{ ft}^2/\text{sec}^2$	9	12	15	1.8	21.	24

A stepwise procedure was used based on the finite difference form of the equations resulting from the conservation of mass, momentum, and energy in the relaxation zone. With the state equation added, they are

$$\Delta u/u + \Delta \rho/\rho = 0 , (62)$$

$$u\Delta u + (1/\rho)\Delta p = 0 , (63)$$

$$\Delta h + u\Delta u = 0$$
 , and (64)

$$p = \rho RT$$
 (65)

These equations can be combined to yield:



$$\Delta u = -\frac{2u}{7RT - 5u^2} \Delta E_V \quad , \text{ and} \quad (66)$$

$$\Delta p = - (\rho u) \Delta u \qquad . \tag{67}$$

If one knows ΔE_V and the local conditions, then Δu and Δp can be computed, and new values of u, p, ρ , and T can be calculated at the end of the interval which corresponds to the change in $E_{V^{\bullet}}$. The length of the interval was calculated from

$$\Delta x = \frac{u\tau}{E_V(T) - E_{V_{local}}} \Delta E_V , \qquad (68)$$

where $\mathrm{E}_{\mathrm{V}}(\mathrm{T})$ was computed from the energy relation for a linear harmonic oscillator

$$E_{V}(T) = \frac{R\theta}{e^{\theta/T} - 1}$$
(69)

and T was obtained from

$$\tau = K_3 T^{1/2} p^{-1} e^{K_4/T^{1/3}}$$
, (70)

where for nitrogen,

$$Ks = 3.12 \times 10^{-8} \text{ psf-sec/(}^{\circ}R)^{1/2}$$
 , (71)

$$K_4 = 187.332 (^{\circ}R)^{1/3}$$
 , and

$$\theta = 6008.2$$
 OR

The initial conditions for the stepwise computation were calculated with $\gamma = 1.4$.



The computer program consisted of the following steps:

- 1. Input initial conditions, including ΔE_{V}
- 2. Calculate $E_V(T)$
- 3. Calculate τ
- 4. Calculate ∆x
- 5. Calculate Δu
- 6. Calculate △p
- 7. $x_i = x_{i-1} + \Delta x$
- 8. u_i = u_{i-1} + ∆u
 - 9. p_i = p_{i-1} + △p
- 10. $\rho = \rho u/u$
- 11. $E_{V_i} = E_{V_i 1} + \Delta E_V$
- 12. $T = p/\rho R$

The detailed computer program was written in Scatran language and since this method of programming is not particularly common, the actual program will not be given here. The computations were accomplished with no difficulty.



APPENDIX III

COMPUTATIONAL PROCEDURE FOR CHEMICAL NON-EQUILIBRIUM DOWNSTREAM OF NORMAL SHOCK WAVES

Dissociation processes were computed for normal shock waves in nitrogen at six Mach numbers, two altitudes, and one stream dissociation level. The conditions are listed below.

ALTITUDE, FT.	I	MACH NUI	MBERS			α_{1}
150,000	12	15	18	21	24	0
250,000	12	15	18	21	24	0

The equations for these computations are similar to those used in the vibrational calculations presented in Appendix II.

$$\Delta u/u + \Delta \rho/\rho = 0 \tag{72}$$

$$u\Delta u + 1/\rho \Delta p = 0 \tag{73}$$

$$\Delta H + u \Delta u = 0 \tag{74}$$

$$p = \rho RT \tag{75}$$

The enthalpy change across an increment of length measured from the shock front was computed from

$$\Delta H = (1 - \alpha_R) \Delta H_f^{N_2}(T_R) - (1 - \alpha_L) \Delta H_f^{N_2}(T_L) + \alpha_R \Delta H^N_f(T_R)$$
$$- \alpha_L \Delta H_f^N(T_L) , \qquad (76)$$



where subscript L indicates the left or upstream side of the interval.

Since

$$\alpha_{\rm R} = \alpha_{\rm L} + \Delta \alpha \qquad \text{and} \qquad (77)$$

$$T_{\rm R} = T_{\rm L} + \Delta T \qquad , \qquad \label{eq:TR}$$

and the heats of formation were computed using expressions of the form

$$\Delta H_{f}^{N_{2}} = \frac{A_{1}}{T} + B_{1} + C_{1}T + D_{1}T^{2} \qquad \text{and} \qquad (78)$$

$$\Delta H_{f}^{N} = \frac{E_{1}}{T} + F_{1} + G_{1}T + H_{2}T^{2} , \qquad (79)$$

Eq. (76) can be written as follows:

$$\Delta H = \Delta T \left[-\frac{A_{1}}{T_{R}T_{L}} + C_{1} + D_{1} (T_{R} + T_{L}) \right]$$

$$+ \alpha_{L} \Delta T \left[\frac{(A_{1} - E_{1})}{T_{R}T_{L}} + (G_{1} - C_{2}) + (H_{1} - D_{1})(T_{R} + T_{L}) \right]$$

$$+ \Delta \alpha \left[\frac{(E_{1} - A_{1})}{T_{R}} + (F_{1} - B_{1}) + (G_{1} - C_{1})T_{R} + (H_{1} - D_{1})T_{R}^{2} \right].$$

If the first two terms on the right side of Eq. (80) are written as DH_1 and the last term is written as $D\alpha$ [DHDA], then Eq. (80) has the form

$$\Delta H = DH_1 + D\alpha [DHDA]$$
; (81)

Then when $\textbf{T}_{\textbf{T}_{i}}$ is known and $\Delta \textbf{T}$ is specified, $\textbf{D}\textbf{H}_{\textbf{1}}$ and DHDA are known.

Contrails

The computer program is then established as follows: (Variables without subscripts in the program are left side values.)

- 1. Read in initial conditions $(\alpha, p, \rho, R, T, u, \Delta T)$
- 2. C₁ = ρu
- 3. X = 0
- $4. \quad \triangle X = 0$
- 5. Calculate $\left(\frac{\Delta \alpha}{\Delta X}\right)_{X=0}$
- 6. Calculate $\left(\frac{\Delta \alpha}{\Delta X}\right)$
- 7. Provided $\frac{\Delta \alpha}{\Delta X} < 0.01 \left(\frac{\Delta \alpha}{\Delta X}\right)_{X=0}$, write output and go to (1.)
- 8. $T_L = T$
- 9. $T_R = T + \Delta T$
- 10. Calculate DH1
- 11. Calculate DHDA
- 12. Iterate on $\Delta\alpha$ until E(K 1) < 0.1 \times 10⁻⁶, where E(K) = $\Delta\alpha$ $\Delta\alpha$ (K)

13.
$$\Delta\alpha(K) = \Delta\alpha(K-1) - E(K-1) \left[\frac{\Delta\alpha(K-1) - \Delta\alpha(K-2)}{E(K-1) - E(K-2)} \right]$$

14.
$$\Delta H = DH_1 + [DHDA] \Delta \alpha(K)$$

15.
$$\Delta u = -\frac{\Delta H}{u}$$

16.
$$u_R = u + \Delta u$$

17.
$$P_R = P + C_1 \Delta u$$

18.
$$\rho_R = \frac{c_1}{u_R}$$

19.
$$\Delta \alpha = \frac{P_R}{\rho_R R T_R} - (1 + \alpha)$$



20.
$$E(K) = \Delta \alpha - \Delta \alpha(K)$$

21.
$$T = T_R$$

22.
$$u = u_R$$

23.
$$\rho = \rho_R$$

24.
$$\alpha = \alpha + \Delta \alpha$$

25.
$$\Delta X = \frac{\Delta \alpha}{(\Delta \alpha / \Delta X)}$$

26.
$$X = X + \Delta X$$

- 27. Write outputs (X, $\frac{\Delta\alpha}{\Delta X}$, α , P, ρ , T, u.)
- 28. Return to statement 6.

Again, Scatran language was employed in the detailed program.



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1. ORIGINATING ACTIVITY (Corporate author)	2 a RE	PORT SECURITY CLASSIFICATION		
The Ohio State University		Unclassified		
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Columbus, Ohio		N/A		
3. REPORT TITLE				
Similitude for Normal Shock Waves in	n Non-Equilibrium Fl	.ows		
4. DESCRIPTIVE NOTES (Type of report and inclusive dates)				
5. AUTHOR(5) (Last name, first name, initial)				
Thomas, R. E., Brooke, D., Petrie, S	ь. L.			
6. REPORT DATE	7# TOTAL NO. OF PAGES	7b. NO. OF REFS		
October 1965	39	20		
8a. CONTRACT OR GRANT NO.	Sa. ORIGINATOR'S REPORT	NUMBER(S)		
AF 33(657)-10416	M1	N. 5		
b. PROJECT NO.	Technical	. No• 5		
1426 c. Task No.	95. OTHER REPORT NO(S) (Any other numbers that may be sasigned		
142604	_			
d.	AFFDL-TR-65-91			
10. A VAIL ABILITY/LIMITATION NOTICES	, , , , , , , , , , , , , , , , , , , ,			
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Similarity parameters are developed which govern the length of nonequilibrium zones behind normal shock waves. Non-equilibrium effects produced by both vibrational relaxation and dissociation are considered. The parameters can also account for arbitrary levels of free-stream vibrational energy or dissociation level.

The validity of the parameters is examined using numerical computations of the properties of the non-equilibrium fields. These computations are made with the aid of experimentally based rate expressions.

The parameters, when written in a form describing the variation of non-equilibrium zone length with Mach number, are shown to have acceptable accuracy.

DD 150RM 1473

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14. KEY WORDS	LINKA		LINK B		LINK C		
	RET WORDS	ROLE	WT	ROLE	WT	ROLE	wT
	NON-EQUILIBRIUM SIMILITUDE VIBRATIONAL NON-EQUILIBRIUM DISSOCIATION NON-EQUILIBRIUM NORMAL SHOCK WAVES						
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