A METHOD FOR COMPUTING NONEQUILIBRIUM CHANNEL FLOW OF A MULTICOMPONENT GASEOUS MIXTURE IN THE NEAR-EQUILIBRIUM REGION

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SUMMARY

A method for computing one-dimensional, steady, nonequilibrium channel flow of an arbitrary mixture of diatomic and monatomic gases is presented. The method assumes the chemical and vibrational nonequilibrium rate processes are not coupled. The numerical formulation permits accurate evaluation of all variables appearing in the rate equations, and it precludes the necessity for computing expressions which become indeterminate in the near-equilibrium region.

INTRODUCTION

The flow of a multicomponent gaseous mixture which is influenced by thermochemical nonequilibrium has proven to be difficult to predict in the near-equilibrium region. In the analysis of a flow of this kind, the equations which describe the fluid dynamical processes must be solved simultaneously with equations which describe the nonequilibrium rate processes. These rate equations take the form of a coupled system of nonlinear differential equations, and in order to proceed toward a prediction of the flow, it is necessary to use numerical methods.

A numerical solution of the equations that govern the flow is possible in principle, but has not been demonstrated to be practical for all cases that may arise. Early investigators found excessive amounts of computation necessary in order to achieve numerical stability in the near-equilibrium regions (refs. 1, 2, 3). The instability arises in part from the necessity for evaluating expressions which, as equilibrium is approached, become indeterminate in the sense that their straightforward calculation leads to large numerical errors. Several methods (refs. 4, 5, 6) that have been of practical value were devised for the approximate numerical integration of such so-called "stiff equations," although they did not entirely remove the underlying cause of the difficulties. In these early studies, the interest was centered primarily on the physics of the problem, and the numerical difficulties were regarded as an inconvenience.

Recently, three new methods have appeared that greatly reduce the computing time in the near-equilibrium regions of the flow (refs. 7, 8, 9). These later papers indicate a growing interest in the mathematical problem which, evidently, has not been solved satisfactorily.
The nature of the problem may be defined by recalling that regions requiring special treatment are frequently encountered in numerical calculations. These are usually regions in which some physical quantity approaches an asymptotic value. A standard remedy is to find a closed-form solution of a simplified set of equations that apply in the asymptotic region. A difficulty at first appears to preclude the use of this device in the present problem. The trouble arises from the fact that the equations are nonlinear over extensive near-equilibrium regions so that a closed-form solution cannot be found. The method, however, can be applied if the equations are linearized independently in each small step of the numerical calculation, as was done by Moretti (ref. 8). At first, it appears unwieldy to incorporate such a procedure in a numerical integration program, but the resulting reduction in computing time gives good reason to do so (refs. 8, 9, 10). Also, such a linearization procedure provides the only method available at present for computing accurately the so-called reaction variables that appear in the rate equations.

The present method differs from that of Moretti (ref. 8) in that accurate evaluation of the reaction variables is included. To accomplish this, considerable manipulation of the original rate equations is necessary. However, upon completion of these steps, a system of equations is obtained that applies for equilibrium, near-equilibrium, or nonequilibrium flows. The method to be presented is based on the requirement that means be found for computing, as accurately as might be specified, all quantities appearing in the equations. This requirement was previously employed in conjunction with a simplified model for air (ref. 10) and has been discussed in connection with more general reacting systems (ref. 11).

Specifically, this report contains a method for computing one-dimensional, steady, nonequilibrium channel flow. The method pertains to an arbitrary multicomponent mixture of ideal diatomic and monatomic gases, free from transport effects and from interaction between the chemical and vibrational nonequilibrium rate processes. The numerical formulation makes unnecessary the computation of expressions which become numerically indeterminate in the near-equilibrium region, but it requires the solution of an eigenvalue problem at each field point of the one-dimensional flow.

The numerical difficulties inherent to calculating the eigenvalues of an arbitrary matrix are well known. However, with the numerical formulation of this report, the matrix in question is similar, at every field point, to a real symmetric matrix which is easily constructed. This fact is used to greatly simplify the computational problem.

**SYMBOLS**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>matrix of coefficients (see eq. (A1))</td>
</tr>
<tr>
<td>$A^{-1}$</td>
<td>inverse of matrix A</td>
</tr>
<tr>
<td>$A^T$</td>
<td>transpose of matrix A</td>
</tr>
</tbody>
</table>
A(x)  cross-sectional area of the channel at point x
D(t)  diagonal matrix with diagonal elements $e^{-\lambda_it}$ ($i = 1, 2, \ldots, r$)
D_i(t)  diagonal matrix with diagonal elements $\frac{1}{\lambda_i}$ ($i = 1, 2, \ldots, r$)
E  matrix whose column vectors are the eigenvectors of matrix $A$
e_{Dj}  energy of dissociation per mole of species $j$
e_j  internal energy per mole of species $j$
\tilde{e}_j  combined rotational, electronic, and translational energies per mole of species $j$
e_v  vibrational energy per mole of a given species
\overline{\ne}_v(T)  equilibrium vibrational energy per mole of a given species at temperature $T$
\ne_{vj}  vibrational energy per mole of species $j$
f  natural vibrational frequency for a given molecular species assuming it is a classical harmonic oscillator
H  matrix (see eq. (38c))
h  enthalpy per unit mass of the gas mixture
h_{ij}  element in the $i$th row and $j$th column of the matrix $H$
(see eq. (38c))
h_0  Planck's constant
I  identity matrix
k  Boltzmann's constant
k_{bi}  backward rate coefficient of the $i$th reaction
k_{fi}  forward rate coefficient of the $i$th reaction
K_i(T)  equilibrium constant of the $i$th reaction
k_{n,n+1}  probability that a molecule vibrating in the $n$th energy level will make a transition to the $(n + 1)$th level in unit time
M  matrix (see eq. (38b))
M_j  chemical formula of species $j$
m_{ij}  element in the $i$th row and $j$th column of matrix $M$
\( N_0 \)  
Avogadro's number

\( n_{kj} \)  
total number of atoms of element \( k \) in species \( j \)

\( p \)  
pressure

\( Q_{ij} \)  
rate of production of species \( M_j \) by the \( i \)th reaction per unit volume

\( R \)  
universal gas constant

\( r \)  
number of chemical reactions

\( s \)  
number of chemical species

\( T \)  
temperature

\( t \)  
time

\( U \)  
see equation (27) and explanation thereafter

\( u \)  
speed of flow

\( V \)  
see equation (27) and explanation thereafter

\( x \)  
distance along the axis of the channel

\( \alpha_i \)  
constant appearing in equation (40)

\( \beta_i \)  
integer equal to \( v_{i}' - v_i \)

\( \beta_{ij} \)  
integer equal to \( v_{ij}' - v_{ij} \)

\( \gamma_j \)  
concentration of the \( j \)th species in moles per unit mass of the gas mixture

\( \Delta e_{vj} \)  
increment in \( e_{vj} \) during the interval \( \Delta t \)

\( \Delta T \)  
increment in \( T \) during the interval \( \Delta t \)

\( \Delta t \)  
incremental interval of time

\( \Delta y_j \)  
increment in \( y_j \) during the interval \( \Delta t \)

\( \Delta \rho \)  
increment in \( \rho \) during the interval \( \Delta t \)

\( \Delta x_i \)  
increment in \( X_i \) during the interval \( \Delta t \)

\( \epsilon_n \)  
energy of the \( n \)th vibrational level of a molecule

\( A \)  
diagonal matrix whose elements are the eigenvalues of the matrix \( A \)
\[ \lambda_i \] \text{ith eigenvalue of the matrix } A \\
\[ \mu_n \] \text{number of molecules of a given species which are in the } n\text{th vibrational energy level} \\
\[ v_i \] \text{integer equal to } \sum_{j=1}^{s} v_{ij} \\
\[ v_i' \] \text{integer equal to } \sum_{j=1}^{s} v_{ij}' \\
\[ v_{ij} \] \text{stoichiometric coefficient of species } M_j \text{ on the left side of chemical equation } i \\
\[ v_{ij}' \] \text{stoichiometric coefficient of species } M_j \text{ on the right side of chemical equation } i \\
\[ \rho \] \text{density of gas mixture} \\
\[ \sigma \] \text{sum of all species concentration coefficients, } \gamma_j \ (j = 1, 2, \ldots, s) \\
\[ \tau_j \] \text{vibrational relaxation time for the } j\text{th species} \\
\[ \chi_i \] \text{reaction variable (see eq. (5))} \\
\[ \vec{\chi} \] \text{column vector whose elements are } \chi_i \ (i = 1, 2, \ldots, r) \\

\text{Subscript} \\
(\quad)_0 \text{used to indicate the numerical value of the quantity taken at the beginning of the interval } \Delta t \\

\text{ANALYSIS} \\

Although they have been developed elsewhere, the basic equations for non-equilibrium channel flow will be derived here. This derivation will provide a background for the numerical method used in their solution. \\

\text{Chemical Rate Equations} \\

It is assumed that \( s \) chemical species, \( M_j \ (j = 1, 2, \ldots, s) \) are involved in \( r \) chemical equations. These equations are represented by
\[
\sum_{j=1}^{S} v_{ij} M_j \stackrel{k_{fi}}{\Rightarrow} \sum_{j=1}^{S} v_{ij}' M_j \quad (i = 1, 2, \ldots, r)
\]

where \( v_{ij} \) and \( v_{ij}' \) are stoichiometric coefficients, the \( M_j \) are the chemical formulas of the species, and \( k_{fi} \) and \( k_{bi} \) are the forward and backward rate coefficients, respectively, of the \( i \)th reaction.

The \( i \)th reaction produces a quantity of species \( M_j \) at the rate \( Q_{ij} \) (moles/unit volume/unit time). For a fluid without gradients of concentration, pressure, or temperature, the law of mass action leads to the following expression for \( Q_{ij} \)

\[
Q_{ij} = \beta_{ij}(k_{fi} \rho \prod_{j=1}^{S} y_{ij} - k_{bi} \rho \prod_{j=1}^{S} y_{ij}')
\]

In this equation, \( y_j \) (moles/unit mass) is the molar concentration of species \( M_j \) (\( j = 1, 2, \ldots, s \)), \( \rho \) is the fluid density, and

\[
v_i = \sum_{j=1}^{S} v_{ij}, \quad v_i' = \sum_{j=1}^{S} v_{ij}', \quad \text{and} \quad \beta_{ij} = v_{ij}' - v_{ij}
\]

It is assumed that equation (2) holds for a flowing gas.

The equilibrium constant for concentrations of the \( i \)th reaction, \( K_i(T) \) is a known function of the temperature, \( T \), and at equilibrium,

\[
K_i(T) = \frac{k_{fi}(T)}{k_{bi}(T)} \quad (i = 1, 2, \ldots, r)
\]

It will be assumed that this relationship holds when the reaction is not in equilibrium as well.

The total rate of change of \( y_j \) is given by

\[
\rho \frac{dy_j}{dt} = \sum_{i=1}^{r} Q_{ij} \quad (j = 1, 2, \ldots, s)
\]
Thus
\[
\rho \frac{d\gamma_j}{dt} = \sum_{i=1}^{r} \beta_{ij} \left( k_{fi} \rho \prod_{l=1}^{s} \gamma_{il} - k_{bi} \rho \prod_{l=1}^{s} \gamma_{il} \right) (j = 1, 2, \ldots, s)
\]  
(3)

These equations can be written
\[
\frac{d\gamma_j}{dt} = \sum_{i=1}^{r} \beta_{ij} k_{fi} \rho^{v_{i-1}} \left( \prod_{l=1}^{s} \gamma_{il} \right) \gamma_i (j = 1, 2, \ldots, s)
\]  
(4)

where the dimensionless variables \( \chi_i \) are defined by
\[
\chi_i = 1 - \frac{1}{k_i(T)} \rho^{\beta_i} \prod_{l=1}^{s} \gamma_{il} \quad (i = 1, 2, \ldots, r)
\]  
(5)

and \( \beta_i = v_i - v_1 \). (See ref. 3.) In near-equilibrium regions, the \( \chi_i \) approach zero, and they cannot be computed accurately from equations (5). Their accurate evaluation is essential if equations (4) are to be used, since the \( \frac{d\gamma_j}{dt} \) cannot be set equal to zero in near-equilibrium regions. In the method to be developed here, equations (4) will not be evaluated numerically, but the method is capable of producing accurate values of the \( \chi_i \) if they are desired. When equations (5) are differentiated with respect to time, there is obtained a set of relations between the \( \chi_i \) \( (i = 1, 2, \ldots, r) \), the \( \gamma_j \) \( (j = 1, 2, \ldots, s) \), and the fluid dynamics variables \( \rho \) and \( T \).

\[
\frac{d\chi_i}{dt} = -\frac{1}{k_i(T)} \rho ^{\beta_i} \sum_{l=1}^{s} \left( \frac{\beta_{il}}{\gamma_l} \right) \left( \frac{d\gamma_l}{dt} \right) \left( \prod_{l=1}^{s} \gamma_{il} \right)
\]

\[
- \frac{1}{k_i^2(T)} \left( -\frac{dK_i}{dT} \right) \left( \frac{dT}{dt} \right) \rho^{\beta_i} \prod_{l=1}^{s} \gamma_{il}
\]

\[
- \frac{1}{k_i(T)} \rho^{\beta_i} \prod_{l=1}^{s} \gamma_{il} \left( \frac{\beta_{il}}{\rho} \right) \left( \frac{d\rho}{dt} \right) (i = 1, 2, \ldots, r)
\]  
(6)

Equations (6) are useful because they contain no forms which become indeterminate at some point in the flow field, including the near-equilibrium region.
Equations (4), (5), and (6) can be combined to obtain another set of equations which will also be used in the computation of the flow.

\[
\frac{dX_i}{dt} = - \sum_{l=1}^{r} a_{il} X_i + F(T, X_i) \frac{dT}{dt} + G(\rho, X_i) \frac{d\rho}{dt} \quad (i = 1, 2, \ldots, r) \tag{7}
\]

where

\[
a_{il} = (1 - X_i) \left( \sum_{j=1}^{s} \frac{\beta_{ij} \beta_{lj}}{\gamma_j} \right) \left( \frac{1}{H_{ij}} \sum_{j=1}^{s} \frac{\gamma_j}{\rho} \right) \quad (i = 1, 2, \ldots, r)
\]

and

\[
F(T, X_i) = (1 - X_i) \left( \frac{1}{K_{i}(T)} \right) \left( \frac{dK_i}{dT} \right) \quad (i = 1, 2, \ldots, r)
\]

\[
G(\rho, X_i) = (X_i - 1) \left( \frac{\beta_{i}}{\rho} \right) \quad (i = 1, 2, \ldots, r)
\]

**Vibrational Rate Equations**

It is assumed that the molecules of the gaseous mixture are free to vibrate only at a discrete set of energy levels

\[
\varepsilon_n = \left( n + \frac{1}{2} \right) h_0 f \quad (n = 0, 1, 2, \ldots)
\]

where \( h_0 \) is Planck's constant and \( f \) is the natural frequency for the species in question assuming it is a classical harmonic oscillator. It is further assumed that changes in energy can occur only between adjacent levels.

The probability that a molecule vibrating in the \( n \)th level will make a transition to the \((n + 1)\)th level in a unit time is designated by \( k_{n,n+1} \). With this notation, \( k_{0,1} \) and \( k_{1,0} \) are the probabilities of excitation and de-excitation per unit time, respectively, between the ground state and the first excited energy level. Let \( \mu_n \) be the number of molecules in the \( n \)th vibrational energy level. Then

\[
\frac{d\mu_n}{dt} = k_{n-1,n}\mu_{n-1} - k_{n,n-1}\mu_n + k_{n+1,n}\mu_{n+1} - k_n,n+1\mu_n \tag{8}
\]
In reference 12 it is developed that

\[ k_{0,1} = k_{1,0} \exp \left( \frac{-\hbar \omega_f}{kT} \right) \]  \hspace{1cm} (9)

where \( k \) is the Boltzmann constant. For other energy levels

\[ k_{n,n+1} = k_{n+1,n} \exp \left( \frac{-\hbar \omega_f}{kT} \right) \]

and from the quantum-mechanical study of transition probabilities

\[ k_{n,n-1} = nk_{1,0} \]  \hspace{1cm} (10)

If equation (8) is combined with equations (9) and (10), it is possible to obtain

\[ \frac{d\mu_n}{dt} = k_{1,0} \left\{ (n + 1)\mu_{n+1} - n\mu_n + \left[ \exp \left( \frac{-\hbar \omega_f}{kT} \right) \right] \left[ n\mu_{n-1} - (n + 1)\mu_n \right] \right\} \]  \hspace{1cm} (11)

Let \( N_0 \) be Avogadro's number, and

\[ N = \sum_{n=0}^{\infty} \mu_n \]

If \( e_v \) is used to denote the vibrational energy above the ground \((n = 0)\) state of a given species, per mole of species

\[ e_v = \frac{N_0}{N} \sum_{n=0}^{\infty} e_n\mu_n = \frac{N_0 \hbar \omega_f}{N} \sum_{n=0}^{\infty} n\mu_n \]

Therefore

\[ \frac{de_v}{dt} = \frac{N_0 \hbar \omega_f}{N} \sum_{n=1}^{\infty} n \frac{d\mu_n}{dt} \]

When equation (11) is combined with this last equation, it is possible to manipulate the resulting expression into the form.
The expression

\[ \tilde{E}_V(T) = \frac{N_0 h_0 f}{\exp\left(\frac{-h_0 f}{kT}\right) - 1} \]

is defined to be the vibrational energy, per mole of species, corresponding to equilibrium conditions at temperature \( T \). Also, the relaxation time, \( \tau \), is defined by the relation

\[ \frac{1}{\tau} = k_{1,0} \left[ 1 - \exp\left(\frac{-h_0 f}{kT}\right) \right] \]

With these definitions, equation (12) can be written in a more compact form.

\[ \frac{de_v}{dt} = \frac{[\tilde{E}_V(T) - e_v]}{\tau} \] (14)

Since \( k_{1,0} \) is a function of density, temperature, and chemical species, \( \tau \) is a function of these variables. It is customary to write, for the \( j \)th chemical species, the vibrational nonequilibrium equations in the form

\[ \frac{de_{v_j}}{dt} = \frac{[\tilde{E}_{V_j}(T) - e_{v_j}]}{\tau_j(\rho, T)} \quad (j = 1, 2, \ldots, s) \] (15)

The vibrational energy of species \( j \) is related to the total internal energy per mole, \( e_J \), of species \( j \) by the equation

\[ e_J = \tilde{e}_J + e_{v_j} + e_{Dj} \] (16)

where \( \tilde{e}_J(T) \) is a function of temperature which expresses the rotational, electronic, and translational energies per mole of species \( j \). The term \( e_{Dj} \), a constant, is the energy of dissociation per mole of species \( j \).
Fluid Dynamical Equations

Since the flow under consideration is to be one-dimensional and steady, all quantities used in its description are functions of a single independent variable. The channel is presumed to be described by some function of \( x \), the distance along the axis of the channel from some fixed point. However, the flow variables will be considered as functions of time, \( t \). In the conservation equations which follow, the speed of the flow is represented by \( u \), the pressure by \( p \), the cross-sectional area of the channel by \( A \), and the enthalpy per unit mass by \( h \). The conservation equations are

\[
\text{Mass} \quad \rho u A = c_1 \tag{17}
\]

\[
\text{Energy} \quad \frac{1}{2} u^2 + h = c_2 \tag{18}
\]

\[
\text{Momentum} \quad \frac{1}{2} u^2 + \int \frac{dp}{\rho} = c_3 \tag{19}
\]

The numbers \( c_1, c_2, \) and \( c_3 \) are constants of integration.

It is assumed that either a function \( A(x) \) or a function \( p(x) \) is given. When \( A(x) \) is given, the cross-sectional area of the channel is prescribed; when \( p(x) \) is given, the pressure is a known function along the channel.

For a mixture of gases composed of \( s \) species, the thermal equation of state is

\[
p = \left( \sum_{j=1}^{s} \gamma_j \right) \rho \mathcal{R} T
\]

In this equation, \( \mathcal{R} \) is the universal gas constant. In later equations, the notation

\[
\sum_{j=1}^{s} \gamma_j = \sigma
\]

will be used. Thus

\[
p = \sigma \rho \mathcal{R} T
\]

By differentiating equation (21) with respect to time, and using

\[
\frac{d}{dt} = \frac{dx}{dt} \frac{d}{dx} = u \frac{d}{dx}
\]
it is found that

\[ \frac{uT}{p} \frac{dp}{dx} = \frac{dT}{dt} + \frac{T}{\rho} \frac{dp}{dt} + \frac{T}{\sigma} \sum_{j=1}^{s} \frac{dy_j}{dt} \]  \tag{22} 

Equation (22) is useful when \( p(x) \) is specified. When \( A(x) \) is given instead, equation (22) can be adapted by using the equations for conservation of mass and momentum. To this end, the conservation of mass equation can be written

\[ (uA) \frac{dp}{dt} + (\rho A) \frac{du}{dt} + (\rho u) \frac{dA}{dt} = 0 \]  \tag{23} 

and from the conservation of momentum

\[ u \frac{du}{dx} + \frac{1}{\rho} \frac{dp}{dx} = 0 \]

or

\[ \frac{du}{dt} = - \frac{1}{\rho} \frac{dp}{dx} \]  \tag{24} 

When equations (23) and (24) are combined, there is obtained

\[ \frac{dp}{dx} = u \frac{dp}{dt} + \frac{\rho u^2}{A} \frac{dA}{dx} \]  \tag{25} 

Finally, by substituting the right side of equation (25) for \( \frac{dp}{dx} \) in equation (22), it is seen that

\[ \frac{u^2}{AR\sigma} \frac{dA}{dx} = \frac{dT}{dt} + \frac{T}{\rho} \left( 1 - \frac{u^2}{\rho} \right) \frac{dp}{dt} + \frac{T}{\sigma} \sum_{j=1}^{s} \frac{dy_j}{dt} \]  \tag{26} 

This equation will be useful when \( A(x) \) is specified.

In general

\[ \frac{dT}{dt} + \frac{T}{\rho} U \frac{dp}{dt} + \frac{T}{\sigma} \sum_{j=1}^{s} \frac{dy_j}{dt} = V \]  \tag{27} 

When \( A(x) \) is specified, \( U = [1 - (u^2/\rho T)] \) and \( V = (u^3/AR\sigma)(dA/dx) \). When \( p(x) \) is specified, \( U = 1 \) and \( V = (uT/p)(dp/dx) \).
Equation (27) is one of the two fluid dynamical equations which will be used in the numerical solution of the nonequilibrium flow. The other such relation is derived from the equations for conservation of energy and momentum.

The specific enthalpy, \( h \), is given by

\[
h = e + \frac{p}{\rho}
\]

For a mixture of \( s \) chemical species, the internal energy, \( e \), per unit mass is

\[
e = \sum_{j=1}^{s} \gamma_j e_j
\]

Therefore

\[
h = \sum_{j=1}^{s} \gamma_j e_j + \frac{p}{\rho}
\] (28)

When this equation is differentiated with respect to time, there is obtained

\[
\frac{dh}{dt} = \sum_{j=1}^{s} \gamma_j \frac{de_j}{dt} + \frac{1}{\rho} \frac{dp}{dt} - \frac{\sigma RT}{\rho} \frac{dp}{dt}
\] (29)

When the equations for the conservation of energy and momentum are differentiated and then combined, it is possible to show that

\[
\frac{dh}{dt} = \frac{1}{\rho} \frac{dp}{dt}
\] (30)

From equation (16),

\[
\frac{de_j}{dt} = \frac{d\tilde{e}_j}{dt} + \frac{de_{v_j}}{dt} \quad (j = 1, 2, \ldots, s)
\]

and since \( d\tilde{e}_j/dT \) is a known function of \( T \), it is convenient to write

\[
\frac{de_j}{dt} = \frac{d\tilde{e}_j}{dT} \frac{dT}{dt} + \frac{de_{v_j}}{dt} \quad (j = 1, 2, \ldots, s)
\] (31)
When equations (29), (30), and (31) are combined, there results

\[
\left( \sum_{j=1}^{s} \gamma_j \frac{d\tilde{e}_j}{dT} \right) \frac{dT}{dt} + \sum_{j=1}^{s} \gamma_j \frac{d\nu_j}{dt} + \sum_{j=1}^{s} \epsilon_j \frac{d\nu_j}{dt} - \frac{\sigma R T}{\rho} \frac{d\rho}{dt} = 0 \quad (32)
\]

Equation (32) together with equation (27) will be used with the equations of the nonequilibrium rate processes in the numerical procedure which is to be described.

**NUMERICAL PROCEDURE**

For one-dimensional channel flow, the field points can be stationed along a line which extends the length of the channel. The variables \( \rho, T, \gamma_j, \) and \( \nu_j (j = 1, 2, \ldots, s) \) from which all other flow variables can be obtained must be computed at each of these stations.

As a fluid element moves downstream from one station to the next, an interval of time \( \Delta t \) elapses, and there are corresponding increments \( \Delta \rho, \Delta T, \Delta \gamma_j, \) and \( \Delta \nu_j. \) Let it be assumed that the fluid element is at a given station at time \( t_0 \) and at the next downstream station at time \( (t_0 + \Delta t). \) Then

\[
\begin{align*}
\rho(t_0 + \Delta t) &= \rho(t_0) + \Delta \rho \\
T(t_0 + \Delta t) &= T(t_0) + \Delta T \\
\gamma_j(t_0 + \Delta t) &= \gamma_j(t_0) + \Delta \gamma_j \quad (j = 1, 2, \ldots, s) \\
\nu_j(t_0 + \Delta t) &= \nu_j(t_0) + \Delta \nu_j \quad (j = 1, 2, \ldots, s)
\end{align*}
\]

The computational problem is to find numerical values for the increments \( \Delta \rho, \Delta T, \Delta \gamma_j, \) and \( \Delta \nu_j \) when numerical values of the flow variables are known at the upstream station. Since values for all quantities are assumed known at the beginning of the interval \( (t_0, t_0 + \Delta t), \) there is no loss in generality in taking \( t_0 = 0 \) and denoting values at the beginning of the interval by the subscript \( 0. \) Thus

\[
\begin{align*}
\rho(\Delta t) &= \rho_0 + \Delta \rho \\
T(\Delta t) &= T_0 + \Delta T \\
\gamma_j(\Delta t) &= (\gamma_j)_0 + \Delta \gamma_j \quad (j = 1, 2, \ldots, s) \\
\nu_j(\Delta t) &= (\nu_j)_0 + \Delta \nu_j \quad (j = 1, 2, \ldots, s)
\end{align*}
\]
Computation of the Increments $\Delta \varepsilon_{vj}$

As a consequence of the assumption that vibrational and chemical relaxation rates are not coupled, an expression for the $\Delta \varepsilon_{vj}$ ($j = 1, 2, \ldots, s$) can be found independently of the increments $\Delta y_j$. Since $\rho$ and $T$ are functions of time, equations (1.5) can be written

$$
\frac{d \varepsilon_{vj}}{dt} = \frac{(\bar{\varepsilon}_{vj} - \varepsilon_{vj})_o}{(\tau_j)_o} \quad (j = 1, 2, \ldots, s)
$$

It might be presumed, then, that the increment $\Delta \varepsilon_{vj}$ could be computed from

$$
\Delta \varepsilon_{vj} = \left[\frac{(\bar{\varepsilon}_{vj} - \varepsilon_{vj})_o}{(\tau_j)_o}\right] \Delta t \quad (j = 1, 2, \ldots, s)
$$

However, use of these equations are not practical because of the behavior of the right-hand side in the near-equilibrium region of the flow. In the near-equilibrium region, $1/\tau_j$ is very large while $(\bar{\varepsilon}_{vj} - \varepsilon_{vj})$ is very small. This makes an accurate evaluation of $\Delta \varepsilon_{vj}$ impossible even for small $\Delta t$. Apart from this, the use of $(\bar{\varepsilon}_{vj} - \varepsilon_{vj})_o$ over the entire interval, $\Delta t$, is of questionable validity. The quantities $\tau_j$, $\bar{\varepsilon}_{vj}$, and $\varepsilon_{vj}$ can be described as slowly varying in the near-equilibrium region, because their change during a short-time interval is small enough that their value during the interval can be approximated by a constant. On the other hand, $(\bar{\varepsilon}_{vj} - \varepsilon_{vj})$ can change by several times its own magnitude during a small interval of time when the upstream station is in the near-equilibrium region.

A means of avoiding these numerical difficulties is provided by the behavior of $\bar{\varepsilon}_{vj}$. Since it is a slowly varying function, $d\bar{\varepsilon}_{vj}/dt$ can be considered constant over an interval $\Delta t$. Likewise, $\tau_j$ can be considered constant over the interval.

With this in mind, the following equations are derived from equations (15).

$$
\frac{d \bar{\varepsilon}_{vj}}{dt} - \frac{d \varepsilon_{vj}}{dt} = -\left(\frac{\bar{\varepsilon}_{vj} - \varepsilon_{vj}}{\tau_j}\right) + \frac{d \bar{\varepsilon}_{vj}}{dt} \quad (j = 1, 2, \ldots, s)
$$

These can also be written

$$
\frac{d}{dt} (\bar{\varepsilon}_{vj} - \varepsilon_{vj}) = -\frac{1}{\tau_j} (\bar{\varepsilon}_{vj} - \varepsilon_{vj}) + \frac{d \bar{\varepsilon}_{vj}}{dt} \quad (j = 1, 2, \ldots, s) \quad (33)
$$

Over the interval $\Delta t$, $\tau_j = (\tau_j)_o$ and

$$
\frac{d \bar{\varepsilon}_{vj}}{dt} = \frac{\Delta \bar{\varepsilon}_{vj}}{\Delta t}
$$
Hence, over this interval, equations (33) become linear differential equations with constant coefficients. Their solution is found to be

\[
[\bar{e}_{vj}(t) - e_{vj}(t)] = \frac{\Delta \bar{e}_{vj}}{\Delta t} (\tau_j)_0 + \left[ (\bar{e}_{vj} - e_{vj})_0 - (\tau_j)_0 \right] \frac{\Delta \bar{e}_{vj}}{\Delta t} \left\{ \exp \left[ - \frac{t}{(\tau_j)_0} \right] \right\}
\]

\( j = 1, 2, \ldots, s \)

where \( 0 \leq t \leq \Delta t \). From this solution, the increment in \((\bar{e}_{vj} - e_{vj})\) corresponding to \( \Delta t \) can be found

\[
\Delta(\bar{e}_{vj} - e_{vj}) = \left\{ \exp \left[ - \frac{\Delta t}{(\tau_j)_0} \right] - 1 \right\} \left[ (\bar{e}_{vj} - e_{vj})_0 - (\tau_j)_0 \frac{\Delta \bar{e}_{vj}}{\Delta t} \right]
\]

\( j = 1, 2, \ldots, s \) \hspace{1cm} (34a)

Equations (34a) show that as \((\tau_j)_0 \to 0\) (equilibrium is approached), the increments \(\Delta(\bar{e}_{vj} - e_{vj}) \to (\bar{e}_{vj} - e_{vj})_0\). There is no difficulty in computing these increments in the near-equilibrium region by means of equations (34a).

The increments \(\Delta e_{vj}\) can now be determined accurately.

\[
\Delta e_{vj} = \Delta \bar{e}_{vj} - (\bar{e}_{vj} - e_{vj}) \quad (j = 1, 2, \ldots, s)
\]

and

\[
\Delta \bar{e}_{vj} = \left( \frac{d \bar{e}_{vj}}{dT} \right)_0 (\Delta T) = \left( \frac{d \bar{e}_{vj}}{dT} \right)_0 \Delta T \quad (j = 1, 2, \ldots, s)
\]

These last two sets of equations are combined with equations (34a) to give

\[
\Delta e_{vj} = \left( \frac{d \bar{e}_{vj}}{dT} \right)_0 \Delta T - \left\{ \exp \left[ - \frac{\Delta t}{(\tau_j)_0} \right] - 1 \right\} \left[ (\bar{e}_{vj} - e_{vj})_0 - \frac{1}{(\tau_j)_0} \left( \frac{d \bar{e}_{vj}}{dT} \right)_0 \Delta T \right]
\]

\( j = 1, 2, \ldots, s \) \hspace{1cm} (34b)

\textbf{Computation of the Increments } \Delta X_i

When the increments \(\Delta e_{vj}\) \((j = 1, 2, \ldots, s)\) have been found by the method just outlined, there remain the \((s + 2)\) increments \(\Delta \rho, \Delta T, \text{ and } \Delta y_j\) \((j = 1, 2, \ldots, s)\) yet to be computed. These will be found by solving a system of \((s + 2)\) linear equations in which the variables are the \((s + 2)\) increments in question. However, these equations contain the increments \(\Delta X_i\) \((i = 1, 2, \ldots, r)\) taken by the variables \(X_i\) during the interval \(\Delta t\). It will be shown that upon solution of an eigenvalue problem, each \(\Delta X_i\) becomes a linear function of \(\Delta \rho\) and \(\Delta T\).
The variables \( X_i \) \((i = 1, 2, \ldots, r)\) satisfy the coupled system of rate equations (7)

\[
\frac{dX_i}{dt} = - \sum_{l=1}^{r} a_{il} X_l + F(T, X_i) \frac{dT}{dt} + G(\rho, X_i) \frac{d\rho}{dt}
\]

where

\[
a_{il} = (1 - X_i) \left( \sum_{j=1}^{s} \frac{\beta_{ij} \beta_{lj}}{\gamma_j} \right) \left( k_{fi}^{0} \alpha \sum_{j=1}^{s} \gamma_j \right) \quad (i = 1, 2, \ldots, r)
\]

\[
F(T, X_i) = (1 - X_i) \left[ \frac{1}{K_i(T)} \right] \left( \frac{dK_i}{dT} \right)
\]

\[
G(\rho, X_i) = -(1 - X_i) \left( \frac{\beta_i}{\rho} \right)
\]

With the exception of \( X_i \) itself, all the variables which appear in the coefficients \( a_{il} \), \( F(T, X_i) \), and \( G(\rho, X_i) \) are assumed to be slowly varying in the sense that they change by only a small percentage of their magnitude during an interval \( \Delta t \). Hence, they will be approximated by a constant value over this interval. In the near-equilibrium region, however, the variables \( X_i \) \((i = 1, 2, \ldots, r)\) can change by several times their own magnitude during the interval. This magnitude must be small because \( X_i \rightarrow 0 \) as equilibrium is approached. However, in any region of channel flow, including the near-equilibrium region, \((1 - X_i)\) can change by only a small percentage of its value during a small interval of time.

This fact allows the coupled, first-order system, equations (7), to be "linearized" by taking the coefficients to be constant over the interval \( \Delta t \). Equations (7) are then written

\[
\frac{dX_i}{dt} = - \sum_{l=1}^{r} (a_{il})_o X_l + [F(T, X_i)]_o \frac{dT}{\Delta t} + [G(\rho, X_i)]_o \frac{d\rho}{\Delta t}
\]

\((i = 1, 2, \ldots, r) \quad (0 \leq t \leq \Delta t) \quad (35)\)

When the constants \( N_i \) are defined through the equation

\[
N_i = \frac{[F(T, X_i)]_o}{\Delta t} \Delta T + \frac{[G(\rho, X_i)]_o}{\Delta t} \Delta \rho \quad (i = 1, 2, \ldots, r)
\]

the differential equations (35) can be written in vector form

\[
\frac{d\vec{X}}{dt} = -A\vec{X} + \vec{N}
\]

(36)
where

\[
\begin{bmatrix}
X_1 \\
X_2 \\
\vdots \\
X_r
\end{bmatrix}, \quad \begin{bmatrix}
\bar{N}_1 \\
\bar{N}_2 \\
\vdots \\
\bar{N}_r
\end{bmatrix}, \quad \text{and} \quad A = \begin{pmatrix}
(a_{11})_0 & (a_{12})_0 & \cdots & (a_{1r})_0 \\
(a_{21})_0 & (a_{22})_0 & \cdots & (a_{2r})_0 \\
\vdots & \vdots & \ddots & \vdots \\
(a_{r1})_0 & (a_{r2})_0 & \cdots & (a_{rr})_0
\end{pmatrix}
\]

Although numerical values cannot be assigned to \( N_i \) (\( i = 1, 2, \ldots, r \)) until \( \Delta T \) and \( \Delta \rho \) have been found, this must not obscure the fact that each \( N_i \) can be considered to be a constant over the interval \( \Delta t \).

If \( \bar{X}(t) \) is a vector function which satisfies the differential equation (36) such that \( \bar{X}_0 = \bar{X}(0) \), then each \( \Delta \bar{X}_i \) (\( i = 1, 2, \ldots, r \)) is determined by the equation

\[
\Delta \bar{X} = \bar{X}(\Delta t) - \bar{X}(0)
\]

Consequently, a general solution must be found for equation (36).

Toward this end, a transformation will be used to replace equation (36) with an uncoupled system. Theorem 3 in the appendix shows that such a transformation exists. This theorem states that there are eigenvectors, \( \eta_i \) (\( i = 1, 2, \ldots, r \)), of the matrix \( A \) which are linearly independent at every point in the flow. A simplified method for finding the eigenvalues and eigenvectors of \( A \) is provided by theorems 1 and 2 in the appendix.

If \( E \) is the matrix whose \( i \)th column is the eigenvector \( \eta_i \) which corresponds to the eigenvalue \( \lambda_i \) of \( A \), then \( E \) is nonsingular since its column vectors are linearly independent (see ref. 13). Moreover,

\[
A = E \Lambda E^{-1}
\]

where \( \Lambda \) is the diagonal matrix whose diagonal elements are the eigenvalues of \( A \).

\[
\Lambda = \text{diag} (\lambda_1, \lambda_2, \ldots, \lambda_r) = \begin{pmatrix}
\lambda_1 \\
\lambda_2 \\
\vdots \\
\lambda_r
\end{pmatrix}
\]
Equation (36) can be written
\[
\frac{d\vec{x}}{dt} = -(E \Lambda E^{-1})\vec{x} + \vec{N}
\]
or
\[
E^{-1} \frac{d\vec{x}}{dt} = -\Lambda E^{-1}\vec{x} + E^{-1}\vec{N}
\]
Setting \( \vec{\psi} = E^{-1}\vec{x} \) yields
\[
\frac{d\vec{\psi}}{dt} = -\Lambda\vec{\psi} + E^{-1}\vec{N}
\] (37)

Equation (37) is an uncoupled system because \( \Lambda \) is a diagonal matrix of constants.

If \( \vec{\psi}(t) \) is a general solution of equation (37) then
\[
\vec{x}(t) = E\vec{\psi}(t)
\]
is a general solution of equation (36).

The general solution, \( \vec{\psi}(t) \), is found by obtaining a general solution \( \vec{\psi}_h(t) \) of the homogeneous equation
\[
\frac{d\vec{\psi}}{dt} = -\Lambda\vec{\psi}
\]
then adding to it any particular solution, \( \vec{\psi}_p(t) \) of the equation (37).
\[
\vec{\psi}(t) = \vec{\psi}_h(t) + \vec{\psi}_p(t)
\]

The solution, \( \vec{\psi}_h(t) \), of the homogeneous equation is easily verified to be
\[
\vec{\psi}_h(t) = D(t)\vec{c}
\]
where
\[
\vec{c} = \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_r \end{pmatrix} \quad \text{and} \quad D(t) = \begin{pmatrix} e^{-\lambda_1t} & & \\ & e^{-\lambda_2t} & \\ & & \ddots \\ & & & e^{-\lambda_rt} \end{pmatrix}
\]
A particular solution, $\dot{\psi}_p(t)$ of equation (37), can be obtained by solving

$$\dot{\psi} = -A\psi + E^{-1}\dot{N}$$

This gives

$$\dot{\psi}_p = D_1(t)E^{-1}\dot{N}$$

where the diagonal matrix $D_1$ can take two possible forms. If all the eigenvalues of $A$ are nonzero

$$D_1(t) = \Lambda^{-1} = \text{diag}\left(\frac{1}{\lambda_1}, \frac{1}{\lambda_2}, \ldots, \frac{1}{\lambda_r}\right)$$

The possibility that some of the eigenvalues may vanish, however, cannot be excluded. This will happen, for example, when there are more chemical equations than distinct chemical species. Each eigenvalue of $A$ which vanishes must have its reciprocal in $D_1(t)$ replaced by $t$. For example, if the second and $r$th eigenvalues vanish, $D_1(t)$ takes the form

$$D_1(t) = \text{diag}\left(\frac{1}{\lambda_1}, t, \frac{1}{\lambda_3}, \ldots, \frac{1}{\lambda_{r-1}}, t\right)$$

Finally,

$$\dot{\psi}(t) = \dot{\psi}_h(t) + \psi_p(t)
= D(t)\dot{c} + D_1(t)E^{-1}\dot{N}$$

Therefore

$$\dot{x}(t) = [Ed(t)]\dot{c} + [Ed_1(t)E^{-1}]\dot{N}$$

It is possible to determine the constants $C_1, C_2, \ldots, C_r$ from the equation

$$\dot{x}_o = \dot{x}(0) = [Ed(0)]\dot{c} + [Ed_1(0)E^{-1}]\dot{N}$$

From the definition of $D(t)$, it is seen that $D(0) = I$, the identity matrix. Consequently,

$$\dot{c} = E^{-1}\dot{x}_o - [D_1(0)E^{-1}]\dot{N}$$

and this yields

$$\dot{x}(t) = Ed(t)\left[E^{-1}\dot{x}_o - [D_1(0)E^{-1}]\dot{N}\right] + [Ed_1(t)E^{-1}]\dot{N}$$

(38a)

The increments, $\Delta x_i$ ($i = 1, 2, \ldots, r$), for the interval $\Delta t$ are found from

$$\Delta x = \dot{x}(\Delta t) - \dot{x}_o$$
Therefore

\[ \Delta \mathbf{x} = [\mathbf{E} \mathbf{D}(\Delta t) \mathbf{E}^{-1} - \mathbf{I}] \mathbf{x}^0 + [\mathbf{E} \mathbf{D}_1(\Delta t) \mathbf{E}^{-1} - \mathbf{E} \mathbf{D}(\Delta t) \mathbf{D}_1(0) \mathbf{E}^{-1}] \mathbf{x}^N \]

For a fixed value of \( \Delta t \), the diagonal matrices \( \mathbf{D}(\Delta t) \) and \( \mathbf{D}_1(\Delta t) \) become matrices with constant elements. For purposes of notation, let

\[ [\mathbf{E} \mathbf{D}(\Delta t) \mathbf{E}^{-1} - \mathbf{I}] = \mathbf{M} = m_{ij} \quad (i, j = 1, 2, \ldots, r) \quad (38b) \]

and

\[ [\mathbf{E} \mathbf{D}_1(\Delta t) \mathbf{E}^{-1} - \mathbf{E} \mathbf{D}(\Delta t) \mathbf{D}_1(0) \mathbf{E}^{-1}] = \mathbf{H} = h_{ij} \quad (i, j = 1, 2, \ldots, r) \quad (38c) \]

Then

\[ \Delta \mathbf{x} = \mathbf{Mx}^0 + \mathbf{Hx}^N \]

In terms of the increments \( \Delta \rho \) and \( \Delta T \), this is written

\[ \Delta x_i = \sum_{j=1}^{r} m_{ij}(x_j)^0 + \left[ \sum_{j=1}^{r} h_{ij} \frac{F(T, x_j)^0}{\Delta t} \right] \Delta T + \left[ \sum_{j=1}^{r} h_{ij} \frac{G(\rho, x_j)^0}{\Delta t} \right] \Delta \rho \]

\[ (i = 1, 2, \ldots, r) \quad (39) \]

**Computation of the Increments \( \Delta \rho, \Delta T, \text{ and } \Delta \gamma_j \)**

With equations (6) and (39) combined there is obtained

\[ \left[ \frac{1}{K_1(T)} \frac{dK_1}{dT} \right]_o \Delta x_i - \alpha_i \left[ \sum_{l=1}^{s} h_{il} \frac{F(T, x_i)^0}{\Delta t} \right] \Delta T - \left\{ \frac{\beta_{ij}}{\rho} \right\}_o + \alpha_i \left[ \sum_{l=1}^{s} h_{il} \frac{G(\rho, x_i)^0}{\Delta t} \right] \Delta \rho \]

\[ - \sum_{j=1}^{s} \left( \frac{\beta_{ij}}{\gamma_j} \right)_o \Delta \gamma_j = \alpha_i \sum_{l=1}^{r} m_{il}(x_l)^0 \quad (i = 1, 2, \ldots, r) \quad (40) \]

where

\[ \alpha_i = \left[ \frac{K_1(T)}{\rho} \frac{\beta_{1}}{} \right]_o \]

\[ \frac{s}{j=1} \beta_{ij} \gamma_j \]
The two linear equations below are easily obtained from equation (27) and a combination of equations (32) and (34b)

\[
\Delta T + \left( \frac{T}{\sigma} \right)_o \sum_{j=1}^{s} \Delta y_j + \left( U \frac{T}{\rho} \right)_o \Delta \rho = (V)_o \Delta t
\]  

\[
\left\{ \sum_{j=1}^{s} \left( \gamma_j \right)_o \left[ \left( \frac{dS_j}{dT} \right)_o + \frac{d\bar{S}_{ij}}{dT} \right] \left( 1 + \frac{(\tau_j)_o}{\Delta t} \left[ \exp \left[ \frac{-\Delta t}{(\tau_j)_o} \right] - 1 \right] \right) \right\} \Delta T - \left( \frac{g\Delta T}{\rho} \right)_o \Delta \rho 
\]

\[
+ \sum_{j=1}^{s} (e_j)_o \Delta y_j = \sum_{j=1}^{s} \left( \gamma_j \right)_o \left\{ \exp \left[ \frac{-\Delta t}{(\tau_j)_o} \right] - 1 \right\} \left( \bar{S}_{ij} - e_{ij} \right)_o
\]

Equations (40), (41), and (42) comprise a system of \((r + 2)\) linear equations in the \((s + 2)\) unknowns \(\Delta T, \Delta \rho, \) and \(\Delta y_j \) \((j = 1, 2, \ldots, s)\). If it were possible that \(r = s\) and that equations (40) form a linearly independent set, these \((s + 2)\) equations can be solved for the increments in question. However, both conditions cannot be satisfied simultaneously, and supplementary linear equations in the variables \(\Delta T, \Delta \rho, \) and \(\Delta y_j \) \((j = 1, 2, \ldots, s)\) are needed. These supplementary equations can be obtained, just as in equilibrium from atom conservation equations.

The system of equations (40) always contains a linearly independent subset which can be determined by reference to the original chemical equations (1). The chemical equations (1) can be ordered so that each succeeding equation, after the first, contains a chemical species not appearing in any of the previous equations. If this ordering exhausts all of equations (1), there will be some number, say \(r_1\) \((\text{where } r_1 < r)\), of equations (40) which is linearly independent. This linearly independent subset of equations can be determined before any computation is begun, and the required atom conservation equations can be adjoined.

In the \(s\) species, there are a fixed number, \(m\), of different elements. Let \(n_{k,j}\) be the total number of atoms of element \(k\) \((k = 1, 2, \ldots, m)\) in species \(j\). The total number of atoms of element \(k\) must be constant so that

\[
\sum_{j=1}^{s} n_{k,j} \frac{dy_j}{dt} = 0 \quad (k = 1, 2, \ldots, m)
\]

When \(dy_j/dt\) is replaced by \(\Delta y_j/\Delta t\) and both sides of this equation are multiplied by \(\Delta t\), there is obtained
\[
\sum_{j=1}^{m} n_{kj} \Delta y_j = 0 \quad (k = 1, 2, \ldots, m)
\]

From these \( m \) linear equations, the required supplementary equations can be obtained.

It should be noted that equations (40) were derived independently from the fluid dynamical equations (17), (18), and (19). They can be used, therefore, in conjunction with other sets of fluid equations which arise in, for example, three-dimensional flow, or unsteady flow.

CONCLUDING REMARKS

In order to compute accurately the nonequilibrium channel flow of a multicomponent gaseous mixture, a numerical formulation is needed which applies to the equilibrium and near-equilibrium regions of the flow as well as the nonequilibrium region. The needed formulation is obtainable when a proper choice has been made for the dependent variables, and the rate equations in these variables are linearized over small intervals of time. By a properly chosen transformation, these rate equations can also be uncoupled, and the problem of obtaining expressions for the reaction variables reduces to solving a system of linear, uncoupled, first-order differential equations. The solution is, of course, easily obtained. However, in order to determine the needed transformation, it is necessary to solve an eigenvalue problem. It has been found that the needed transformation exists for all regions of the channel, and a method has been developed which reduces the eigenvalue problem to finding the eigenvalues of a symmetric matrix. This greatly simplifies the computational problem because numerical methods for finding eigenvalues of a general matrix are unreliable in their accuracy.

The integration procedure used in reference 10 can be regarded as a special application of the present method. In that work matrix methods were not required because of the low rank of the system. The method is presently being applied to a more general case. It appears that the necessary matrix manipulations can be performed accurately, and without adding greatly to the computing time per case experienced in reference 10.

Ames Research Center
National Aeronautics and Space Administration
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APPENDIX A

PROPERTIES OF THE MATRIX \( A \)

The \( r \times r \) matrix \( A = [a_{ij}] \) of equation (36) has its elements defined in equations (7).

\[
a_{ij} = (1 - x_i) \left( \sum_{j=1}^{S} \frac{\beta_{ij} \beta_{lj}}{\gamma_j} \right) \left( k_{fl} v_{l-1} \sum_{j=1}^{S} v_{lj} \right)
\]  

(A1)

This can be written

\[
a_{ij} = p_i b_{il} q_j
\]

where

\[
p_i = (1 - x_i) \quad \text{and} \quad q_j = \left( k_{fl} v_{l-1} \sum_{j=1}^{S} v_{lj} \right)
\]

and

\[
b_{il} = \left( \sum_{j=1}^{S} \frac{\beta_{ij} \beta_{lj}}{\gamma_j} \right)
\]

It is seen that \( b_{il} = b_{li} \) and hence the matrix \( B = [b_{ij}] \) is an \( r \times r \) real symmetric matrix. Since \( x_i < 1 \), it follows that \( p_i > 0 \) \((i = 1, 2, \ldots, r)\). Likewise, from its definition, \( q_j > 0 \) \((j = 1, 2, \ldots, r)\).

Let \( P = \text{diag} (p_1, p_2, \ldots, p_r) \) and \( Q = \text{diag} (q_1, q_2, \ldots, q_r) \). Then, from the construction of \( P, B, \) and \( Q \), it follows that

\[
A = PBQ
\]

Both \( P \) and \( Q \) are diagonal positive definite real matrices and \( B \) is real symmetric.

**Theorem 1.**

Let \( A = PBQ \) where \( B \) is real symmetric and where \( P \) and \( Q \) are real, diagonal, and positive definite.

\[
P = \text{diag} (p_1, p_2, \ldots, p_r) \quad \text{and} \quad p_i > 0 \quad (i = 1, 2, \ldots, r)
\]

\[
Q = \text{diag} (q_1, q_2, \ldots, q_r) \quad \text{and} \quad q_i > 0 \quad (i = 1, 2, \ldots, r)
\]
Then, the eigenvalues of \( A \) are the same as the eigenvalues of a real symmetric matrix

\[ F = DBD \]

where

\[ D = \text{diag} (\sqrt{p_1/q_1}, \sqrt{p_2/q_2}, \ldots, \sqrt{p_r/q_r}) \]

**Proof:**

Since \( P \) and \( Q \) are diagonal with rank \( r \), each has an inverse. It is possible, then, to define a matrix

\[ S^{-1} = PQ^{-1} = \text{diag} (p_1/q_1, p_2/q_2, \ldots, p_r/q_r) \]

Also, let

\[ T = QBQ \]

Then

\[ A = PBQ = PQ^{-1}QBQ = S^{-1}T \]

Now

\[ \lambda I - A = [\lambda I - S^{-1}T] = [S^{-1}][\lambda S - T] \]

where

\[ S = \text{diag} (q_1/p_1, q_2/p_2, \ldots, q_r/p_r) \]

Consequently

\[ |\lambda I - A| = |S^{-1}| \cdot |\lambda S - T| \]

From the definition of \( S^{-1} \), it is seen that \( |S^{-1}| \neq 0 \). Thus \( |\lambda I - A| = 0 \) if and only if \( |\lambda S - T| = 0 \). This shows that the eigenvalues of \( A \) are precisely the roots of \( |\lambda S - T| = 0 \).

Now define the matrix \( R \) by

\[ R = \text{diag} (\sqrt{p_1/q_1}, \sqrt{p_2/q_2}, \ldots, \sqrt{p_n/q_n}) \]

This definition is made so that \( RSR = I \). Consequently

\[ |R| \cdot |\lambda S - T| \cdot |R| = |\lambda I - RTR| \]

Again, \( |R| \neq 0 \) so that the roots of \( |\lambda S - T| = 0 \) are the eigenvalues of the matrix

\[ F = RTR \]

This shows that the eigenvalues of \( F \) are the same as the eigenvalues of \( A \).
It will be shown that $F$ is symmetric. Since $R$, $Q$, and $B$ are all symmetric,

$$R^T = R, \quad Q^T = Q, \quad \text{and} \quad B^T = B$$

Then

$$F^T = R^T(QBQ)^T = R^TQ^TB^TB^TQ^T = RQBQR = F$$

Since $R$ and $Q$ are diagonal, they commute. Let

$$D = RQ = (\sqrt{p_1q_1}, \sqrt{p_2q_2}, \ldots, \sqrt{p_nq_n})$$

Then

$$F = DBD$$

Q.E.D.

**Theorem 2.**

Let $A$ and $F$ be the matrices of theorem 1, and let $R = \text{diag} \left(\sqrt{p_1/q_1}, \sqrt{p_2/q_2}, \ldots, \sqrt{p_r/q_r}\right)$. If $\lambda$ is an eigenvalue of $F$ and $\xi$ its corresponding eigenvector, then $\eta = R\xi$ is the eigenvector of $A$ corresponding to $\lambda$.

**Proof:**

Theorem 1 shows that $\lambda$ is an eigenvalue of both $F$ and $A$. Since $\xi$ is the corresponding eigenvector of $F$,

$$F\xi = (RQBQ)\xi = \lambda\xi$$

Thus

$$PQ^{-1}R^{-1}(RQBQ)\xi = \lambda PQ^{-1}R^{-1}\xi$$

The matrices $R$ and $Q$ commute since they are both diagonal. Hence

$$(PBQ)R\xi = \lambda PQ^{-1}R^{-1}\xi$$

Now $PQ^{-1}R^{-1} = R$, since $PQ^{-1} = \text{diag} \left(p_1/q_1, p_2/q_2, \ldots, p_r/q_r\right)$. Also $A = PBQ$, so that the above equation is

$$AR\xi = \lambda R\xi$$

Define $\eta$ by

$$\eta = R\xi$$

Then

$$A\eta = \lambda \eta$$

so that $\eta$ is the eigenvector of $A$ corresponding to $\lambda$. Q.E.D.
Theorem 3.

The eigenvectors $\vec{v}_i (i = 1, 2, \ldots, r)$ of the matrix $A = PBQ$ of theorem 1 are linearly independent.

Proof: Let $F = DBD$ be the matrix used in theorem 1. Since $F$ is real symmetric, there is a nonsingular matrix $H$ such that

$$H^{-1}FH = \text{diag} (\lambda_1, \lambda_2, \ldots, \lambda_r)$$

where $\lambda_1, \lambda_2, \ldots, \lambda_r$ are the eigenvalues of the matrix $F$. The possibility that some eigenvalues may have multiplicity greater than unity is not excluded. Let $L = \text{diag} (\lambda_1, \lambda_2, \ldots, \lambda_r)$. Then

$$FH = HL$$

Denote the column vectors of $H$ by $\vec{\xi}_1, \vec{\xi}_2, \ldots, \vec{\xi}_r$. These column vectors of $H$ are the eigenvectors of $F$, for

$$F\vec{\xi}_i = \lambda_i \vec{\xi}_i \quad (i = 1, 2, \ldots, r)$$

It is to be noted that the $\vec{\xi}_i$ are linearly independent since $H$ is nonsingular.

Now consider the matrix

$$G = RH$$

where

$$R = \text{diag} (\sqrt{p_1/q_1}, \sqrt{p_2/q_2}, \ldots, \sqrt{p_r/q_r})$$

The matrix $G$ is nonsingular since it is the product of two nonsingular matrices, $R$ and $H$. Thus, its column vectors form a linearly independent set. But the column vectors of $G$ are

$$\vec{v}_i = R\vec{\xi}_i$$

The result of theorem 2 shows that these are the eigenvectors of $A = PBQ$.

Q.E.D.
REFERENCES


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—National Aeronautics and Space Act of 1958

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