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Finite Difference Methods of Solution of the Boundary-Layer Equations

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Nomenclature

c_i = mass fraction of species i, ρ_i/ρ
c_{pi} = specific heat at constant pressure of species i, ft²/(sec²°R)
$\bar{c}_p$ = frozen specific heat at constant pressure of the mixture $\sum_i c_i c_{p_i}$, ft²/(sec²°R)
D_{ij} = multicomponent diffusion coefficient, ft²/sec
$\mathfrak{D}_{ij}$ = binary diffusion coefficient, ft²/sec
D_i^T = thermal diffusion coefficient, lb sec/ft
h = enthalpy, $\sum_i h_i c_i$, ft²/sec²
h_i = enthalpy of species i, ft²/sec²
k = thermal conductivity of mixture, lb/(sec° R)
l = density-viscosity product, $\rho\mu/(\rho\mu)_r$
L_{ij} = multicomponent Lewis-Semenov number, $\bar{c}_p\rho\mathfrak{D}_{ij}/k$
$\mathfrak{L}_{ij}$ = binary Lewis-Semenov number $\bar{c}_p\rho\mathfrak{D}_{ij}/k$
L_i^T = thermal Lewis-Semenov number, $\bar{c}_p D_i^T/k$
$\bar{M}$ = molecular weight of the mixture, $1/\left(\sum_i c_i/M_i\right)$, lb/lb-mole
M_i = molecular weight of species i, lb/lb-mole
NI = number of chemical species
Pr = Prandtl number $\bar{c}_p\mu/k$
p = pressure, lb/ft²
p_0' = normal shock stagnation pressure, atm
R = universal gas constant, lb ft²/(lb-mole sec² °R)
R_N = nose radius, ft
r = distance from axis in axisymmetric problems, ft
T = temperature, °R
T_0' = normal shock stagnation temperature, °K
T_K = temperature, °K
u,v = velocity components tangential and normal to body surface, fps
V = transformed normal velocity [Eq. (3a)]
V_∞ = freestream velocity, fps
w_i = mass rate of formation of species i, lb sec²/(ft⁴ sec)
x = distance along surface from leading edge or stagnation point, ft
y = distance along normal from surface, ft
μ = viscosity, lb sec/ft²
ρ = density, lb sec²/ft⁴
ρ_i = density of species i, lb sec²/ft⁴

Subscripts

b,w = conditions at body surface
e = conditions at outer edge of shock layer or boundary layer
r = quantities evaluated at some reference condition
∞ = freestream conditions

Superscripts

$j = 0$ = two-dimensional body
$j = 1$ = axisymmetric body

I. Review of Numerical Techniques

THE step-by-step solution of the first-order boundary-layer equations was considered by Prandtl[1] as early as 1938. A review of the early work (up to 1955) on numerical solutions of the boundary-layer equations is given in Ref. 2, whereas a more recent review of the Russian literature* is given in Refs. 3 and 4. There has been a rapid development of numerical techniques in recent years, and these can be divided into the following categories: 1) difference-differential procedure; 2) method of integral relations; 3) finite difference schemes.

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The difference-differential procedure was originally developed by Hartree and Womersley[5] and has been applied by Leight[6] and Manohar[7] to the boundary-layer equations. Smith and colleagues[8–13] have exploited and developed this procedure even further, and have applied it to a variety of problems. In this scheme, the derivatives in the direction along the surface are usually replaced with finite difference relations, and the partial differential equations reduce to ordinary differential equations with two-point boundary conditions. The ordinary differential equations are solved as an initial-value problem which requires an iteration procedure to satisfy the boundary conditions at the outer edge. The difference-differential approach has been used by Zamurayev[14] and Le Maréchal and Ronat,[15] but these authors linearize the ordinary differential equations and obtain the solution in an iterative manner with a finite difference method. Steiger and Sepri[16] have investigated the solution of the boundary layer with the difference-differential procedure where the normal derivatives are replaced by finite difference relations. This results in a system of first-order ordinary differential equations of the initial-value type, and these equations are of the "stiff" type also. This approach has been developed further by Lubard and Schetz.[17]

The method of integral relations is a special case of the method of weighted residuals, as has been discussed by Finlayson and Scriven.[18] This method is due to Dorodnitsyn[19] and has been employed in a number of Russian papers.[19–22] The procedure has also been employed by Pallone and colleagues,[23,24] and investigated further by Bethel.[25,26] This technique reduces the partial differential equations to a system of ordinary differential equations of the initial-value type.

Recently Kendall and Bartlett[27] have used the integral method to replace the normal derivatives, while the differential-difference procedure of replacing the tangential derivatives has also been employed. The partial differential equations are thus reduced to a system of nonlinear algebraic equations which must be solved at each step along the body.

After the early finite difference techniques,[28–36] which have been reviewed in Ref. 2, the emphasis was on the solution of the boundary-layer equations in the Crocco form, as exemplified by Refs. 37–41. The approach was partially used by Eichelbrenner; the procedure was developed further, and preliminary examples were computed by Flügge-Lotz using a desk calculator. This work was extended by Baxter and Flügge-Lotz, and a digital computer was utilized for the finite difference solution. In this work, an explicit finite difference scheme was employed in which the step size along the wall is restricted by stability considerations. In order to avoid the stability restrictions required in explicit schemes, Kramer and Lieberstein[42] employed an implicit scheme with the Crocco form of the equations.†

Another difference scheme that has been used by Raetz[43] for solving the three-dimensional boundary-layer equations is that of Dufort-Frankel. This scheme is stable, but care must be taken to insure that the truncation error is sufficiently small. In differencing the partial differential equation, a term has been added to the equations, and this term will only be small if the appropriate ratio of the step sizes is taken.

Besides employing various finite difference procedures, the form of the boundary-layer equation can be changed. The von Mises transformed boundary-layer equations have been solved with an explicit finite difference scheme by Mitchell and Thomson.[44,45] The advantage of this form of the boundary-layer equations is that the continuity equation has been eliminated. There is a singularity at the wall which introduces difficulties, but these have been overcome in the papers by Mitchell and Thomson.

The solution of the boundary-layer equations in untransformed or physical coordinates appears to be the next development in the numerical schemes. In the paper by Flügge-Lotz and Yu,[46] an explicit finite difference procedure was applied to the compressible equations. This proved rather unsuccessful, as the stability requirements are very stringent and the replacement of the continuity equation caused many problems. In the paper by Wu,[47] the treatment of the continuity was such that more stable solutions were obtained with an explicit difference scheme. Also, by transforming the compressible equations into incompressible form, with the Howarth-Dorodnitsyn relation, the stability requirements are not as restrictive when a constant step size across the boundary layer is used and when the step size is the same for both coordinate systems. For these conditions, the physical distance for the first grid point away from the wall is much larger in the Howarth-Dorodnitsyn variables. In Russia, Chudov and Brailovskaya[48,49] also studied the solution of the boundary-layer equations in physical coordinates; however, an implicit six-point finite difference scheme was used. The governing equations are replaced with finite differences such that the coupling between equations is initially neglected. Then an iteration process is employed to obtain the desired accuracy of the dependent variables with coupling and nonlinear effects included. This type of procedure has been developed into a standard program for equations of the boundary-layer type by Paskonov.[50] In this program a procedure is described which allows the step size across the boundary layer to vary. At about the same time, in the United States a similar implicit technique was developed independently for the boundary-layer equations in physical coordinates by Flügge-Lotz and Blottner.[51] The main difference between this work and that of Chudov and Brailovskaya is that coupling between the equations is allowed. This results in a tridiagonal matrix with matrix elements, which is somewhat more complicated to solve than the uncoupled equations. The boundary-layer equations transformed with the Howarth-Dorodnitsyn relations was also investigated by Flügge-Lotz and Blottner, and both a four-point and a six-point (Crank-Nicolson) difference scheme were considered. For hypersonic boundary-layer flows, the transformed equations with the six-point implicit scheme is the better procedure.

One of the problems with all the previous methods is the starting of the solution of the equations. Initial profiles of the dependent variables are required across the boundary layer at some point, and the solution then proceeds downstream. For sharp bodies one would want to start the solution at the tip, whereas for a blunt body the solution should start at the stagnation point. At the tip of a sharp body, the boundary thickness goes to zero and the finite difference scheme is inappropriate in the physical coordinates.‡ If the boundary-layer equations are transformed into similarity variables (relations developed by Mangler, Görtler, Howarth-Dorodnitsyn, Levy, and Lees), then in the transformed plane the boundary layer is nearly of uniform thickness for many flow situations. Also the partial differential equations reduce to ordinary differential equations at the tip of a body or at a stagna ion point. The solution of these ordinary differential equations provides initial conditions for a finite difference solution which can start at the beginning of the body. This type of procedure was applied to a binary gas mixture with finite chemical reaction rate by Blottner.[52] The transformed boundary-layer equations were replaced with an implicit six-point finite difference scheme, and coupling between

† The Crocco form of the equations is attractive because the continuity equation has been eliminated and the independent variable u/u_e, which is related to the thickness of the boundary layer, goes from zero to one. If the velocity within the boundary layer exceeds the edge velocity, the Crocco form of the equations is difficult to apply.

‡ The boundary-layer equations at the tip of a body are also physically inappropriate, as continuum theory is not valid; and when it is, more complete equations are required. However, from a mathematical point of view, one can still consider the boundary-layer solution.

the equations was included. This procedure was extended to the air boundary layer with seven chemical species and finite reaction rates by Blottner.[53] The chemically reacting boundary layer has been solved with an explicit finite difference scheme by Galowin and Gould.[54] The boundary-layer equations are transformed into von Mises coordinates before the derivatives are replaced with difference quotients. In this study for flow on blunt bodies, the swallowing of the inviscid flow by the boundary layer is taken into account.

The application of the finite difference technique to second-order boundary-layer theory has been made by Davis and Flügge-Lotz[55] and Fannelop and Flügge-Lotz[56] for axisymmetric and two-dimensional bodies, respectively. An implicit finite difference technique similar to that developed by Flügge-Lotz and Blottner[51] was employed. In linearizing the finite difference equation, certain terms are evaluated at the known grid point rather than at the point halfway between the known and the unknown points. For stagnation-point flows, Davis and Flügge-Lotz found it advantageous to use linear extrapolation to approximate the unknown quantities at the halfway point. This procedure requires that two profiles of the dependent variable be known.

In a paper by Fussell and Hellums,[57] an implicit finite difference procedure is applied to the similarity form of the boundary-layer equation. The momentum equation has a third-order derivative and results in a pentadiagonal matrix, while the energy equation becomes a tridiagonal matrix. The procedure recommended in this paper is to use a 10-point symmetric implicit finite difference scheme, with the equations replaced initially by a linear difference equation. An iteration procedure is used until the nonlinear difference equations corresponding to the grid points employed have been solved.

An explicit finite difference scheme has been used by Kleinstein[58] to solve the boundary-layer equations in von Mises variables. This work is for a compressible perfect gas, and the approach is similar to that of Mitchell and Thomson[44] and Galowin and Gould,[54] where an incompressible gas and a reacting gas are employed, respectively. Later a revision of this work was reported by Kleinstein,[59] and a description and operation instructions for the program were given by Nabi.[60]

For boundary-layer programs at General Applied Science Laboratories, Lane[61] initially recommended that an explicit finite difference technique be used. Later Lane, Lieberman, and Fox[62] used an implicit finite difference scheme to solve the compressible boundary-layer equations in physical coordinates. The momentum and energy equations are uncoupled, and iterations are performed until a solution of the nonlinear coupled equations is obtained. This method is that of Brailovskaya and Chudov.[48,49] Lieberman, Lane, and Fox[63] have also investigated boundary-layer flow of air in chemical equilibrium and with finite rate chemistry. In this work an implicit finite difference scheme is used near the initial station to start the solution, and then reverts to an explicit scheme downstream.

The numerical solution of reacting boundary layers has also been investigated by Gruenich and Pindroh.[64] The difference-differential method of Smith[8–13] is used for the momentum and energy equations, whereas an implicit scheme is used for the species equations. In this method an iteration procedure is required to solve the momentum equation, and two trial solutions are required for the energy equation.

In the implicit finite difference procedure developed by Flügge-Lotz and Blottner,[51] it was assumed that both the normal and tangential velocity components and the temperature distribution are known from similarity solutions across the boundary layer. In a recent paper by Ting,[65] the compatibility conditions for the velocity components have been investigated further than in the original work of Prandtl. The proper formulation is to specify the tangential velocity component and then to determine the normal velocity component from the compatibility conditions. This approach has been incorporated into the implicit finite difference scheme originally developed by Flügge-Lotz and Blottner, and this technique has been examined further by Krause.[66] The normal velocity component is obtained in an iterative manner by requiring that the continuity, momentum, and energy equations are satisfied at each step. The finite difference procedure is the same as that of Flügge-Lotz and Blottner, except the normal velocity component is assumed initially in order to solve the momentum and energy equations. Then the continuity equation is solved to obtain a better value of the normal velocity component that is averaged with the initially assumed value to obtain a new estimate of the normal velocity component. This type of procedure is repeated until convergence is obtained.

To avoid third-order derivatives in the governing equations, when the boundary-layer equations are transformed into similarity form, a transformed normal velocity is introduced by Blottner[52] and the continuity equation is retained. Fannelop[67] has applied the same type of transformation but has introduced the stream function such that the continuity equation is satisfied. However, in introducing the stream function, the momentum equation is still written as a second-order equation. The new partial differential equation for momentum involves f and $\partial f/\partial \xi$. The value of f can be readily obtained from an integration once the value of the tangential velocity component across the boundary layer is known. The values of f and $\partial f/\partial \xi$ are required for the solution of the momentum equation, and the solution of this equation gives the tangential velocity component. The values of the quantities f and $\partial f/\partial \xi$ for the difference equation are evaluated by employing a linear extrapolation of the values of these quantities at two previous profiles.

A multicomponent reacting gas with thermal diffusion effects included has been investigated by Moore,[68] where the implicit finite difference scheme was provided by Farrington.[69] The similarity coordinates are used with a stretching of the normal coordinate near the surface. A Crank-Nicolson implicit finite difference scheme is used with the equations uncoupled. The final solution is obtained after an iteration procedure is performed that corrects the linearized terms and approximations made to uncouple the governing equations. In this work it was observed that stability problems occurred for the Crank-Nicolson scheme with boundary condition involving derivatives. This problem was eliminated by using a four-point implicit scheme at the first grid point away from the wall.

An implicit finite difference scheme of the boundary-layer equations in nearly the Crocco form has been studied by Schönauer.[70] Rather than using the shearing stress as a dependent variable, a quantity proportional to the square of the velocity gradient is used. The independent variable for the coordinate normal to the surface is the tangential velocity that is nondimensionalized with the velocity at the edge of the boundary layer, and the independent variable therefore varies from 0 to 1.

A method has been given by Schennikov[71] for constructing finite difference schemes for the boundary layer on the basis of the laws of conservation. The governing equations are written as the divergence of a vector quantity, and its components depend upon the equation being considered. Then the Gauss theorem is employed to express the divergence of the vector as two integrals. The integrals are then expanded with the trapezoidal formula and normal derivatives are replaced with central differences. The result of these operations is a system of nonlinear finite difference equations with coupling between the equations involving the dependent variables.

An implicit finite difference has been developed by Patankar and Spalding[72] for solving boundary-layer equations. The governing equations are transformed with a von Mises-type coordinate system, where the stream function is an inde-

pendent variable across the layer. A nondimensional stream function is defined such that it varies from 0 to 1 from the wall to the outer edge. A parameter in the nondimensional stream function is determined as the calculation proceeds such that the grid adjusts its width so as to conform to the thickness of the layer. The finite difference scheme is the Crank-Nicolson implicit scheme, except the convection terms are based on an integrated average over a small control volume. This results in the streamwise derivative being approximated as a weighted average of the derivatives at the point of interest and those on both sides of this point. This method of differencing the equations is similar to that used by Shchennikov.[71]

The boundary-layer flow on a rotating cone has been obtained with a finite difference method by Koh and Price.[73] The governing equations are transformed with similarity-type variables, and the stream function is introduced in the manner employed by Fannelop[67] as previously described. An implicit finite difference scheme of the Crank-Nicolson type is employed, and linear difference equations are written such that the coupling between equations is neglected initially. The linear difference equations are solved in an iterative manner which gives the solution of the coupled nonlinear difference equations.

The finite difference procedure has also been employed for the Rayleigh problem and a flat-plate boundary-layer flow, with radiation effects included by Solan and Cohen[74] and Sibulkin and Dispaux,[75] respectively. The boundary-layer equations are transformed with the von Mises transformation initially, and then new independent variables are introduced which transform the equations to the similarity-type form. In the absence of radiation or at the leading edge of the flat plate, the governing equations become ordinary differential equations, or similarity solutions are obtained. The partial differential equations are solved with a Crank-Nicolson six-point finite difference scheme. The resulting difference equations are nonlinear algebraic equations and are solved by an iteration scheme given by Douglas.[76] A finite difference method proposed by Douglas[76] was also investigated for the Rayleigh problem, but stability restriction required a relatively small step along the body. In this method nine points at three time levels are employed and the resulting difference equations are linear and are readily solved.

The boundary-layer equations for real equilibrium gases have been solved with an implicit finite difference method by Levine.[77] This method is that employed by Blottner,[52] where the difference equations are coupled.

A transformation that maps the infinite region of the boundary-layer flow into a finite interval has been used by Sills.[78] The transformed governing equations are then solved with an implicit finite difference scheme similar to that employed by Paskonov.[50]

In this paper a technique for solving the boundary-layer equations for a multicomponent flow with finite chemical reactions is presented. This procedure has evolved over a number of years, and an earlier version was reported in Ref. 79. The motivation for the present finite difference scheme is the desire for a method for solving the governing equations where there are many chemical species in the flow (for example, 25). The technique is described in the following sections, and typical results are presented for the boundary-layer flow on a sharp cone and hyperboloid§ at re-entry conditions.

II. Governing Equations

The general equations for a multicomponent nonequilibrium gas are given in Ref. 80, and the resulting equations for the boundary layer have been given in Ref. 53. The boundary-layer equations are transformed into similarity form in order to obtain them in a form more appropriate for numerical solution. The new independent variables are

$$\xi(x) = \int_0^x (\rho\mu)_r u_e r_b^{2j}\, dx \tag{1a}$$

$$\eta(x,y) = \frac{u_e r_b^j}{(2\xi)^{1/2}} \int_0^y \rho\, dy \tag{1b}$$

and the derivatives become

$$\partial/\partial x = (\rho\mu)_r u_e r_b^{2j}\partial/\partial\xi + (\partial\eta/\partial x)(\partial/\partial\eta) \tag{2a}$$

$$\partial/\partial y = [\rho u_e r_b^j/(2\xi)^{1/2}](\partial/\partial\eta) \tag{2b}$$

When the new dependent variables

$$V = [2\xi/(\rho\mu)_r u_e r_b^{2j}][f'\,\partial\eta/\partial x + \rho v r_b^j/(2\xi)^{1/2}] \tag{3a}$$

$$f' = u/u_e \tag{3b}$$

$$\theta = T/T_e \tag{3c}$$

are introduced and the transformations are applied, the boundary-layer equations become the following in the transformed plane:

Continuity equation:

$$2\xi(\partial f'/\partial\xi) + \partial V/\partial\eta + f' = 0 \tag{4a}$$

Momentum equation:

$$2\xi\frac{\partial f'}{\partial\xi} + \left(\frac{V - l'}{f'}\right)\frac{\partial f'}{\partial\eta} + \beta\left[f' + \frac{\bar{M}_e}{\bar{e}\bar{M}}\frac{\theta}{f'}\right] - \frac{l}{f'}\frac{\partial^2 f'}{\partial\eta^2} = 0 \tag{4b}$$

Energy equation:

$$2\xi f'\frac{\partial\theta}{\partial\xi} + \left(V - \frac{\bar{c}'}{\bar{c}_p} + d + b\right)\frac{\partial\theta}{\partial\eta} - \alpha l\left(\frac{\partial f'}{\partial\eta}\right)^2 + \left(-\alpha\beta\frac{\bar{M}_e}{\bar{M}\bar{e}} + \bar{e}\right)\theta f' - \frac{\bar{c}}{\bar{c}_p}\frac{\partial^2\theta}{\partial\eta^2} - \frac{a}{\theta}\left(\frac{\partial\theta}{\partial\eta}\right)^2 + \frac{e}{\bar{c}_p T_e}\sum_{i=1}^{NI} h_i\left(\frac{w_i}{\rho}\right) = 0 \tag{4c}$$

Species equations:

$$2\xi f'\frac{\partial c_i}{\partial\xi} + (V - b_i')\frac{\partial c_i}{\partial\eta} - b_i\frac{\partial^2 c_i}{\partial\eta^2} - \frac{\bar{a}_i}{\theta}\frac{\partial^2\theta}{\partial\eta^2} - \frac{\bar{a}_i'}{\theta}\frac{\partial\theta}{\partial\eta} + \left(\frac{\bar{a}_i}{\theta^2}\right)\left(\frac{\partial\theta}{\partial\eta}\right)^2 - \bar{b}_i' - e\left(\frac{w_i}{\rho}\right) = 0 \tag{4d}$$

where

$$\bar{a}_i = \frac{lL_i^T}{Pr},\quad a = \frac{1}{\bar{c}_p}\sum_{i=1}^{NI}\bar{a}_i c_{pi}$$

$$b_i = \frac{lLe_i}{Pr},\quad \bar{b}_i = \frac{l}{Pr}\sum_{\substack{k=1\\k\neq i}}^{NI}\Delta\bar{b}_{i,k}\frac{\partial c_k}{\partial\eta}$$

$$b = -\sum_{i=1}^{NI}\frac{c_{pi}\bar{b}_i}{\bar{c}_p},\quad \bar{c} = \frac{l\bar{c}_p}{Pr},\quad d = -\sum_{i=1}^{NI}\frac{c_{pi}}{\bar{c}_p}b_i\frac{\partial c_i}{\partial\eta}$$

$$e = \frac{2\xi}{u_e(d\xi/dx)},\quad \bar{e} = \frac{2\xi}{T_e}\frac{dT_e}{d\xi},\quad \bar{e} = \rho_e u_e\frac{du_e/dx}{dp_e/dx}$$

$$\alpha = u_e^2/\bar{c}_p T_e,\quad \beta = (2\xi/u_e)(du_e/d\xi) = e(du_e/dx)$$

$$l' = \partial l/\partial\eta,\ \bar{a}'_i = \partial\bar{a}_i/\partial\eta,\ b'_i = \partial b_i/\partial\eta,\ \bar{b}_i' = \partial\bar{b}_i/\partial\eta$$

The preceding equations differ from those given in Ref. 53 by the quantity $\bar{e}$ which has been set equal to -1 in that Ref. For the classical boundary-layer approach, the inviscid

§ The employment of this problem and body geometry was requested of participants in the AGARD Seminar.

flow body streamline results are used as the conditions at the edge of the boundary layer. For this case, $\bar{e} = -1$. For the more general case where swallowing of the inviscid flow into the boundary layer is taken into account, the value of $\bar{e}$ must be determined from the expression given previously.

In the aforementioned relations, the mass flux relative to the mass-average velocity, j_i, has been used and was written as

$$j_i = -\frac{\mu}{Pr}\left\{\sum_{k=1}^{NI} \bar{b}_{ik}\frac{\partial c_k}{\partial y} + \frac{L_i{}^T}{T}\frac{\partial T}{\partial y}\right\} \tag{5}$$

where

$$b_{ik} = \begin{cases} Le_i & i = k \\ \Delta\bar{b}_{ik} & i \neq k \end{cases}$$

$$Le_i = \sum_{\substack{j=1 \\ j\neq 1}}^{NI} \frac{c_j}{M_j} \Bigg/ \sum_{\substack{j=1 \\ j\neq 1}}^{NI} \frac{c_j}{M_j\mathfrak{L}_{ij}}$$

$$\Delta\bar{b}_{ik} = Le_i - \left[\frac{M_i}{\bar{M}}L_{ik} + \left(1 - \frac{M_i}{M_k}\right)\sum_{j=1}^{NI} L_{ij}c_j\right]$$

If the Lewis-Semenov numbers, $\mathfrak{L}_{ij}$, are constant for all the species or if a trace species is being considered, the term $\Delta\bar{b}_{ik}$ is zero. In Eq. (5), the pressure diffusion term is neglected due to the boundary-layer assumption, and the forced diffusion term is assumed zero.

The equation of state is also required and is written as

$$\rho = \left[p_e \Big/ RT \sum_{i=1}^{NI}\left(\frac{c_i}{M_i}\right)\right] = p_e\bar{M}/RT \tag{6}$$

where it is assumed the gas consists of a mixture of chemically reacting perfect gases with the pressure change across the boundary layer neglected.

The chemical mass rate of production of species i per unit volume, w_i, is obtained from the Law of Mass Action, and the desired form is given in Ref. 53. The gas model for air and the chemical kinetics employed are the same as described in Ref. 81. Also the thermodynamic and transport properties of the individual species and the mixture are required. These properties are obtained from the same relations and information as was employed in Ref. 81. The multicomponent Lewis-Semenov numbers were obtained from relations given in Ref. 82, which are written as

$$L_{ij} = \bar{F}_{ij} - (M_i/M_j)\bar{F}_{ii} \tag{7}$$

The quantities $\bar{F}_{ij}$ are coefficients in a matrix which is the inverse of the matrix with the following coefficients:

$$F_{ij} = \frac{c_i}{\mathfrak{L}_{ij}} + M_j \sum_{\substack{l=1 \\ l\neq i}}^{NI} \frac{c_l}{M_l\mathfrak{L}_{il}}, \quad i \neq j \tag{8a}$$

$$F_{ij} = 0, \quad i = j \tag{8b}$$

The binary Lewis-Semenov numbers are obtained using the definition and binary diffusion coefficients, which are expressed as

$$\mathfrak{D}_{ij} = (\bar{\mathfrak{D}}_{ij}/\bar{p})\ 1.0764 \times 10^{-3} \qquad (\text{ft}^2/\text{sec}) \tag{9}$$

where $\bar{p}$ = pressure in atmospheres, and

$$\bar{\mathfrak{D}}_{ij} = e^C T_K{}^{A\ln T_K + B} \qquad (\text{cm}^2\ \text{atm/sec})$$

The preceding expression for $\bar{\mathfrak{D}}_{ij}$ was used to curve-fit tabulated binary diffusion coefficients given by Yos.[83] A revised table of values was used for the NO—NO^+ interaction as given in a later paper by Yos.[84] The collision cross sections for the atomic and molecular interactions in these results were obtained from calculations of Mason et al.[85,86] Some of the interaction cross sections were calculated as averages of the other interaction cross sections, whereas the cross sections for the interactions N—O_2 and N—NO were assumed the same as N—N_2. Also the interaction cross sections for NO^+ with a neutral species have been taken the same as the N—O^+ and O—N^+ cross sections. The curve-fit coefficients for the various binary diffusion coefficients are given in Table 1.

Table 1 Diffusion curve fit constants

Interaction	A	B	C
N—O	−0.0043383	1.9119177	−11.891342
N—N_2	0.0191055	1.4904448	−10.358828
N—O_2	0.0191055	1.4904448	−10.358828
N—NO	0.0191055	1.4904448	−10.358828
O—O_2	0.0216586	1.3875747	− 9.7389971
O—N_2	0.0168907	1.5276702	−10.629306
N_2—O_2	0.0435927	0.9784219	− 8.3354916
O—NO	0.0183441	1.4750189	−10.265935
O_2—NO	0.0410864	1.0124720	− 8.4455480
N_2—NO	0.0315955	1.2225368	− 9.4862934
O—NO^+	0.0003467	1.8941393	−12.978394
N—NO^+	0.0003467	1.8941393	−12.978394
O_2—NO^+	0.0003467	1.8941393	−12.978394
N_2—NO^+	0.0003467	1.8941393	−12.978394
NO—NO^+	0.0039930	1.5689336	−11.441502

The conditions at the surface and outer edge of the boundary layer determine the necessary boundary conditions for the foregoing equations. At the wall, it is assumed that the tangential velocity is zero and the surface temperature is specified, and these conditions are expressed as

$$u(x, 0) = 0; \quad T(x, 0) = T_b(x) \tag{10a, b}$$

In addition, the boundary condition on the mass flux of a species i at the surface, $(\rho_i v_i)_b$, is

$$(\rho_i v_i)_b = \dot{m}_i = (c_i\rho v)_b + (j_i)_b \quad (i = 1, 2, \ldots, NI) \tag{10c}$$

The mass flux of a species at the surface depends on the surface material and what phenomena occur at the gas-surface interface. The surface conditions employed are given with the numerical examples presented.

The total mass flux at the surface can be determined from

$$\rho v = \sum_{i=1}^{NI} (\dot{m}_i)_b \tag{11}$$

and this is the boundary condition employed with the continuity equation.

The flow at the edge of the boundary layer is determined from the inviscid nonequilibrium flow around the body. The boundary conditions at the outer edge of the boundary layer are

$$u \to u_e; \quad T \to T_e; \quad c_i \to c_{ie} \quad (i = 1, 2, \ldots, NI) \tag{12}$$

where u_e, T_e, and the c_{ie}'s are obtained from the inviscid flow. The technique for matching the inviscid flow with the boundary layer is discussed where the numerical results are presented.

III. Finite Difference Procedure

The problem of multicomponent chemically reacting boundary layers for pure air, or as many as 11 chemical species, has been solved with a finite difference procedure by Blottner.[53] When the partial differential equations are replaced with the finite difference equations, the resulting difference equations are coupled, as more than one of the unknown independent variables appear in each equation. Hence, the equations must be solved simultaneously. Since these equations are of a special form, the procedure requires the inversion of 12 × 12 matrices (number of species plus one), where there will be as many of these matrices as points across the boundary layer

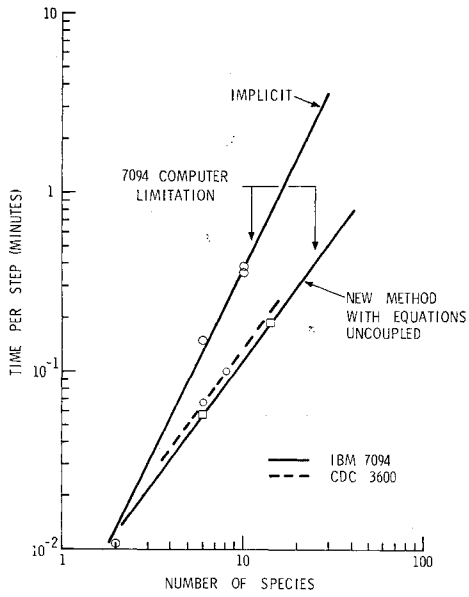

Fig. 1 Computation time for various numbers of chemical species (binary diffusion).

(50 in this program). All the coefficients of the matrices must be saved (stored in the computer memory), which requires 7200 storage locations. The storage requirements for these matrices increases rapidly when the number of species is increased. This program, with 11 chemical species and 20 reactions, requires nearly the full capacity of the IBM 7094 computer with 32K memory. The computation time for this method increases rapidly when the number of species becomes large. At best, one would expect the computation time to vary nearly directly with the number of species. For matrix inversions, the computation time is proportional to the number of rows or columns of the matrix cubed. Since many matrix inversions are performed, the computation time must be proportional to the number of species to a power greater than one and less than three. The actual time required per step for the present implicit procedure is shown in Fig. 1. Due to the rapid increase in computation time and storage requirements, the implicit procedure does not seem appropriate when one is interested in boundary-layer flows with ablation contaminants where there can be a large number of chemical species.

The question might be asked, why not use an explicit procedure where the computation time is nearly proportional to the number of species and the storage requirements are probably a minimum? For boundary-layer computations, the explicit method has not proved very successful, as stability requirements demand that the step size be exceedingly small, which will result in an excessive over-all computation time. In addition, there are problems in starting the solution at the tip or stagnation point of the body.

A method is described below which has the desirable stability characteristics of the implicit procedure (large step size), with the computing time being nearly proportional to the number of species, as in the explicit scheme. The procedure is similar to the implicit procedure of the Crank-Nicolson type which has been employed previously, except the difference equations are written such that only one dependent variable appears in each equation. Therefore, the resulting implicit difference equations are solved for each dependent variable separately.¶

Another variation of this procedure has also been investigated and is a "predictor-corrector" procedure similar to the method employed by Douglas and Jones.[87] With this method, the variables are predicted at a half-step forward, and then these quantities are used to give the value of the variables a complete step ahead. The truncation error for such a procedure is of the order of the step size $(\Delta x)^2$. The procedure described below consists of only the corrector part of the preceding method, with variables required at the half step evaluated at the known step, and has a truncation error of the order of the step size. Although the present method (corrector only) is less accurate for the same step size as the predictor-corrector procedure, the predictor-corrector method requires approximately twice the amount of computer time as the present method. When the step size of the present method is reduced to one-half of the predictor-corrector step size, the computation time of the two methods is nearly the same and the accuracy appears to be about the same. Hence, the two methods appear almost equivalent as far as computer time required, but the present method is easier to program and requires less storage.

The boundary-layer equations, with the exception of the continuity equation, are of the following form:

$$(\partial^2 W/\partial\eta^2) + \alpha_1(\partial W/\partial\eta) + \alpha_2 W + \alpha_3 + \alpha_4 2\xi(\partial W/\partial\xi) = 0 \tag{13}$$

where W represents any of the dependent variables. The coefficients in the preceding equation are obtained after the boundary-layer equations (4) have been linearized, with the following relations:

$$1/f' = (1/f'_{m,n})(2 - f'/f'_{m,n}) \tag{14a}$$

$$\frac{1}{f'} W = \left(\frac{W}{f'}\right)_{m,n} + \frac{W}{f'_{m,n}} - \left(\frac{W}{f'}\right)_{m,n} \frac{f'}{f'_{m,n}} \tag{14b}$$

$$e \sum_{i=1}^{NI} h_i \left(\frac{w_i}{\rho}\right) = \sum_{i=1}^{NI} \left[\bar{W}_i \Delta h_i{}^F - e\theta h_i \frac{\partial}{\partial\theta}\left(\frac{w_i}{\rho}\right)\right]_{m,n} + \theta T_e \sum_{i=1}^{NI} \left[\bar{W}_i C_{1_i} + \frac{eh_i}{T_e} \frac{\partial}{\partial\theta}\left(\frac{w_i}{\rho}\right)\right]_{m,n} \tag{14c}$$

$$w_i/\rho = W_i{}^0 - W_i{}^1 c_i \tag{14d}$$

In the preceding relations, the quantities without subscripts are evaluated in the neighborhood of the point (m,n). The coefficients in Eq. (13) become

Momentum equation:

$$\alpha_1{}^1 = -(V - l')/l \tag{15a}$$

$$\alpha_2{}^1 = -2\beta f'/l - F/f' \tag{15b}$$

$$\alpha_3{}^1 = -(\beta/l)[-(f')^2 + \bar{M}_e\theta/\bar{e}\bar{M}] + F \tag{15c}$$

$$\alpha_4{}^1 = -f'/l \tag{15d}$$

where

$$F = \frac{\partial^2 f'}{\partial\eta^2} + \alpha_1{}^1 \frac{\partial f'}{\partial\eta} - \frac{\beta}{l}\left[(f')^2 + \frac{\bar{M}_e\theta}{\bar{e}\bar{M}}\right] = \frac{2\xi f'}{l} \frac{\partial f'}{\partial\xi}$$

Energy equation:

$$\alpha_1{}^2 = [\bar{c}' - \bar{c}_p(V + d + b)]/\bar{c} \tag{15e}$$

$$\alpha_2{}^2 = \left\{\bar{c}_p f'\left(\alpha\beta \frac{\bar{M}_e}{\bar{e}\bar{M}} - \bar{e}\right) - \sum_{i=1}^{NI}\left[\bar{W}_i C_{1_i} + \frac{eh_i}{T_e}\frac{\partial}{\partial\theta}\left(\frac{w_i}{\rho}\right)\right]\right\}\Big/\bar{c} \tag{15f}$$

$$\alpha_3{}^2 = \left\{\bar{c}_p \alpha l\left(\frac{\partial f'}{\partial\eta}\right)^2 - \frac{1}{T_e}\sum_{i=1}^{NI}\left[\bar{W}_i \Delta h_i{}^F - \theta e h_i \frac{\partial}{\partial\theta}\left(\frac{w_i}{\rho}\right)\right]\right\}\Big/\bar{c} \tag{15g}$$

¶ In Russia, this idea of solving the equations individually has also been developed.[4]

$$\alpha_4^2 = -f'\bar{c}_p/\bar{c} \tag{15h}$$

Species equation ($i = 3, 4, \ldots, NI + 2$):

$$\alpha_1^i = -(V - b_1')/b_i \tag{15i}$$

$$\alpha_2^i = -eW_i^1/b_i \tag{15j}$$

$$\alpha_3^i = (eW_i^0 + \bar{b}_i')/b_i \tag{15k}$$

$$\alpha_4^i = -f'/b_i \tag{15l}$$

The boundary layer is divided with a grid of size $\Delta\eta$ and $\Delta\xi$ with $\xi = m \cdot \Delta\xi$ and $\eta = n \cdot \Delta\eta$. It is assumed that f', θ, and the c_i's are known at the grid points in the mth column and unknown in the $(m + 1)$th column. In the present implicit scheme, the derivatives are replaced with linear difference quotients, and the partial differential equations are evaluated at $(m + \frac{1}{2}, n)$. However, the equations are written with a parameter Θ which will give the various finite difference schemes as indicated below:

$$\Theta = \begin{cases} 0 & \text{Explicit} \\ \frac{1}{2} & \text{Crank-Nicolson (present scheme)} \\ 1 & \text{Implicit} \end{cases}$$

With the function $W(\xi,\eta)$ representing the dependent variables, the difference quotients are written as

$$\partial W/\partial\xi = (W_{m+1,n} - W_{m,n})/\Delta\xi \tag{16a}$$

$$\partial W/\partial\eta = [\Theta(W_{m+1,n+1} - W_{m+1,n-1}) + (1 - \Theta)(W_{m,n+1} - W_{m,n-1})]/(2\Delta\eta) \tag{16b}$$

$$\partial^2 W/\partial\eta^2 = [\Theta(W_{m+1,n+1} - 2W_{m+1,n} + W_{m+1,n-1}) + (1 - \Theta)(W_{m,n+1} - 2W_{m,n} + W_{m,n-1})]/\Delta\eta^2 \tag{16c}$$

$$W = \Theta W_{m+1,n} + (1 - \Theta)W_{m,n} \tag{16d}$$

$$W \cdot Z = (1 - 2\Theta)W_{m,n}Z_{m,n} + \Theta(W_{m,n}Z_{m+1,n} + Z_{m,n}W_{m+1,n}) \tag{16e}$$

When these difference quotients and expressions are used with the partial differential equations (13), the finite difference equations become the simultaneous (involving only one dependent variable across the boundary layer) linear algebraic equations

$$A_n{}^i W^i{}_{m+1,n+1} + B_n{}^i W^i{}_{m+1,n} + C_n{}^i W^i{}_{m+1,n-1} = D_n{}^i \tag{17}$$

where

$n = 2, 3, \ldots, N - 1$		
$i = 1$	Momentum equation	$W^1 = f'$
$i = 2$	Energy equation	$W^2 = \theta$
$i = 3$	First species equation	$W^3 = c_1$
$i = 4$	Second species equation	$W^4 = c_2$
.	.	.
.	.	.
.	.	.
$i = NI + 1$	$NI - 1$ species equation	$W^{NI+1} = c_{NI-1}$

The coefficients in the preceding equations with $L_i{}^T = 0 (\bar{a}_i = a = 0)$ are

$$A_n{}^i = \Theta P(1 + \Delta\eta\alpha_1{}^i/2) \tag{18a}$$

$$B_n{}^i = \bar{\delta} + \Theta P(-2 + \alpha_2{}^i\Delta\eta^2) \tag{18b}$$

$$C_n{}^i = \Theta P(1 - \Delta\eta\alpha_1{}^i/2) \tag{18c}$$

$$D_n{}^i = -(1 - \Theta)P[(1 + \Delta\eta\alpha_1{}^i/2)W_{m,n+1} + (-2 + \alpha_2{}^i\Delta\eta^2)W_{m,n} + (1 - \Delta\eta\alpha_1{}^i/2)W_{m,n-1}] + \bar{\delta}W_{m,n} - P\Delta\eta^2\alpha_3{}^i \tag{18d}$$

where

$$P = \Delta\xi/(2\xi\Delta\eta^2\alpha_4{}^i); \quad \bar{\delta} = 1$$

In the preceding coefficients, the α^i's are determined from relations (15), where all quantities are evaluated at the mth column of grid points across the boundary layer. The independent variable ξ is evaluated at (m) for the explicit, $(m + \frac{1}{2})$ for the Crank-Nicolson, and $(m + 1)$ for the implicit schemes. In the relation (15g) it was found necessary to express the following derivative in the energy equation as:

$$(\partial f'/\partial\eta)^2 = (f'_{m,n+1} - f'_{m,n-1})(f'_{m+1,n+1} - f'_{m+1,n-1})/4\Delta\eta^2$$

It should be noted that the momentum equation is solved before the energy equation in order that the values of f' at the $(m + 1)$th column are available for the preceding expression.

From truncation-error considerations, the mass fraction in relation (14d) would be evaluated as shown; however, such a form can encounter stability problems. Although stability is usually considered to be practically unaffected by lower-order terms, as discussed by Richtmyer,[88] in actual computations with finite step size, these terms can control the stability. As considered by Richtmyer, stability is concerned with what happens in the limit as the mesh sizes approach zero. Therefore, such stability analyses cannot be completely satisfactory when finite mesh sizes are employed. If $W_i{}^0$ and $W_i{}^1$ were constants, then it appears that stable solutions are obtained without any restrictions on the step sizes. However, $W_i{}^0$ and $W_i{}^1$ are not constant, and stability problems can occur if the step size becomes too large, but the formulation below appears to minimize unstable solutions. The convergence of the system of difference equations to the differential equations has not been investigated. However, Douglas[76] states that an implicit or Crank-Nicolson difference scheme is convergent for an equation of the type (13).

In relation (14d) the mass fraction is evaluated at $(m + 1)$ for all difference schemes and the evaluation of relation (15j) must be changed. For the species equation, the value of α_2 becomes

$$\alpha_2{}^i = \begin{cases} -eW_i{}^1/(\Theta b_i) & \text{in } B_n{}^i \\ 0 & \text{in } D_n{}^i \end{cases}$$

At a stagnation point or at the tip of a sharp body, $\xi = 0$ and the partial differential equations (13) become ordinary differential equations and provide initial profiles to start the solution along the body. The ordinary differential equations can be solved with the same finite difference procedure employed for the partial differential equations. The coefficients in Eq. (18) for the ordinary differential equations are the same except the following quantities become $\Theta = P = 1$; $\bar{\delta} = 0$ and $F = 0$.

To complete the system of Eqs. (17), the boundary conditions are written in the following form:

$$W^i{}_{m+1,1} = H^i W^i{}_{m+1,2} + F^i W^i{}_{m+1,3} + h^i \tag{19a}$$

$$W^i{}_{m+1N} = g^i \tag{19b}$$

The boundary conditions for the momentum and energy equations [conditions (10a, 10b, 12a, and 12b)] are readily written in the previously described form. The mass flux of species i at the wall is expressed as

$$\dot{m}_i = P_i + Q_i(c_i)_b = c_i\rho v + j_i \tag{20}$$

The relative mass flux with $L_i{}^T = 0$ is written as

$$j_i = -(1/\overline{W})\{Le_i(\partial c_i/\partial\eta) + \Delta b_i\} \tag{21}$$

where

$$\overline{W} = \frac{Pr_b(2\xi)^{1/2}}{l_b(\rho\mu)_i r_b{}^j u_e}; \quad \Delta b_i = \sum_{\substack{k=1 \\ k\neq i}}^{NI} \Delta b_{ik}\left(\frac{\partial c_k}{\partial\eta}\right)_m$$

The derivative in the preceding expression is written as

$$\frac{\partial c_i}{\partial \eta} = \frac{1}{2\Delta\eta}(-3c_{i_1} + 4c_{i_2} - c_{i_3})_{m+1} \tag{22}$$

The relations (20–22) can now be employed to determine the wall boundary condition coefficients H^i, F^i, and h^i. The remaining boundary condition coefficients for the momentum and energy equation are given below, whereas the edge condition for the species equations comes from relation (12c);

Momentum:

$$H^1 = 0; \quad F^1 = 0; \quad h^1 = 0; \quad g^1 = 1 \tag{23a}$$

Energy:

$$H^2 = 0; \quad F^2 = 0; \quad h^2 = T_b/T_e; \quad g^2 = 1 \tag{23b}$$

Species for $i = 1,2, \ldots, NI$:

$$H^{i+2} = 4/D_i; \quad F^{i+2} = -1/D_i$$
$$h^{i+2} = [2\Delta\eta/(Le_i)_b](P_i\overline{W} + \Delta b_i)/D_i; \quad g^{i+2} = c_{ie} \tag{23c}$$

where

$$D_i = 3 + [2\Delta\eta/(Le_i)_b]\overline{W}[(\rho v)_b - Q_i]$$
$$(\rho v)_b = \sum_{i=1}^{NI} \dot{m}_i = \sum_{i=1}^{NI} (P_i + Q_i c_i)$$

The quantities in these relations are evaluated at the mth step where they can be determined without an iteration process. The values of P_i and Q_i depend on the boundary conditions at the wall and are determined by the mass flux $\dot{m}_i$ of the species, as was discussed in an earlier section. The total mass flux is determined from the sum of the individual species mass flux.

The difference equation (17) and the boundary conditions (19) form a system of linear algebraic equations of the tridiagonal type. These are readily solved with the technique discussed by Richtmyer.[88] Since the equations are uncoupled, a choice of the order for solving the dependent variables must be made. Experience has shown that this order is important. The tangential and normal velocity are solved for first, and the species must be solved for before the temperature. The continuity equation is then used to obtain $V_{m+1/2,n}$ with the finite difference representation

$$V_{m+1/2,n} = V_{m+1/2,n-1} - \Delta\eta\left(\frac{\xi}{\Delta\xi} + \frac{1}{4}\right)(f'_{m+1,n} + f'_{m+1,n-1}) + \Delta\eta\left(\frac{\xi}{\Delta\xi} - \frac{1}{4}\right)(f'_{m,n} + f'_{m,n-1}) \tag{24}$$

In the preceding finite difference procedure, certain quantities should be evaluated at $(m + \frac{1}{2})$, but have used the known values at (m). An iteration could be employed such that the values at $(m + \frac{1}{2})$ would be used when convergence is obtained. However, the present calculations have shown that this is not necessary.

In solving the boundary-layer equations, the finite difference procedure is applied in the transformed ξ, η coordinate system. The results must be related back to the physical x, y coordinate system. Also the edge conditions are given as a function of x and are required for the finite difference solution as a function of ξ. The procedure of specifying $\Delta x(x_{m+1} = x_m + \Delta x)$ and then finding $\Delta\xi$ has been employed. The transformed coordinate ξ is related to x by the ordinary differential equation [see Eq. (1a)]

$$d\xi/dx = (\rho\mu)_r u_e r_b^{2j} \tag{25}$$

The conditions at the edge of the boundary layer as a function of x and the body radius r_b are required to solve the foregoing equation. For a sharp or blunt conical body, the body radius is an algebraic expression whereas, for a hyperboloid, an ordinary differential equation must be solved to obtain r_b as a function of x.

For the value of ξ as a function of x, the ordinary differential Eq. (25) has to be solved numerically for most body shapes. When the Runge-Kutta method is applied to this equation, the following is obtained:

$$\xi_{m+1} = \xi_m + \Delta\xi$$

where

$$\Delta\xi = \tfrac{1}{6}\Delta x[\lambda(x_M) + 4\lambda(x_M + \tfrac{1}{2}\Delta x) + \lambda(x_M + \Delta x)]$$
$$\lambda(x_M) = [(\rho\mu)_r u_e r_b^{2j}]_{x=x_M}$$

The value of ξ at $(m + \frac{1}{2})$ can be obtained from

$$\xi_{m+1/2} = \xi_m + \tfrac{1}{2}\Delta\xi$$

The conditions at the edge of the boundary layer, u_e, T_e, p_e, and c_{i_e}'s (air species only), are required as a function of x. A table of these edge properties as a function of x is employed, with Lagrange interpolation used to obtain the edge conditions and the derivatives of the edge conditions for any value of x.

IV. Discussion of Numerical Results

The present technique for solving the boundary-layer equations has been used to obtain the flow on a sharp cone and a hyperboloid. These examples are used as test cases to illustrate the present implicit finite difference scheme when applied to an air gas model with finite reaction rates. The first case is a sharp cone at 150-kft altitude, 22-kfps velocity, and a wall temperature of 1000°K with the gas undissociated at the surface. This problem has been investigated by the author[53] previously and also by Galowin and Gould,[54] Gruenich and Pindroh,[64] and Moore.[68] Although sharp-cone results have been presented in Ref. 24, Moore has shown that these results differ significantly from finite difference solutions. He attributed these differences to the inaccuracies associated with the use of polynomials in Ref. 24.

The present results for the peak electron density are given in Fig. 2 and are compared to the results of other authors. The present results employ 28 points across the boundary layer and an initial value of $\Delta x_0 = 0.001$, and the step size increases according to the relation $\Delta x = \Delta x_0\,(2m - 1)$, where $m = 1, 2, 3, \ldots, M$ as each step is taken. A total of 122 steps are taken to obtain the solution to 14.884 ft. The present method has been employed with all the binary Lewis-Semenov numbers equal to 1.4 and with complete multicomponent diffusion included. The multicomponent diffusion results are slightly higher than the binary diffusion results, but the difference would not be distinguishable if both were plotted in Fig. 2. When the present method employs the reaction rates of Ref. 53, the peak electron density is close to the value given in Ref. 53. The difference between the various results is mainly due to reaction rates, transport properties, and thermodynamic properties. When Moore[68] used the rates of Ref. 53, his prediction of the peak electron density was in close agreement with Ref. 53. The difference from the present results can be attributed to the reaction rates used. The results of Gruenich and Pindroh[64] employ the same reaction rates as those of Ref. 53, but Sutherland's viscosity law is used and electronic excitation is ignored in the thermodynamic properties. The results of Galowin and Gould[54] are different because of the reaction rates and transport properties that are employed.

The boundary-layer flow on a hyperboloid has been investigated at conditions corresponding to an altitude of 100 kft and a velocity of 20 kfps, with a wall temperature of 1000°K.** This case is a way to verify if a numerical tech-

** This is case A, requested for the AGARD seminar.

Table 2 Properties at edge of boundary layer

	X(ft.)	P_e(psf)	U_e(fps)	T_e(°R)	C_{O_2}	C_{N_2}	C_O	C_N	C_{NO}	C_{NO^+}
1	0.	1.2772E+04	0.	1.2603E+04	4.6176E-04	5.8273E-01	2.2608E-01	1.7538E-01	1.4884E-02	6.2807E-04
2	3.3333E-03	1.2751E+04	3.1854E+02	1.2597E+04	4.6176E-04	5.8273E-01	2.2608E-01	1.7538E-01	1.4884E-02	6.2807E-04
3	5.0000E-03	1.2726E+04	4.7781E+02	1.2590E+04	4.6176E-04	5.8273E-01	2.2608E-01	1.7538E-01	1.4884E-02	6.2807E-04
4	6.6667E-03	1.2691E+04	6.3709E+02	1.2589E+04	4.6176E-04	5.8273E-01	2.2608E-01	1.7538E-01	1.4884E-02	6.2807E-04
5	7.8943E-03	1.2659E+04	7.3727E+02	1.2589E+04	4.6176E-04	5.8273E-01	2.2608E-01	1.7538E-01	1.4884E-02	6.2807E-04
6	1.0471E-02	1.2575E+04	9.7938E+02	1.2578E+04	4.6080E-04	5.8301E-01	2.2608E-01	1.7510E-01	1.4851E-02	6.2597E-04
7	1.3353E-02	1.2456E+04	1.2516E+03	1.2562E+04	4.5920E-04	5.8329E-01	2.2608E-01	1.7468E-01	1.4803E-02	6.2297E-04
8	1.6362E-02	1.2305E+04	1.5381E+03	1.2541E+04	4.5696E-04	5.8413E-01	2.2624E-01	1.7412E-01	1.4740E-02	6.1876E-04
9	1.7913E-02	1.2218E+04	1.6868E+03	1.2529E+04	4.5568E-04	5.8441E-01	2.2624E-01	1.7370E-01	1.4704E-02	6.1636E-04
10	2.0041E-02	1.2089E+04	1.8921E+03	1.2510E+04	4.5376E-04	5.8497E-01	2.2624E-01	1.7314E-01	1.4644E-02	6.1246E-04
11	2.2564E-02	1.1922E+04	2.1379E+03	1.2484E+04	4.5120E-04	5.8553E-01	2.2624E-01	1.7244E-01	1.4566E-02	6.0766E-04
12	2.4595E-02	1.1779E+04	2.3378E+03	1.2461E+04	4.4896E-04	5.8637E-01	2.2640E-01	1.7188E-01	1.4497E-02	6.0316E-04
13	2.6698E-02	1.1623E+04	2.5471E+03	1.2434E+04	4.4608E-04	5.8694E-01	2.2640E-01	1.7118E-01	1.4416E-02	5.9806E-04
14	3.0447E-02	1.1330E+04	2.9263E+03	1.2380E+04	4.4064E-04	5.8862E-01	2.2632E-01	1.6964E-01	1.4251E-02	5.8756E-04
15	3.3755E-02	1.1059E+04	3.1995E+03	1.2347E+04	4.4128E-04	5.9002E-01	2.2656E-01	1.6824E-01	1.4215E-02	5.8035E-04
16	3.5109E-02	1.0945E+04	3.2929E+03	1.2335E+04	4.4128E-04	5.9058E-01	2.2656E-01	1.6782E-01	1.4200E-02	5.7765E-04
17	3.6774E-02	1.0804E+04	3.4067E+03	1.2319E+04	4.4032E-04	5.9114E-01	2.2656E-01	1.6712E-01	1.4167E-02	5.7435E-04
18	3.9481E-02	1.0572E+04	3.5882E+03	1.2290E+04	4.3808E-04	5.9226E-01	2.2656E-01	1.6613E-01	1.4095E-02	5.6865E-04
19	4.3853E-02	1.0196E+04	3.8714E+03	1.2237E+04	4.3328E-04	5.9394E-01	2.2672E-01	1.6459E-01	1.3948E-02	5.5875E-04
20	4.9474E-02	9.7151E+03	4.2168E+03	1.2165E+04	4.2656E-04	5.9590E-01	2.2672E-01	1.6263E-01	1.3732E-02	5.4555E-04
21	5.6219E-02	9.1516E+03	4.6055E+03	1.2075E+04	4.1728E-04	5.9842E-01	2.2688E-01	1.6011E-01	1.3453E-02	5.2904E-04
22	6.2065E-02	8.6824E+03	4.9202E+03	1.1994E+04	4.0864E-04	6.0066E-01	2.2704E-01	1.5815E-01	1.3198E-02	5.1494E-04
23	6.9260E-02	8.1390E+03	5.2780E+03	1.1895E+04	3.9808E-04	6.0346E-01	2.2736E-01	1.5549E-01	1.2879E-02	4.9783E-04
24	7.8614E-02	7.4937E+03	5.6975E+03	1.1770E+04	3.8464E-04	6.0683E-01	2.2752E-01	1.5241E-01	1.2486E-02	4.7593E-04
25	9.0126E-02	6.7917E+03	6.1538E+03	1.1619E+04	3.6800E-04	6.1075E-01	2.2784E-01	1.4862E-01	1.1988E-02	4.5222E-04
26	1.0509E-01	6.1493E+03	6.5535E+03	1.1440E+04	3.5040E-04	6.1551E-01	2.2816E-01	1.4428E-01	1.1463E-02	4.2101E-04
27	1.2351E-01	5.2555E+03	7.1665E+03	1.1235E+04	3.2640E-04	6.2055E-01	2.2864E-01	1.3955E-01	1.0743E-02	3.9370E-04
28	1.4838E-01	4.4633E+03	7.7179E+03	1.0993E+04	3.0131E-04	6.2644E-01	2.2896E-01	1.3417E-01	1.0014E-02	3.5710E-04
29	1.7969E-01	3.7398E+03	8.2715E+03	1.0717E+04	2.6544E-04	6.3260E-01	2.2976E-01	1.2857E-01	8.9574E-03	3.2169E-04
30	2.2196E-01	3.0667E+03	8.8286E+03	1.0409E+04	2.3469E-04	6.3876E-01	2.3008E-01	1.2282E-01	8.0541E-03	2.7721E-04
31	2.6424E-01	2.6040E+03	9.2646E+03	1.0141E+04	1.9949E-04	6.4409E-01	2.3072E-01	1.1821E-01	6.9979E-03	2.5468E-04
32	3.1120E-01	2.2380E+03	9.6338E+03	9.8955E+03	1.7302E-04	6.4829E-01	2.3120E-01	1.1436E-01	6.1907E-03	2.2923E-04
33	3.8636E-01	1.8412E+03	1.0075E+04	9.5822E+03	1.5184E-04	6.5333E-01	2.3200E-01	1.0964E-01	5.2244E-03	1.9916E-04
34	4.5149E-01	1.6076E+03	1.0363E+04	9.3672E+03	1.2410E-04	6.5670E-01	2.3232E-01	1.0652E-01	4.6302E-03	1.8008E-04
35	5.3165E-01	1.4018E+03	1.0637E+04	9.1536E+03	1.0685E-04	6.6006E-01	2.3264E-01	1.0353E-01	4.0511E-03	1.6222E-04
36	6.3586E-01	1.2151E+03	1.0909E+04	8.9359E+03	9.0080E-05	6.6342E-01	2.3296E-01	1.0049E-01	3.5109E-03	1.4515E-04
37	7.4007E-01	1.0834E+03	1.1116E+04	8.7660E+03	8.0448E-05	6.6594E-01	2.3312E-01	9.8140E-02	3.1238E-03	1.3258E-04
38	8.2023E-01	1.0060E+03	1.1247E+04	8.6599E+03	7.4656E-05	6.6762E-01	2.3312E-01	9.6557E-02	2.9057E-03	1.2498E-04
39	9.2043E-01	9.2915E+02	1.1384E+04	8.5498E+03	6.8768E-05	6.6958E-01	2.3328E-01	9.4834E-02	2.6860E-03	1.1736E-04
40	1.0407E+00	8.5750E+02	1.1518E+04	8.4430E+03	6.3584E-05	6.7126E-01	2.3344E-01	9.3069E-02	2.4847E-03	1.1016E-04
41	1.2812E+00	7.5662E+02	1.1721E+04	8.2876E+03	5.6736E-05	6.7435E-01	2.3360E-01	9.0155E-02	2.2143E-03	9.9927E-05
42	1.4615E+00	7.0394E+02	1.1835E+04	8.2063E+03	5.3600E-05	6.7631E-01	2.3360E-01	8.8362E-02	2.0880E-03	9.4645E-05
43	1.7321E+00	6.4673E+02	1.1965E+04	8.1209E+03	5.0144E-05	6.7855E-01	2.3376E-01	8.6093E-02	1.9892E-03	8.9094E-05
44	1.9124E+00	6.1818E+02	1.2034E+04	8.0814E+03	4.9376E-05	6.7995E-01	2.3376E-01	8.4762E-02	1.9169E-03	8.6393E-05
45	2.0928E+00	5.9492E+02	1.2091E+04	8.0527E+03	4.8704E-05	6.8135E-01	2.3376E-01	8.3530E-02	1.8860E-03	8.4322E-05
46	2.3453E+00	5.6884E+02	1.2158E+04	8.0255E+03	4.9056E-05	6.8275E-01	2.3376E-01	8.1975E-02	1.8641E-03	8.2192E-05
47	2.5978E+00	5.4825E+02	1.2212E+04	8.0097E+03	4.8256E-05	6.8415E-01	2.3376E-01	8.0560E-02	1.8623E-03	8.0662E-05
48	2.9513E+00	5.2589E+02	1.2273E+04	8.0010E+03	4.8800E-05	6.8611E-01	2.3376E-01	7.8767E-02	1.8809E-03	7.9281E-05
49	3.3048E+00	5.0879E+02	1.2321E+04	8.0037E+03	4.9888E-05	6.8751E-01	2.3376E-01	7.7142E-02	1.9196E-03	7.8501E-05
50	3.7997E+00	4.9077E+02	1.2374E+04	8.0198E+03	5.2352E-05	6.8947E-01	2.3376E-01	7.5069E-02	2.0027E-03	7.7991E-05
51	4.2947E+00	4.8040E+02	1.2414E+04	8.0445E+03	5.5136E-05	6.9143E-01	2.3376E-01	7.3192E-02	2.0955E-03	7.8051E-05

nique will operate properly when the gas is near chemical equilibrium. Also, the blunt body requires the solution from a stagnation point downstream where edge conditions change significantly The edge conditions were provided by Lewis,†† and are given in Table 2 as used in the computer program. These conditions are obtained from the inviscid streamline along the surface of the hyperboloid with finite rate chemistry. The pressure along the streamline or body surface is that obtained from modified Newtonian theory. The conditions at the edge of the boundary layer are used as the reference conditions; for example, as required in Eq. (1a). When the body streamline is used, the classical boundary-layer approach is being followed. For the case of chemically reacting flows, there is considerable error in the prediction of the chemical species at the edge of the boundary layer far downstream on the body. The usual approach of taking into account the swallowing of the inviscid flow is not employed. As this case is intended to be a test example, the introduction of swallowing introduces another variable that can influence the results obtained by any method.

The surface boundary conditions employed in this study are such that the wall is either noncatalytic or fully catalytic. For the case of the noncatalytic wall, the terms $\dot{m}_i$, P_i, and Q_i in Eq. (20) are zero for all of the air species. A fully catalytic recombination surface for air is defined as a wall where every dissociated and ionized species that strikes the

†† These conditions were provided by C. H. Lewis in a private communication to participants in the AGARD seminar.

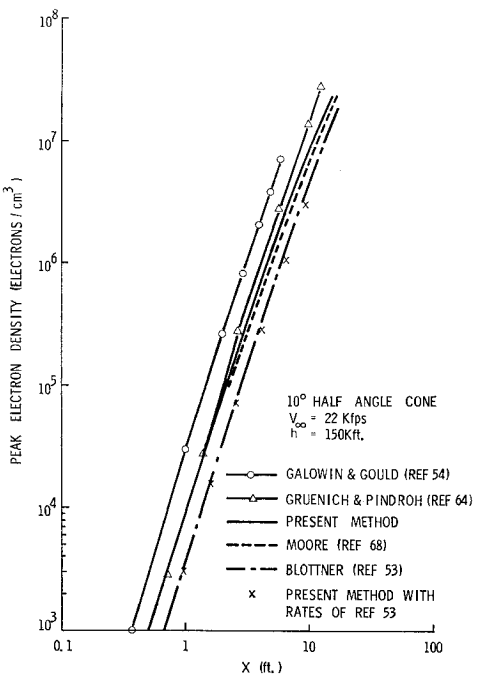

Fig. 2 Peak electron number density on sharp cone.

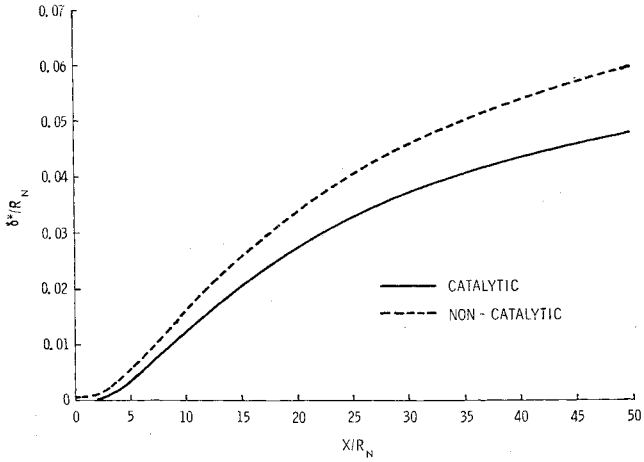

Fig. 3 Displacement thickness along hyperboloid.

surface is converted to a molecular species due to the heterogeneous reactions. For dissociated and ionized species, the P_i's are zero, whereas

$$Q_i = -\rho_b (RT_b/2\pi M_i)^{1/2}, \quad i = \text{O, N, NO, NO}^+$$

For the molecular species, the Q_i's are zero and

$$P_i = -\sum_k \frac{\alpha_k{}^j}{2} \frac{M_i}{M_k} c_{kb} Q_k \qquad \begin{matrix} k = \text{O, N, NO, NO}^+ \\ i = \text{O}_2, \text{N}_2 \end{matrix}$$

where $\alpha_k{}^j$ = amount of element j in species k i = molecular species of element j.

The variation of the radius of the hyperboloid is required as a function of the distance along the surface. This is obtained by solving the ordinary differential equation

$$dr_b/dx = \{1 + (r_b/R_N)^2/[1 + (r_b/R_N)^2 \tan^2\theta]\}^{-1/2}$$

In the results presented, 28 points are employed across the boundary layer, with $\eta = 5.4$ at the outer edge. The step size along the body was increased as the computation proceeded. The step sizes employed were 0.01, 0.025, 0.05, 0.1, 0.25, 0.5, 1.0, and 2.0, where the numbers of steps taken of each were 10, 16, 16, 20, 12, 12, 14, and 12, respectively, for a total of 106 steps. The time required per step along the body is given in Fig. 1 for the case of binary diffusion. For the case of air with multicomponent diffusion, the computation is approximately twice as large. In Fig. 1, the times for the IBM 7094 computer correspond to the computer program employed in Refs. 53 and 79. The times for the CDC 3600 are for the computer program described in this paper.

The boundary-layer flow results for the hyperboloid test case with a catalytic and noncatalytic wall are given in Figs.

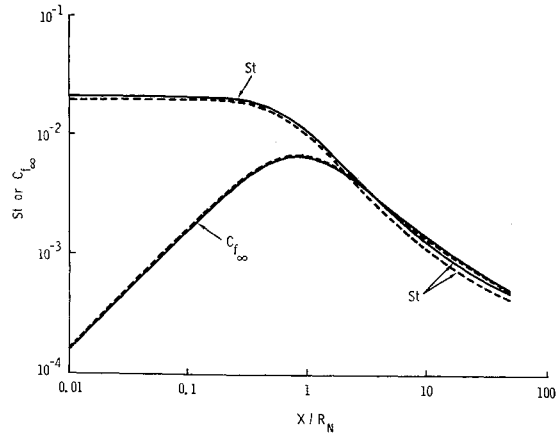

Fig. 4 Stanton number and skin friction along hyperboloid.

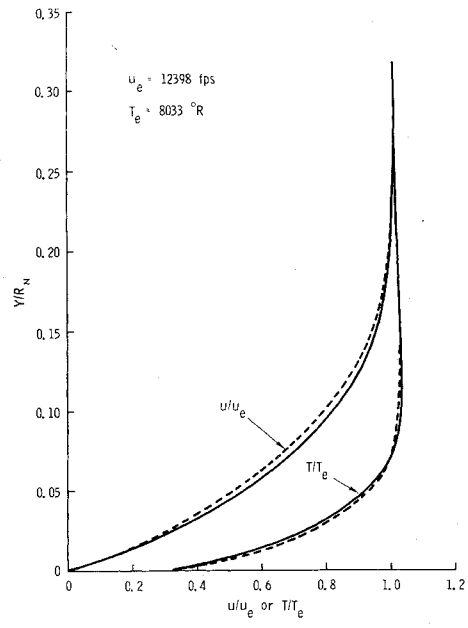

Fig. 5 Velocity and temperature across the boundary layer at $x/R_N = 50$.

3–7. Not too much physical significance should be attached to the results, since the swallowing of the inviscid flow has been neglected. The displacement thickness,

$$\frac{\delta^*}{R_N} = \int_0^{y_e/R_N} \left(1 - \frac{\rho u}{\rho_e u_e}\right) d\left(\frac{y}{R_N}\right)$$

Stanton number,

$$St = \left(k \frac{\partial T}{\partial y} - \sum_{i=1}^{NI} h_i j_i\right)_b \Big/ \rho_\infty V_\infty (H_0 - H_b)$$

and the local skin-friction coefficient,

$$C_{f\infty} = \mu_b (\partial u/\partial y)_b / (\tfrac{1}{2}\rho_\infty V_\infty{}^2)$$

are given in Figs. 3 and 4. The velocity, temperature, and species distribution across the body layer at 50 nose radii downstream for a catalytic and noncatalytic wall are given in Figs. 5, 6, and 7.

The effects of swallowing of the inviscid flow can be taken into account in the boundary-layer program by changing the edge tables (see Table 2). The appropriate edge conditions which should be employed are not clear, but a solution of the nonequilibrium inviscid flow is required with the interaction

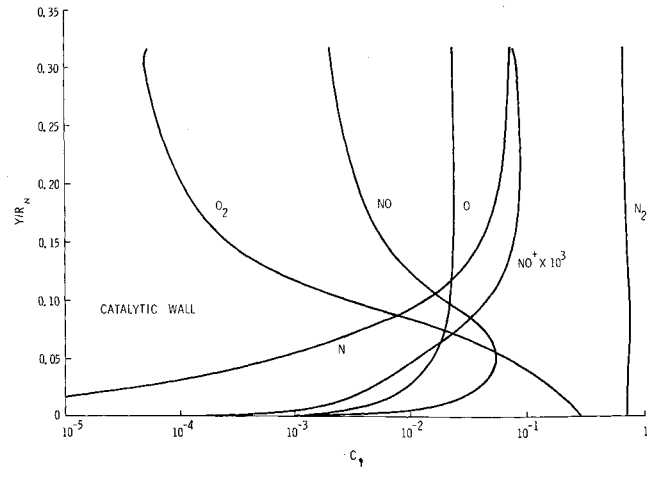

Fig. 6 Mass fraction of chemical species across the boundary layer at $x/R_N = 50$.

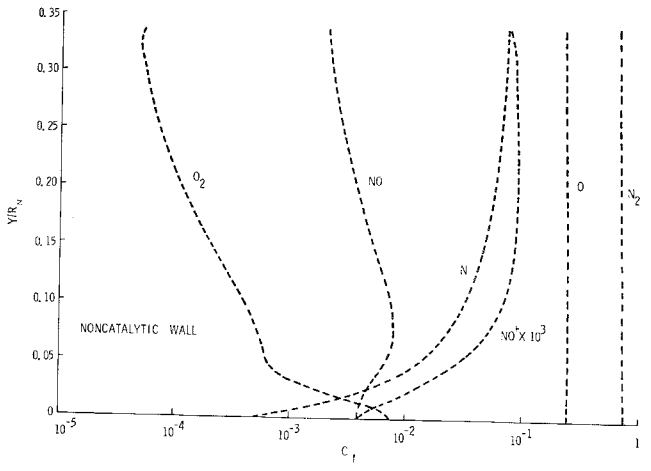

Fig. 7 Mass fraction of chemical species across the boundary layer at $x/R_N = 50$.

of the boundary layer taken into account. If swallowing is taken into account, the local skin-friction coefficient should be a little larger whereas the Stanton number will be slightly larger. The temperature profile at $x/R_N = 50$ in Fig. 5 would be greatly different with swallowing and would have a maximum near the wall which is several times a lower edge temperature. The species profiles of Figs. 6 and 7 would also be changed as the freestream gas would be much less dissociated as part of the entropy layer would have been swallowed at $x/R_N = 50$.

For the solution with a noncatalytic wall, unstable results were obtained with the Crank-Nicolson ($\Theta = 0.5$) method. To avoid this problem, the implicit method with $\Theta = 1.0$ was employed. The results for the sharp-cone test case were compared with $\Theta = 0.5$ and 1.0, and the results were in close agreement downstream on the cone. Near the tip (first few inches) there was a difference between the predictions of the two methods for the mass fraction of the species, with the implicit method giving more accurate results. This type of stability problem has also been observed by Moore[68] and was corrected by using the implicit scheme for the first grid point away from the wall.

The examples indicate that the present method provides a technique for computing the boundary-layer flow with finite reaction rates when there are a large number of chemical species and when the flow is near local chemical equilibrium. With the equations uncoupled and the technique not requiring iterations at each step, the over-all computing time for flows with many chemical species is reasonable.

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