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Abstract

A numerical algorithm has been developed for solving the equations describing chemically reacting supersonic flows. The algorithm employs a two-stage Runge-Kutta method for integrating the equations in time and a Chebyshev spectral method for integrating the equations in space. The accuracy and efficiency of the technique have been assessed by comparison with an existing implicit finite-difference procedure for modeling chemically reacting flows. The comparison showed that the new procedure yielded equivalent accuracy on much coarser grids as compared to the finite-difference procedure with resultant significant gains in computational efficiency.

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Nomenclature

A	cross-sectional area, constant in Arrhenius law
a,b	constants in specific heat equations
C	concentration of species
c	speed of sound
c_p	specific heat at constant pressure
E	activation energy
e_o	total internal energy
$\vec{F}$	flux vector
$\hat{F}_n,\hat{F}_n^{(1)}$	expansion coefficients in Chebyshev series
f	mass fraction
$\vec{H}$	source vector
h_o	total enthalpy
H_T^o	reference enthalpy at standard conditions
I	identity matrix
K	equilibrium constant
k_b	reverse reaction rate
k_f	forward reaction rate
M	molecular weight
N	number of nodes
N_R	number of reactions
N_s	number of species
p	static pressure
p_o	total pressure
R	steady-state residual
R^o	universal gas constant
T_o	total temperature
T	static temperature
T_n	Chebyshev polynomial
t	time
Δt	time step
$\dot{w}$	species production rate
$\vec{U}$	dependent variable vector
u	velocity

x	spatial variable
Δx	spatial step size
γ	stoichiometric coefficient, ratio of specific heats
λ	eigenvalue
ρ	density
ϕ	equivalence ratio

Subscripts

c	based on chemistry
f	based on fluids
i,j	species indices
R	reactions, reference value
s	species
sp	evaluated spectrally

Superscript

$-$	mass weighted value

INTRODUCTION

Research to develop ramjet and supersonic combustion ramjet (scramjet) propulsion systems has been underway at the NASA Langley Research Center for a number of years. A critical element in the design of scramjets and ramjets is the detailed understanding of the complex flow field present in the engine over a range of operating conditions. Numerical modeling of various regions of the engine flow field has proven to be a valuable tool for gaining insight into the nature of these flows. In recent years, computer programs have been developed to model the chemically reacting flow fields in ramjet and scramjet systems.[1] [2] [3] These programs have employed both explicit and implicit finite-difference procedures to solve the equations governing the flow field in the engine combustors. The calculations have often required long computer runs to reach desired steady-state conditions and have been quite costly, due to stiffness introduced in the equations by the finite-rate chemical kinetics that is required for accurate modeling. Also, computer resource limitations have sometimes reduced the degree of spatial resolution that could be achieved in the calculations. These factors have led to the desire for more efficient and more highly accurate algorithms for solving chemically reacting combustor flows.

The system of partial differential equations describing chemically reacting flows (see eq. (4)) is stiff because of the highly disparate time scales that exist among the equations. Certain chemical reactions in an overall combustor kinetics system can take place on an extremely short scale of the order of 10^{-12} seconds, whereas the fluids dynamics may require 10^{-3} to 10 seconds for a typical case to reach steady-state conditions. There are of course several intermediate scales lying between these two extremes. Mathematically, stiffness is often defined by examining the eigenvalues of the Jacobian of the governing equation system and noting that the ratio of the real part of the largest to real part of the smallest eigenvalue is a large number. The former physical definition is perhaps the more useful test of stiffness; it is felt directly in the numerical integration of stiff systems through the required proper choice of the integration time step. We will deal with this requirement now and then follow with a discussion concerning integration of the spatial part of the problem.

Stiffness in the system of equations governing chemically reacting flows typically arises from the source terms in the equations describing production and loss of the chemical species that are present. Large values for these source terms produce rapid changes in the dependent variables being sought, and result in the very short time scales discussed in the previous paragraph. To explore the problem of mixed (short and long) time scales, consider the ordinary differential equation (ODE) system[4]

$$\frac{d\vec{f}}{dt} = [A]\,\vec{f} \tag{1}$$

where $f = [f_1, f_2]^T$, $f(0) = [2,1]^T$ and

$$A = \begin{bmatrix} -500.5 & 499.5 \\ 499.5 & -500.5 \end{bmatrix} .$$

The eigenvalues of [A] are $\lambda_1 = -1000.0$ and $\lambda_2 = -1.0$, and the solution to equation (1) follows as

$$f_1(t) = 1.5\,e^{-t} + 0.5\,e^{-1000t}$$
$$f_2(t) = 1.5\,e^{-t} - 0.5\,e^{-1000t}. \qquad (2)$$

Note that the solutions f_1 and f_2 have a rapidly decaying component corresponding to λ_1 and a much more slowly decaying component corresponding to λ_2. If we were solving this problem numerically, accuracy would require that we advance the solution from the initial conditions using very small time steps. However, once the solution dominated by λ_1 decays, we would prefer to advance the solution using larger time steps that would still maintain an acceptable level of accuracy. Care must be taken in picking a numerical algorithm that will allow this choice of time step. Otherwise, the numerical stability of the solution will continue to be dictated by λ_1 even though its component has decayed, and very small time steps will still be required to maintain stability. In response to this difficulty, several authors, including Bussing and Murman,[5] Stalnaker, et al.,[6] and Smoot, Hecker, and Williams[7] recognized that the stiff source terms in the system of equations governing chemically reacting flow should be evaluated implicitly. Therefore, for our problem, algorithms should be developed with the source terms written implicitly at the new time level in the integration step. Other terms in the governing equations, that do not lead to stiffness, can still be evaluated explicitly.[5 6 7]

Perhaps the best known algorithms for solving stiff systems of ordinary differential equations are those developed by Gear.[8] These schemes employ Adams´ methods of variable order with explicit formulas used to solve non-stiff equations in the system and implicit formulas used to solve the stiff equations. Hindmarsh generalized the Gear algorithms[9] and developed a variant to allow for a variable integration step size.[10] Another class of algorithms for effectively solving stiff ordinary differential equations is the exponential-fitted schemes, described in the work of Liniger and Willoughby[11] and Pratt.[12] These methods fit the solution at two or more integration points with an exponential interpolant rather than polynomial interpolants used in the Gear schemes. The exponential-fitted schemes more naturally follow the exponential behavior of solutions to chemical kinetics problems. Additionally, for decaying solutions, this class of algorithms has an infinite stability radius for both the implicit and explicit variants.[12] A good deal more work has been carried out to develop efficient and accurate algorithms for solving stiff systems of ordinary differential equations resulting from chemical kinetics problems. We will not continue our survey here, but rather we will refer readers to an interesting paper by Bui, Oppenheim, and Pratt[13] that further discusses the area of stiff ODE solvers.

Next, we deal with the computation of spatial derivatives in the governing equations. The importance of accurately modeling spatial derivatives cannot be overemphasized. Chemical reaction does not take place until fuel and oxidant are brought together and macroscopically mixed by convective transport, and then mixed down to the microscopic (molecular) level by diffusive processes. To model these processes, spatial derivatives must be accurately computed. Due to computer storage limitations, higher order numerical methods were indicated. Higher order finite-difference schemes offered one option for computing the spatial derivative. Another option was apparent from earlier work of the second and third authors to develop methods for highly accurate solutions of the Euler equations. Here, Hussaini, et.al.[14] used a spectral collocation method to compute the required spatial derivatives in the governing equations. Using this approach, several problems governed by the Euler equations were successfully solved and accurate solutions were obtained on relatively coarse grids as compared to finite-difference solutions of the same problems. Spectral methods are based on the representation of the solution to a problem f by a finite series of global functions X of the form

$$f(x) = \sum_{n=0}^{N} \hat{a}_n X_n(x), \tag{3}$$

where the $\hat{a}_n$ are the expansion coefficients of the series.[15] The X_n should be a complete orthogonal set. Spatial derivatives of f are then approximated by taking derivatives of the corresponding series (3). If properly applied, the high order approximation (3) yields a very accurate numerical representation for derivatives of f. Spectral methods should therefore satisfy our requirements for approximating spatial derivatives in the equation governing a chemically reacting flow field.

This paper discusses the development of a numerical algorithm for solving the equations governing a chemically reacting flow. The algorithm employs a two-stage partial implicit Runge-Kutta scheme for integrating the equations in time and a Chebyshev spectral collocation method for computing spatial derivatives in the equations. A computer program has been written to apply this algorithm for the solution of a reacting flow problem. The code is currently limited to quasi-one-dimensional inviscid flows with hydrogen-air reaction, which is appropriate for development and evaluation of the algorithm. There appear to be no restrictions prohibiting extension of the algorithm to three-dimensional viscous flows. Chemical reaction is represented in the program with a finite-rate chemistry model, and a real gas thermodynamic model is employed.

ANALYSIS

Governing Equations

The quasi-one-dimensional Euler equations in conservation law form with multiple species undergoing chemical reaction are[16]

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{F}}{\partial x} + \vec{H} = 0, \tag{4}$$

where

$$\vec{U} = \{\rho A,\ \rho u A,\ \rho e_o A,\ \rho f_i A\}^T \tag{5}$$

$$\vec{F} = \{\rho u A,\ \rho u^2 A + pA,\ \rho u h_o A,\ \rho u f_i A\}^T \tag{6}$$

$$\vec{H} = \{0,\ -p\,\frac{dA(x)}{dx},\ 0,\ -\dot{w}_i A\}^T, \tag{7}$$

and

$$h_o = \int_{T_R}^{T} \bar{c}_p dT + \frac{u^2}{2} + \sum_{j=1}^{N_s} (H_T^o)_j\, f_j \tag{8}$$

$$e_o = h_o - \left(\frac{R^o}{\bar{M}}\right)T. \tag{9}$$

If there are N_s chemical species, then, $i = 1,2,\ldots, (N_s - 1)$ and $(N_s - 1)$ equations must be solved for the species f_i. The final species mass fraction

f_{N_s} can then be found by conservation of mass since

$$\sum_{i=1}^{N_s} f_i = 1 \ .$$

Chemistry Model

The chemical reaction of hydrogen and oxygen is modeled in this work with the global finite-rate hydrogen-air chemistry model of Rogers and Chinitz.[17] This model adequately represents the chemical reaction taking place in the problems to be considered, and it also produces an extremely large disparity in the time scales present in the problems. This phenomenon allows the ability of the numerical algorithm to deal with resulting stiffness to be demonstrated.

The Rogers-Chinitz model assumes that the overall reaction of hydrogen and oxygen takes place through two reactions, the first resulting in the formation of hydroxyl radical, and the second combining the hydroxyl radical with hydrogen to form water. The reactions are given by,

$$H_2 + O_2 \underset{k_{b1}}{\overset{k_{f1}}{\rightleftharpoons}} 2OH \tag{10}$$

$$2OH + H_2 \underset{k_{b2}}{\overset{k_{f2}}{\rightleftharpoons}} 2H_2O \tag{11}$$

where the k_f's are the forward reaction rates and the k_b's are the reverse reaction rates. The reverse rates can be found given the forward rate and equilibrium constant K for each reaction, as

$$k_b = k_f/K. \tag{12}$$

The forward reaction rates are computed from the Arrhenius Law,

$$k_{f_i} = A_i T^{N_i} e^{-E_i/R^o T} \tag{13}$$

for each reaction i. For the Rogers-Chinitz model, the rates are given by,[17]

$$k_{f1} = A_1 \; T^{-10} \; e^{-4865/R^o T} \tag{14}$$

$$k_{f2} = A_2 \; T^{-13} \; e^{-42500/R^o T} \tag{15}$$

where

$$A_1 = (8.917 \; \phi + \frac{31.433}{\phi} - 28.95)(10^{47}) \; \frac{cm^3}{mole\text{-}s}$$

$$A_2 = (2.0 + \frac{1.333}{\phi} - 0.833 \; \phi)(10^{64}) \; \frac{cm^6}{mole^2\text{-}s}$$

and

$$K_1 = 26.164 \; e^{-8992/T}$$

$$K_2 = 2.682 \times 10^{-6} \; Te^{69415/T}.$$

Knowing the reaction rates for reactions (10) and (11), the production of the four species present in the model can be found from the law of mass action. For a general reaction,

$$\sum_{j=1}^{N_s} \gamma'_{ij} C_j \; \underset{k_{bi}}{\overset{k_{fi}}{\rightleftharpoons}} \; \sum_{j=1}^{N_s} \gamma''_{ij} C_j , \qquad i = 1,2,\ldots,N_R$$

the law of mass action states that the rate of change of concentration of species j by reaction i is given by,[18]

$$(\dot{C}_j)_i = (\gamma''_{ij} - \gamma'_{ij})\left[k_{fi} \prod_{j=1}^{N_s} C_j^{\gamma'_{ij}} - k_{bi} \prod_{j=1}^{N_s} C_j^{\gamma''_{ij}}\right]. \qquad (16)$$

The rate change in concentration of species j by all N_R reactions is then found by summing the contributions from each reaction,

$$\dot{C}_j = \sum_{i=1}^{N_R} (\dot{C}_j)_i. \qquad (17)$$

Finally, the production rate of species j is found from,

$$\dot{w}_j = \dot{C}_j M_j. \qquad (18)$$

Applying the law of mass action to the global model, equations (10) and (11), gives,[17]

$$\dot{C}_{O_2} = - k_{f1}\, C_{H_2}\, C_{O_2} + k_{b1}\, C_{OH}^2, \qquad (19)$$

$$\dot{C}_{H_2O} = 2(k_{f2}\, C_{OH}^2\, C_{H_2} - k_{b2}\, C_{H_2O}^2), \qquad (20)$$

$$\dot{C}_{H_2} = \dot{C}_{O_2} - \frac{1}{2}\dot{C}_{H_2O}, \qquad (21)$$

$$\dot{C}_{OH} = - (2\, \dot{C}_{O_2} + \dot{C}_{H_2O}). \qquad (22)$$

The source terms for the last i equations in (4) can now be determined, as a function of the dependent variables, by application of equation (18).

Thermodynamics Model

The specific heat at constant pressure, c_p, is nearly a linear function of temperature for each species present in the flow field (H_2, O_2, OH, H_2O, N_2) over the range of temperature being considered. We therefore fit the c_p versus temperature data[19] for each species i with

$$c_{p_i}(T) = a_i T + b_i, \tag{23}$$

where a and b are constants. A mixture specific heat, $\bar{c}_p$, can then be defined by weighting over the species i as

$$\bar{c}_p = \sum_{i=1}^{N_s} c_{p_i} f_i. \tag{24}$$

The total enthalpy of the mixture, made up of the five species, is given by

$$H = \sum_{i=1}^{N_s} f_i \left[\int_{T_R}^{T} c_{p_i} dT + H^o_{T_i} \right] + \frac{u^2}{2} \tag{25}$$

where H^o_T is the reference enthalpy at the reference temperature $T_R = 0$ K.[19] Putting equation (24) into (25) and integrating gives

$$H = \sum_{i=1}^{N_s} f_i \left[\frac{a_i T^2}{2} + b_i T + H^o_{T_i} \right] + \frac{u^2}{2}. \tag{26}$$

Finally, the mixture gas constant, $\bar{R}$, is found by weighting the individual gas constants over the species i as

$$\bar{R} = \sum_{i=1}^{N_s} R_i f_i. \tag{27}$$

Equations (24), (26), and (27) can then be used to define all other required thermodynamic variables.

SOLUTION OF THE GOVERNING EQUATIONS

Chebyshev Spectral Method

The Chebyshev spectral collocation method[15] is used to define the derivatives $\partial\vec{F}/\partial x$ in equations (4). To define $\partial\vec{F}/\partial x$, we expand $\vec{F}$ in terms of the Chebyshev polynomials

$$T_n(x) = \cos(n \cos^{-1} x) \tag{28}$$

in the truncated Chebyshev series

$$F(x) = \sum_{n=0}^{N} \hat{F}_n T_n(x) \tag{29}$$

where the $\hat{F}_n$ are the expansion coefficients of the series. To form a range on x, we introduce the change of variables

$$x = \cos\theta, \qquad 0 < \theta < \pi. \tag{30}$$

Putting equation (30) into (28) and introducing the resulting expression into (29) gives

$$F(x) = \sum_{n=0}^{N} \hat{F}_n \cos n\theta, \tag{31}$$

a Fourier cosine series. To discretize equation (31), we define a set of collocation points x_j by

$$x_j = \cos \frac{\pi j}{N}, \qquad j=0,1,2,\ldots,N \tag{32}$$

and the discrete form of (31) becomes

$$F_j = F(x_j) = \sum_{n=0}^{N} \hat{F}_n \cos \frac{n\pi j}{N}. \tag{33}$$

The inverse of (33) gives the $\hat{F}_n$ as

$$\hat{F}_n = \frac{2}{N\bar{C}_n} \sum_{j=0}^{N} \bar{C}_j^{-1} F_j \cos \frac{n\pi j}{N} \tag{34}$$

where

$$\bar{C}_j = \begin{cases} 2 & j = 0 \text{ or } j = N \\ 1 & 1 < j < (N-1) \end{cases}$$

Examination of equations (33) and (34) shows that the $\hat{F}_n$ can be efficiently evaluated using the fast Fourier transform.[20]

Next, we differentiate F in equation (33) with respect to x giving

$$F'(x) = \sum_{n=1}^{N} \hat{F}_n T_n'(x). \tag{35}$$

A form of equation (35) without derivatives of the Chebyshev polynomials is preferred, so we rewrite (35) in terms of another series

$$F'(x) = \sum_{n=0}^{N} \hat{F}_n^{(1)} T_n(x) \tag{36}$$

and then proceed to relate the coefficients of the two series. The following recursion relation exists between the Chebyshev polynomials and their derivatives[15]

$$\frac{T'_{n+1}}{n+1} - \frac{T'_{n-1}}{n-1} = \frac{2}{C_n} T_n \tag{37}$$

where

$$C_n = \begin{cases} 2 & n = 0 \\ 1 & n > 1 \end{cases} .$$

Putting equation (37) into (36) and algebraically manipulating the resulting expression gives

$$F'(x) = \sum_{n=1}^{N} \frac{C_{n-1}\hat{F}^{(1)}_{n-1}}{2n} T'_n - \sum_{n=1}^{N} \frac{\hat{F}^{(1)}_{n+1}}{2n} T'_n. \tag{38}$$

Introducing equation (35) into (38) and simplifying then results in

$$2n\,\hat{F}_n = C_{n-1}\,\hat{F}^{(1)}_{n-1} - \hat{F}^{(1)}_{n+1} \tag{39}$$

an expression for the $\hat{F}^{(1)}_n$ given the $\hat{F}_n$. The procedure for finding the $\hat{F}^{(1)}_n$ is initialized by setting

$$\hat{F}^{(1)}_{N+1} = 0$$

$$\hat{F}^{(1)}_{N} = 0$$

and then solving for $\hat{F}^{(1)}_{N-1}$ through $\hat{F}^{(1)}_{0}$ by back substitution.[15] Then, knowing all the $\hat{F}^{(1)}_n$, the required spatial derivatives of $\vec{F}$ can be calculated from equation (36). This procedure can again be done efficiently using the fast Fourier transform (FFT).

In summary, the computational procedure to find $\partial\vec{F}/\partial x$ is carried out as follows. First, given initial values of $F_j = F(x_j)$, find the Chebyshev coefficients $\hat{F}_n$ from equation (34) or the FFT. Next, compute the $\hat{F}_n^{(1)}$ from equation (39). Then, knowing the $\hat{F}_n^{(1)}$, compute $\partial\vec{F}/\partial x$ from equation (36) or the FFT. Once $\partial\vec{F}/\partial x$ and the source term $\vec{H}$ (see equations (4)) are known at $t = 0$, the solution may be advanced in time with an appropriate temporal integration scheme. The scheme developed for this work is discussed in the next section of the paper.

Temporal Integrator

Once values for $\partial\vec{F}/\partial x$ and $\vec{H}$ are determined as described above, there remains a system of ordinary differential equations in time that must be solved for the dependent variable vector $\vec{U}$. A number of algorithms were surveyed for integrating this system of ODE's including pure explicit schemes, pure implicit schemes, and mixed explicit-implicit schemes. The pure explicit schemes were in general unattractive because the stiffness of the ODE system made the algorithm inefficient. Pure implicit schemes were also precluded by the difficulty of developing spectral algorithms for the spatial derivatives evaluated implicitly. Hybrid explicit-implicit algorithms therefore appeared to offer the most attractive approach. Following References 5-7, (see page 2) the explicit-implicit split was formed by computing the source term $\vec{H}$ implicitly at the new time level, and computing $\partial\vec{F}/\partial x$ explicitly at the old time level to allow application of the spectral approach. Having made this choice, the equations were then integrated in time using a two-stage

Runge-Kutta technique. The algorithm was developed as follows.

We first discretize equation (4) as noted above giving

$$U_i^{n+1} = U_i^n - \Delta t\left[\left(\frac{\partial F}{\partial x}\right)_{i_{sp}}^n + H_i^{n+1}\right] + O(\Delta t)^2 \tag{40}$$

where n is the old time level and n+1 is the new time level. The vector $\vec{H}^{n+1}$ is then expanded in a Taylor series in time.

$$H^{n+1} = H^n + \Delta t\left(\frac{\partial H}{\partial t}\right)^n + O(\Delta t)^2$$

or

$$H^{n+1} = H^n + K^n(U^{n+1} - U^n) + O(\Delta t)^2 \tag{41}$$

where K^n is the Jacobian of H, $\frac{\partial H}{\partial U}$. Putting equation (41) into (4), simplifying the resulting equation, and then rewriting in delta form gives,

$$[I + \Delta t K_i^n]\Delta U_i^{n+1} = -\Delta t\left[\left(\frac{\partial F}{\partial x}\right)_{i_{sp}}^n + H_i^n\right] \tag{42}$$

where $\Delta U_i^{n+1} = U_i^{n+1} - U_i^n$. Examination of equation (42) shows that the bracketed term on the left-hand side is a block-diagonal matrix, the blocks being n by n submatrices with n the number of equations in the system (4). Since the matrix in equation (42) is diagonal, equation (42) is the most easily solved for ΔU by inverting the blocks, i.e.,

$$\Delta U_i^{n+1} = -\Delta t[I + \Delta t K_i^n]^{-1} R_i^n \tag{43}$$

where $[\ ]^{-1}$ represents a block invert, and

$$R_i^n = \left(\frac{\partial F}{\partial x}\right)_{i_{sp}}^n + H_i^n \tag{44}$$

is the steady-state residual vector. To apply the two-stage Runge-Kutta technique, we divide equation (43) into a predictor and corrector step as follows:

Predictor

$$\begin{aligned} \Delta U_i^{\overline{n+1}} &= -\Delta t\left[I + \Delta t K_i^n\right]^{-1} R_i^n \\ U_i^{\overline{n+1}} &= U_i^n + \Delta U_i^{\overline{n+1}} \end{aligned} \tag{45}$$

Corrector

$$\begin{aligned} \Delta U_i^{n+1} &= -\Delta t\left[I + \Delta t K_i^n\right]^{-1} R_i^{\overline{n+1}} \\ U_i^{n+1} &= U_i^n + \frac{1}{2}\left(\Delta U_i^{\overline{n+1}} + \Delta U_i^{n+1}\right). \end{aligned} \tag{46}$$

Starting with initial conditions for $\vec{U}$, equations (45) and (46) are used to advance the solution from time level n to time level n+1. The process is continued until steady-state conditions, defined as a reduction of ten orders of magnitude in the steady-state residuals, are reached.

The magnitude of the time step in equations (45) and (46) is chosen based on the physical time scales present at any given time in the solution. The fluid-dynamic time step, Δt_f, can be shown numerically to be limited by the Courant condition,

$$\Delta t_f = \frac{\Delta x}{|u| + c} . \tag{47}$$

The chemical relaxation time for a species i is given by[21]

$$t_c = \frac{\rho f_i}{\dot{w}_i} . \tag{48}$$

Changes in this relaxation time are then given by

$$\Delta t_c = \frac{\Delta(\rho f_i)}{\dot{w}_i} \tag{49}$$

since $\dot{w}_i$ remains nearly constant over a time step. For accuracy, we require that the chemical time step be chosen such that no change in specific mass fraction greater than Λ occurs over that time step. Equation (49) then becomes

$$\Delta t_c = \frac{\Lambda}{\dot{w}_i} . \tag{50}$$

Λ is initially set at 0.0001 for the computations that follow. The computational time step Δt is then chosen to be the minimum overall grid points, of the fluid and chemical time step, i.e.,

$$\Delta t = \min(\Delta t_f, \Delta t_c) \tag{51}$$

(We also note here, following our earlier discussion, that other authors[8] [12] restrict the truncation error or the growth of truncation error in the numerical solution to be below some set level, by the appropriate choice of time step. This is also an important constraint to achieve a given level of accuracy. This constraint on Δt has not been applied in the present work, but such an approach should be included as the work further matures).

Initial and Boundary Conditions

The governing equations (4) are hyperbolic and require initial conditions at each point to start the calculation and boundary conditions at the inflow boundary. Initial conditions are computed by first specifying an inflow Mach number and estimating an outflow Mach number. The interior Mach number distribution is then assumed to have a spatial variation which is linear. The total pressure and total temperature are assumed to be constant throughout the domain. Finally, the initial flow is assumed to be isentropic, so that isentropic relations can be used to compute the static pressure and temperature; these conditions are found from

$$\frac{T_o}{T} = 1 + \frac{\gamma-1}{2} M^2 \tag{52}$$

$$\frac{p_o}{p} = \left(\frac{T_o}{T}\right)^{\frac{\gamma}{\gamma-1}}. \tag{53}$$

Knowing the static temperature and pressure and Mach number, the velocity distribution can be computed, and the density distribution can be found from the equation of state. Since the inflow boundary flow remains supersonic, boundary conditions are specified thereby holding conditions fixed at their initial values.

RESULTS

Having now developed a numerical algorithm for solving the equations governing chemically reacting flows, that algorithm will now be used to model the reacting flow in a rapid expansion supersonic diffuser. A rapid expansion diffuser was chosen such that high concentration gradients existed near the inflow boundary, providing a formidable test for the method. Results from the present algorithm were compared with a benchmark calculation from an existing finite-difference chemical kinetics code to validate the method. The comparison also allowed a demonstration of performance of the high-order accurate spectral method on grids which were quite coarse compared to grids required in the finite-difference calculation.

The rapid expansion diffuser is shown in figure 1. The diffuser is two units long, has an initial cross-sectional area of 0.79 and a final cross-sectional area of 3.14. The diffuser wall is defined, as noted, by a shifted sinusoidal. Flow is introduced to the diffuser at $M = 1.4$, a velocity of 1230 m/s, a temperature of 1900 K, and a pressure of 0.081 MPa. The chemical composition of the inflow is defined to be a three-tenths stoichiometric mixture of hydrogen fuel and air.

Starting from the initial state described above, the governing equations were solved, using the algorithm in a time consistent manner, until steady-state conditions were reached. Independent benchmark calculations were also carried out with a previously validated Adams-Moulton implicit finite-difference program. In the results which follow, comparisons between the two methods will be made, first to verify the new procedure, and second to demonstrate its high spatial resolution on relatively coarse grids. A comparison of methods showing a time history of the chemical species is given in figures 2 through 4 for H_2, O_2, OH, and H_2O, respectively. Results are presented at the first grid point interior to the inflow boundary where both the flow field and species gradients are a maximum. Agreement between the Runge-Kutta spectral and the finite-difference calculations is excellent in all cases.

Next, we compare spatial results from the two methods once steady-state conditions have been reached. The finite-difference solution required 101 grid points before a grid independent solution, defined as a graphically imperceptible difference in the steady-state result between the present grid and next coarser grid, was attained. Calculations using the Runge-Kutta spectral code were carried out on 17 and 9 point grids. Comparisons of steady-state results for the two methods are given in figures 5 through 10. Figure 5 shows a comparison of the axial velocity profiles in the diffuser. The 17 point spectral solution and the 101 point finite-difference solution agree quite well throughout the diffuser. The 9 point spectral solution slightly overpredicts the velocity near the inflow boundary, but agrees well throughout the remainder of the diffuser. The overprediction is likely due to the failure of the coarsest spectral grid to predict adequately the high gradients that exist at the beginning of the diffuser. Temperature comparisons, given in figure 6, follow similar trends, with the 17 point spectral solution agreeing well with the benchmark, and the 9 point solution also agreeing well, except near the inflow boundary. Identical trends also occur when axial pressure profiles are compared in figure 7.

Comparisons of axial species distribution computed by the two methods are given in figures 8 through 10. Prediction of the H_2 mass fraction by the spectral method with 17 grid points agrees well with the finite-difference solution throughout the diffuser as can be seen by examining figure 8. The 9 point spectral solution underpredicts the H_2 mass fraction near the inflow boundary, again due to the high spatial gradient in f_{H_2} there, but agreement again becomes good away from the inflow boundary. The spatial distribution of O_2 mass fraction is given in figure 9. The gradients are not as large for this species since O_2 is in excess, and both 17 and 9 point grids agree well with the finite-difference solution. The steady-state species distributions for OH and H_2O are given in figure 10. The spatial gradients are again high for both species near the inflow boundary, and trends similar to those for H_2 are repeated here. Agreement is again quite good when comparing the 17 point spectral and finite-difference results. The 9 point spectral solution still underpredicts gradients near the inflow boundary, however.

A final comparison of methods is given in figure 11 which shows the rate of reduction of steady-state residual with iteration count at the first interior grid point. Since the 17 point Runge-Kutta spectral and the 101 point finite-difference calculations yield comparable accuracy and have the same minimum spatial step size, it is reasonable to assess the relative efficiency of the methods using the result given in this figure. Note that the residual reduction rate by the spectral code is significantly greater than that provided by the finite-difference code. The maximum residual (at any grid point) is reduced with the spectral code by ten orders of magnitude in only 2400 iterations, whereas the finite-difference code requires 6000 iterations to achieve the same level of residual reduction. The more rapid rate of residual reduction translates directly into a superior overall computational efficiency for the spectral Runge-Kutta method.

CONCLUDING REMARKS

A numerical method has been developed for solving the equations governing chemically reacting flow fields. In this method, spatial derivatives are discretized using a Chebyshev spectral collocation technique. Species source terms are calculated using a global hydrogen-air finite-rate chemistry model. The resulting ordinary differential equations in time are integrated using a two-stage partial implicit Runge-Kutta scheme that is effective in handling the stiffness, due to chemical kinetics, that is present in these equations. A computer program has been written using the spectral Runge-Kutta algorithm, and this program has been used to compute the flow in a rapid expansion supersonic diffuser. The diffuser flow field was also computed using an existing implicit finite-difference reacting flow code that had been validated in prior analyses. Comparison of results from the two programs indicated that the Runge-Kutta spectral code was accurate in predicting both the time evolution of the dependent variables and the final steady-state results. In addition, the spectral algorithm produced equivalent accuracy on relatively coarse grids as compared to the fine grid required by the finite-difference calculations. Based on these results, it appears that the Runge-Kutta spectral method offers promise for improving our ability to model chemically reacting flow fields.

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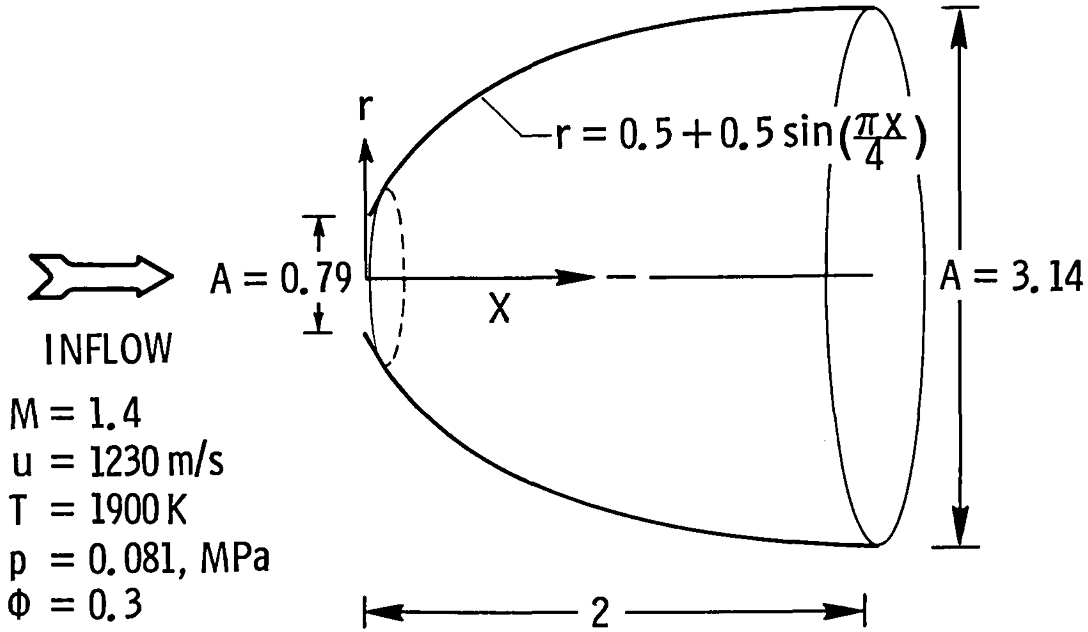

Figure 1. Rapid expansion supersonic diffuser test case.

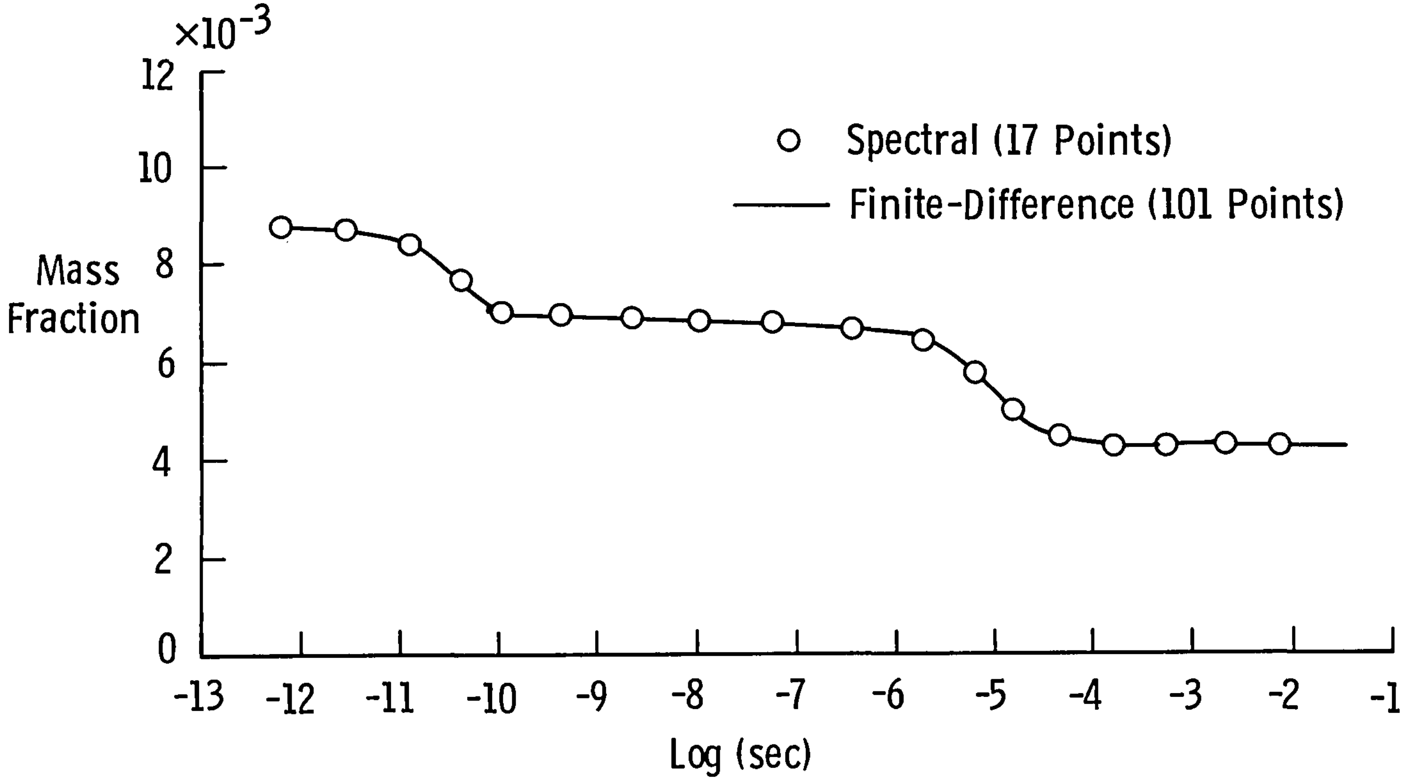

Figure 2. Comparison of time history of hydrogen mass fraction.

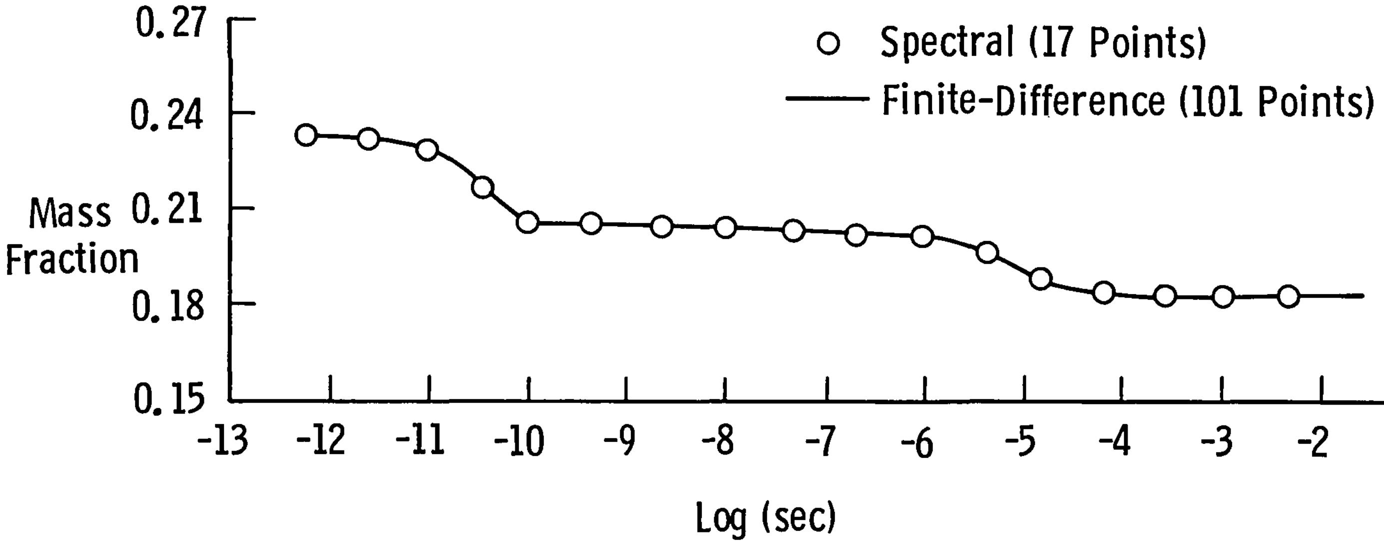

Figure 3. Comparison of time history of oxygen mass fraction.

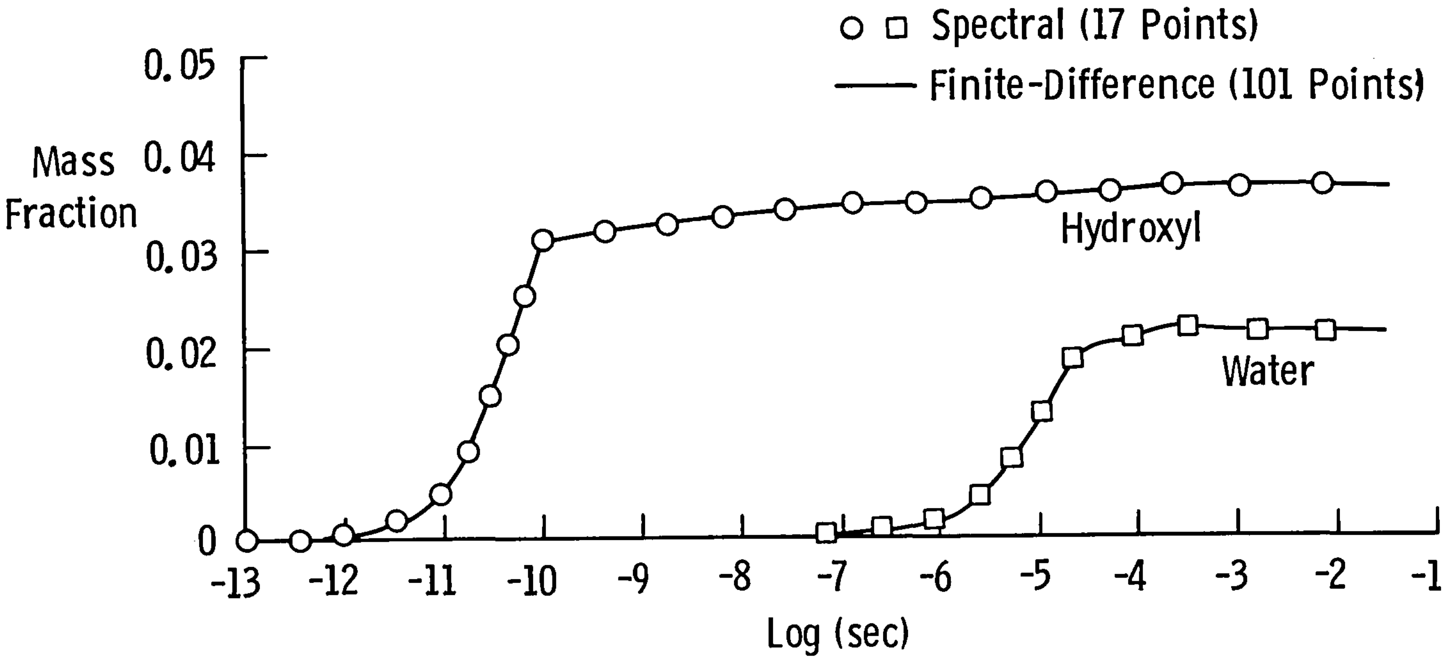

Figure 4. Comparison of time histories of hydroxyl and water mass fractions.

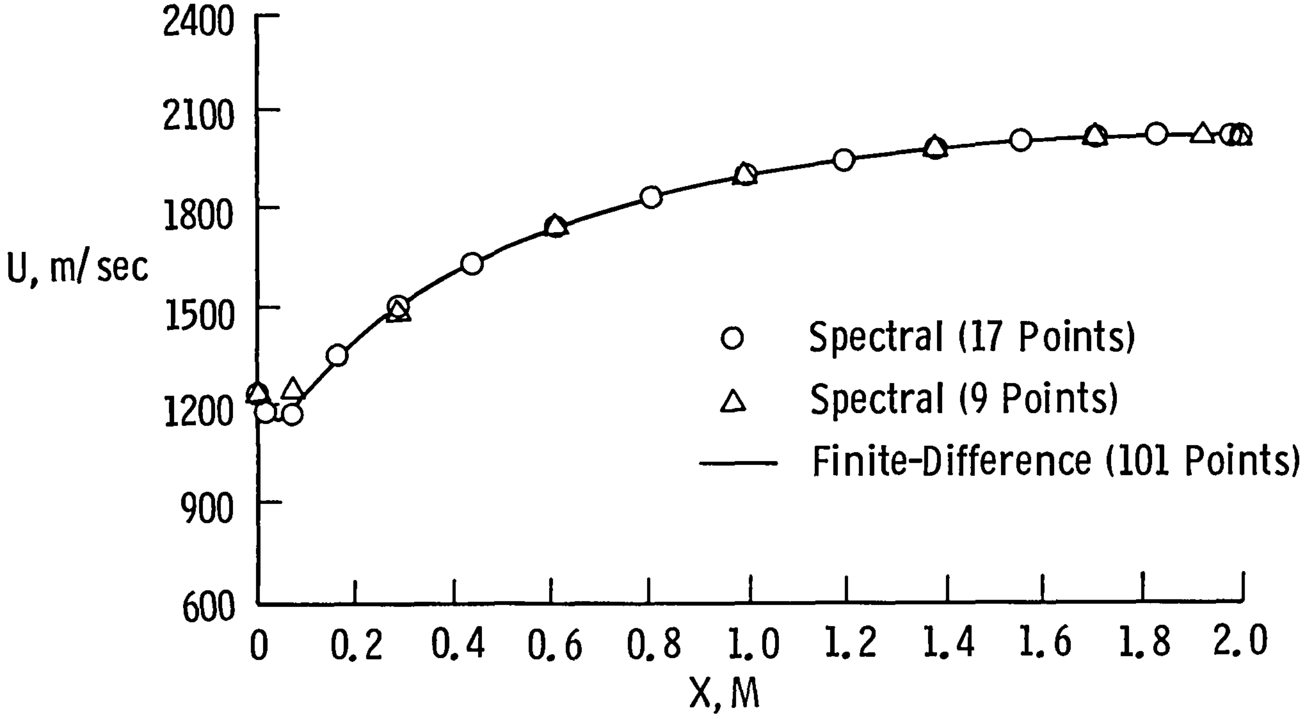

Figure 5. Comparison of axial velocity profiles.

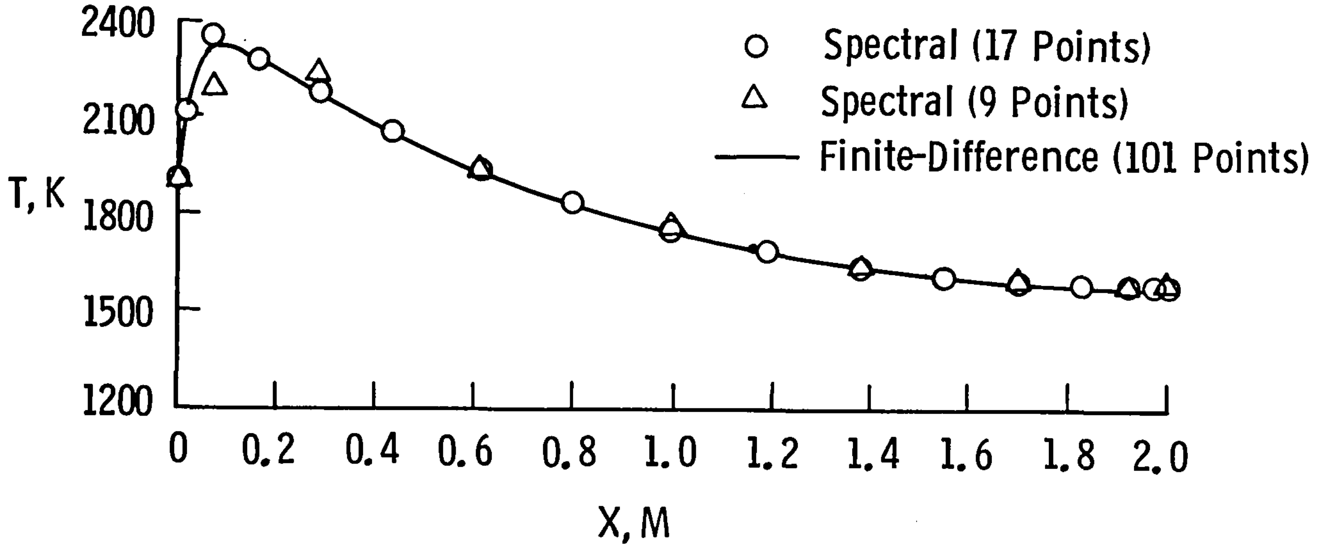

Figure 6. Comparison of axial temperature profiles.

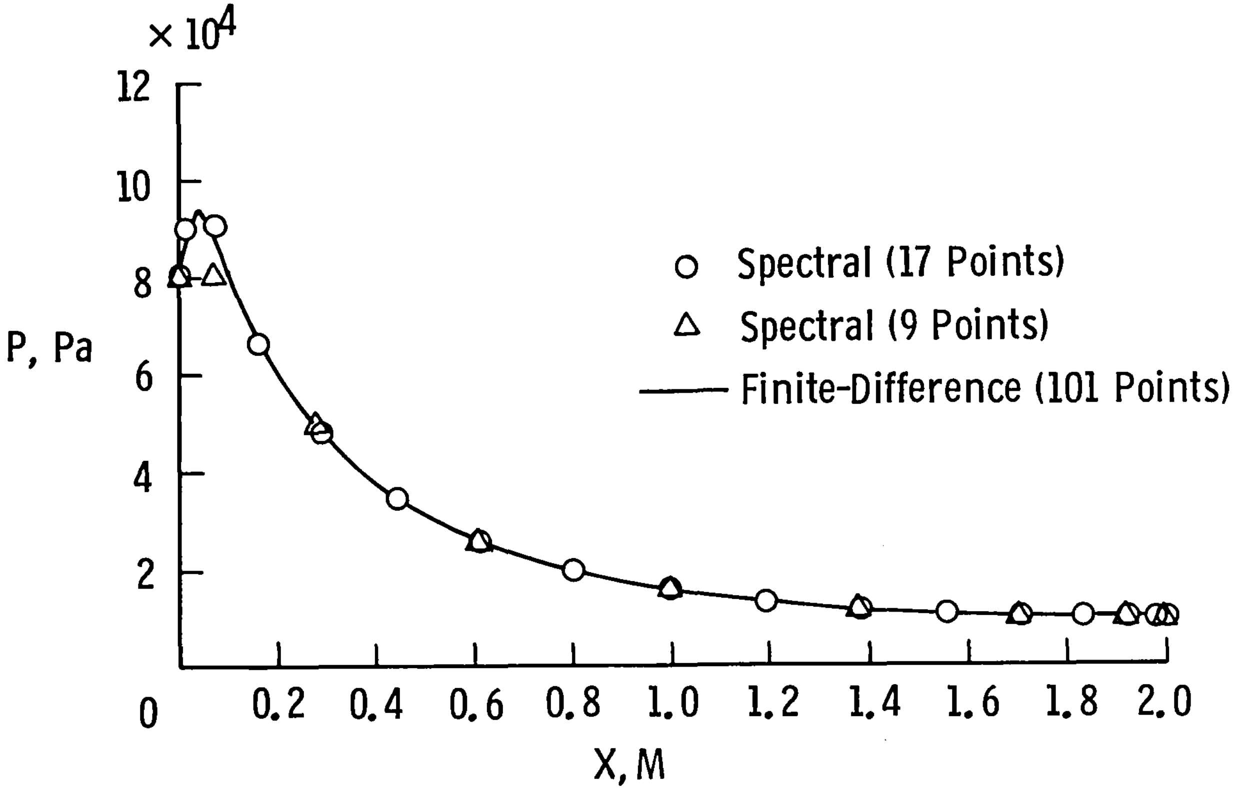

Figure 7. Comparison of axial pressure profiles.

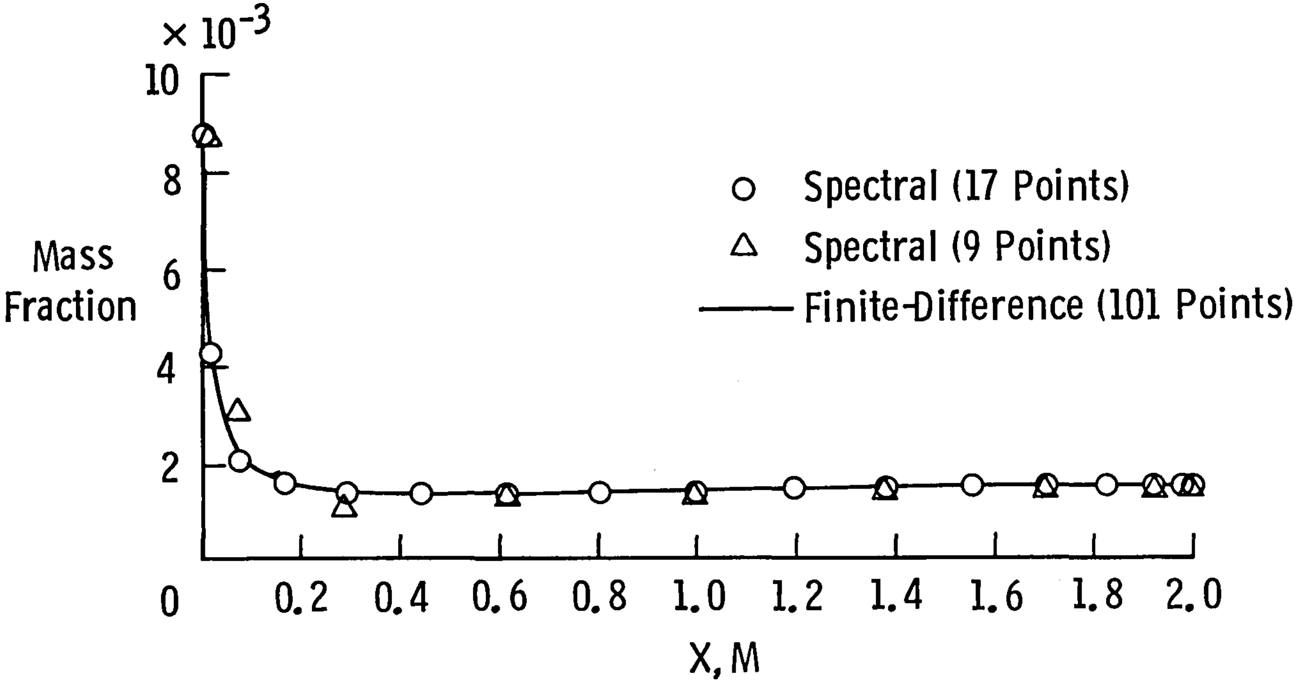

Figure 8. Comparison of axial hydrogen mass fraction profiles.

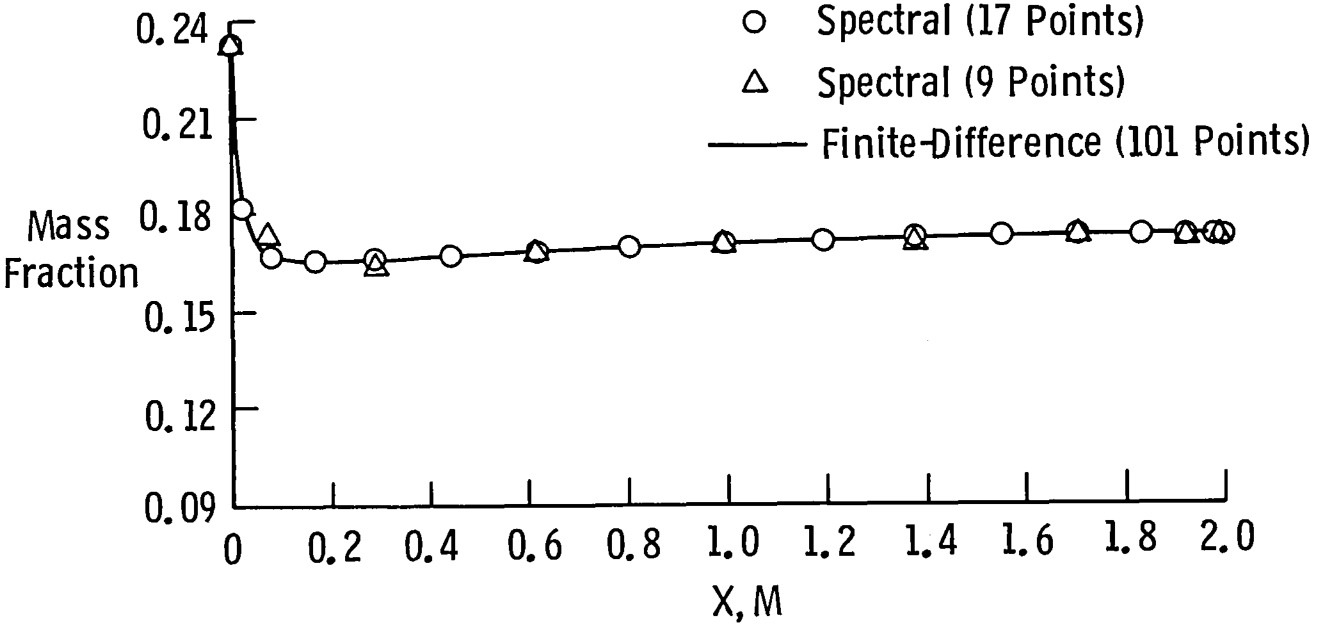

Figure 9. Comparison of axial oxygen mass fraction profiles.

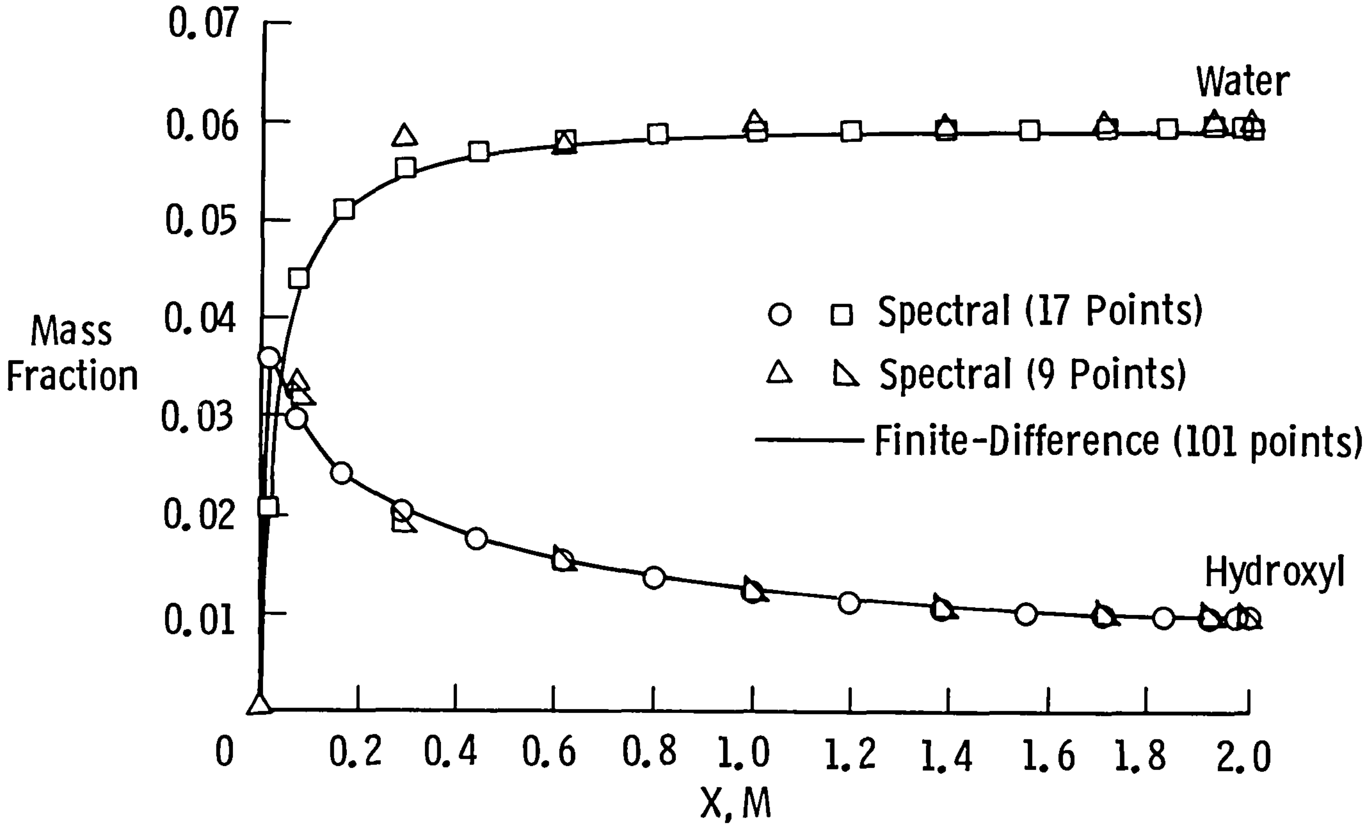

Figure 10. Comparison of axial hydroxyl and water mass fraction profiles.

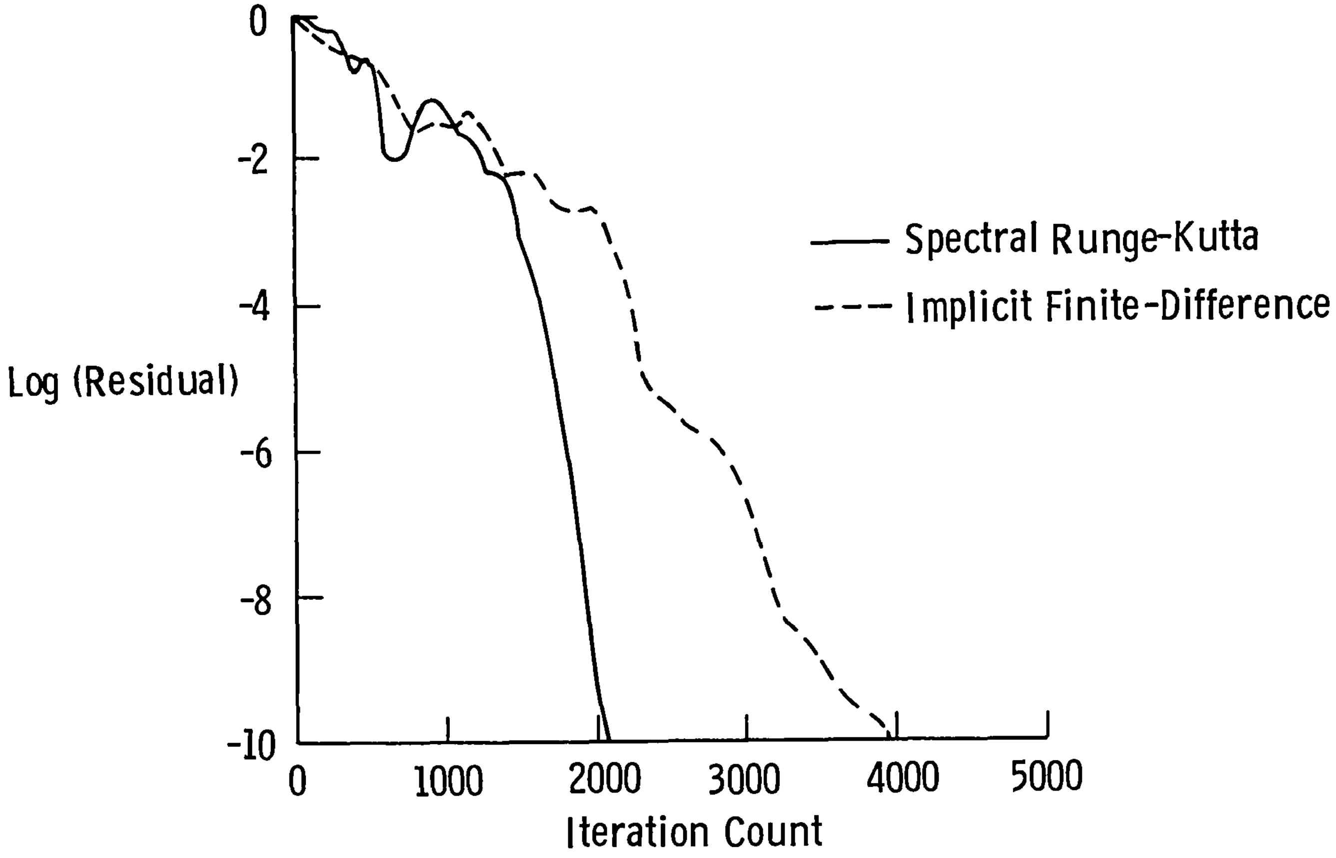

Figure 11. Comparison of steady-state residual reduction rates of the methods.

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16. Abstract

A numerical algorithm has been developed for solving the equations describing chemically reacting supersonic flows. The algorithm employs a two-stage Runge-Kutta method for integrating the equations in time and a Chebyshev spectral method for integrating the equations in space. The accuracy and efficiency of the technique have been assessed by comparison with an existing implicit finite-difference procedure for modeling chemically reacting flows. The comparison showed that the new procedure yielded equivalent accuracy on much coarser grids as compared to the finite-difference procedure with resultant significant gains in computational efficiency.

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