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**An Implicit Finite-Difference Method for Chemical
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an Axisymmetric Supersonic Nozzle.**

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An Implicit Finite-Difference Method for Chemical Nonequilibrium Flow through an Axisymmetric Supersonic Nozzle*

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ABSTRACT

A second-order accurate, noniterative, implicit procedure is developed for the stiff system of equations of a two-dimensional chemically reacting supersonic flow. All equations are solved simultaneously at each grid point by treating the axial derivative terms implicitly, in order to make the scheme stable with respect to the chemical rates. By treating the radial derivative terms explicitly, the scheme becomes simple and has the advantage that only a relatively small computer storage is required. The computational efficiency is compared by investigating the arithmetic operational counts required to solve a linear algebraic equation system constructed in each implicit scheme. It is demonstrated that, although the marching step size of the proposed scheme is restricted due to the explicit treatment of radial derivative terms, the computational efficiency of the proposed scheme is superior to those of other schemes, especially for problems involving a large number of chemically reacting species. The practical computational time of the proposed scheme is also compared with that of an existing explicit-implicit method.

概 要

化学反応を伴った二次元超音速非粘性流の方程式に対して、二次精度を持ち、繰返し計算の不要な陰的差分法を開発した。ノズル軸方向の微分項を陰的差分で評価する事により、近化学平衡領域での数値的不安定性を除去するとともに、半径方向の微分項については陽的な取扱いをして手法のアルゴリズムを簡素化し、かつ必要な計算機記憶容量を大幅に減少している。本計算法の計算効率を見るために、各陰差分法において構成される連立方程式を解くのに要する演算回数を調べた。その結果本手法は、部分的に陽な取扱いをしているために前進ステップ幅が制限されるにもかかわらず、計算効率は他の手法より勝れており、特に関与する化学種の数が多い化学反応の問題では、効率の良さが顕著となる。実際のノズル流問題に要する計算時間は、既存の陽陰混成解法と比較されている。

Nomenclature			
C_i	species mass fraction	h	enthalpy
C_p	specific heat at constant pressure	K	energy source term
F_i	species free energy	M	total mesh number of radial direction
		m	index of radial finite-difference grid point
		N	number of unknowns
		N_s	number of chemical species

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** Kakuda Branch

n	finite-difference step for ξ
P	natural log of pressure
p	pressure
R	universal gas constant divided by global molecular weight
$\bar{R}$	universal gas constant
r	radial coordinate
$r_w(x)$	nozzle wall ordinate, $r'_w = dr_w/dx$
r^*	throat radius
T	temperature
u	axial velocity component
v	radial velocity component
W_i	species molecular weight
x	axial coordinate
α	Mach angle
γ	frozen heat capacity ratio, $\gamma = C_p/(C_p - R)$
η	transformed radial coordinate
ξ	transformed axial coordinate
ρ	density
θ	flow angle
ω_i	species production rate

1. INTRODUCTION

Performance predictions for rocket propulsion systems require a detailed analysis of the flow in the exhaust nozzle. However, the calculation of a two-dimensional nozzle flow with finite-rate chemical reaction is very time consuming, because the number of equations in the mathematical model increases by the number of chemical species considered. This situation necessitates the development of a more efficient computational scheme than that now existing.

It is well known that a numerical integration of chemical species conservation equations in a near equilibrium flow region presents a severe numerical stability problem, and as a result, standard explicit integration methods become impractical in terms of the time needed for computation. For one-dimensional flow problems, this difficulty has been overcome by various numerical methods¹⁾⁻⁷⁾ and an implicit method

is recommended.⁵⁾⁻⁷⁾ However, a stable and practically efficient scheme for two-dimensional problems apparently does not exist.

A commonly used method for analyzing the two-dimensional nonequilibrium nozzle flow is an 'explicit-implicit method',⁸⁾⁻¹²⁾ in which the fluid dynamic equations (equations of global continuity, axial momentum, radial momentum and energy) are integrated using explicit methods, while the species conservation equations are integrated using implicit methods in order to remove the unstable property of the calculation of chemical relaxation equations. The numerical schemes of references 8 and 9 for the calculation of a supersonic flow in a rocket exhaust nozzle employ the method of characteristics for the fluid dynamic equations and a first-order accurate implicit integration method along the streamline for the species conservation equations. Nakahashi et al.¹⁰⁾ developed a performance prediction code for rocket exhaust nozzles, where the MacCormack's difference scheme was used for the fluid dynamic equations and a second-order implicit method for the species conservation equations. Ratliff¹¹⁾ also employs an explicit-implicit method in the study to incorporate the capability of the nonequilibrium chemistry to the shock fitting method for complicated supersonic nozzle flows. As concerning subsonic and transonic flow fields, Stiles and Hoffman¹²⁾ integrate the unsteady fluid dynamic equations explicitly and the species conservation equations implicitly.

However, we can not regard the explicit-implicit method as a sufficiently stable one, because the iteration, which is needed to couple the solutions of the fluid dynamic equations to those of the species conservation equations, often suffers from the ill convergency in the near equilibrium region. This trouble is mainly caused by the large differences in the properties between the fluid dynamic equations and the species conservation equations. Thus, in order to obtain high computational efficiency, the scheme

should be a noniterative one.

In this report, a noniterative finite-difference algorithm has been developed for the stiff equations of a chemically reacting nonequilibrium flow. It consists of a linearization of the system of equations and an implicit treatment of the axial derivative terms. In order to make the algorithm simple and to save computer storage, the radial derivative terms are treated explicitly. After linearizing and differencing, the equations are reduced to a linear algebraic system equation of order $N_s + 4$, where N_s is the number of chemical species.

The computational efficiency is generally the most important factor used in determining the usefulness of a particular numerical approach. In the subject research, the efficiency was investigated by evaluating the arithmetic operational count required for the solution of a linear algebraic equation system constructed in each implicit scheme, by considering the fact that the most computational time is consumed in the solution of linear algebraic equation systems of large order in implicit schemes.

2. CONSERVATION EQUATIONS FOR TWO-DIMENSIONAL KINETIC FLOWS

The basic assumptions made in the derivation of equations for an axisymmetric inviscid flow of reacting gas mixtures are as follows.

- The computational region considered is the supersonic flow field downstream of the nozzle throat and, throughout the region, there are no shock waves.
- Each component of the gas is a perfect gas.
- The flow is assumed to be everywhere in instantaneous translational, rotational, and vibrational equilibrium.

Under these assumptions, a hyperbolic system of equations is written using an axisymmetric coordinate system (x, r) .

$$u \frac{\partial \rho}{\partial x} + v \frac{\partial \rho}{\partial r} + \rho \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial r} \right) + \frac{1}{r} \rho v = 0 \quad (1)$$

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial r} + \frac{a^2}{\gamma} \frac{\partial P}{\partial x} = 0 \quad (2)$$

$$u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial r} + \frac{a^2}{\gamma} \frac{\partial P}{\partial r} = 0 \quad (3)$$

$$u \frac{\partial P}{\partial x} + v \frac{\partial P}{\partial r} - \frac{\gamma}{\rho} \left(u \frac{\partial \rho}{\partial x} + v \frac{\partial \rho}{\partial r} \right) - \frac{\gamma}{a^2} K = 0 \quad (4)$$

$$u \frac{\partial C_i}{\partial x} + v \frac{\partial C_i}{\partial r} - \frac{1}{\rho} \omega_i = 0, \quad i = 1, \dots, N_s \quad (5)$$

and

$$P = \rho RT \quad (6)$$

where

$$P = \ell_n p, \quad a^2 = \gamma p / \rho \quad (7)$$

$$K = \gamma S_1 - (\gamma - 1) S_2 \quad (8)$$

$$S_1 = \sum_{i=1}^{N_s} \left(\frac{\bar{R}}{W_i} \right) \left(\frac{\omega_i}{\rho} \right) T, \quad S_2 = \sum_{i=1}^{N_s} h_i \left(\frac{\omega_i}{\rho} \right) \quad (9)$$

The system enthalpy and gas constant are

$$h = \sum_{i=1}^{N_s} C_i h_i \quad \text{where} \quad h_i = \int_{T_0}^T C_{pi} dT + h_i^0 \quad (10)$$

$$R = \sum_{i=1}^{N_s} C_i \left(\frac{\bar{R}}{W_i} \right) \quad (11)$$

The net species production rate, ω_i , in the preceding equations is determined by the method described below.

A chemical reaction can be written in terms of its stoichiometric coefficients (ν_{ij} and ν'_{ij}) as

$$\sum_{i=1} \nu_{ij} Z_i \rightleftharpoons \sum_{i=1} \nu'_{ij} Z_i \quad (12)$$

where Z_i represents the i^{th} chemical species name and j represents the j^{th} reaction.

Given a system of chemical reactions, the net species production rate ω_i for each species is calculated from

$$\omega_i = W_i \sum_{j=1}^{\Sigma} \rho^{\sum_{l=1}^{\Sigma} \nu_{lj}} (\nu'_{ij} - \nu_{ij}) X_j \quad (13)$$

where

$$X_j = [k_{fj} \prod_{i=1}^{\Sigma} \left(\frac{C_i}{W_i} \right)^{\nu_{ij}} - k_{bj} \rho^{\sum_{l=1}^{\Sigma} (\nu'_{lj} - \nu_{lj})} \prod_{i=1}^{\Sigma} \left(\frac{C_i}{W_i} \right)^{\nu'_{ij}}] M_j \quad (14)$$

The reverse reaction rate, k_{bj} , in the above equation is represented by the Arrhenius form

$$k_{bj} = a_j T^{-n_j} e^{(-b_j/\bar{R}T)} \quad (15)$$

where

- a_j is the pre-exponential coefficients
- n_j is the temperature dependence of the pre-exponential factor
- b_j is the activation energy

The forward reaction rate, k_{fj} , is calculated by using the equilibrium constant, K_j , as

$$k_{fj} = k_{bj} K_j \quad (16)$$

and

$$K_j = e^{-\Delta F/\bar{R}T} (\bar{R}T)^{-\sum_{l=1}^{\infty} (v'_{lj} - v_{lj})} \quad (17)$$

where ΔF is the change in free energy during the reaction process.

$$\Delta F = \sum_{i=1} F_i v'_{ij} - \sum_{i=1} F_i v_{ij} \quad (18)$$

The term M_j is provided so that the reaction rate can be modified for reactions involving a third body, namely

$$\left. \begin{aligned} M_j &= \sum_{i=1} m_{ji} \left(\frac{C_i}{W_i} \right) && \text{for reactions requiring a third body} \\ M_j &= 1 && \text{for all other reactions} \end{aligned} \right\} \quad (19)$$

where the constants m_{ji} are specified.

3. EXPLICIT-IMPLICIT METHOD

Before describing the proposed scheme, it is preferable to make clear the deficiency of the explicit-implicit method. As mentioned in the introductory remarks, the explicit-implicit method integrates the fluid dynamic equations, (1) to (4), explicitly, and the species conservation equations (5) implicitly. This treatment necessitates an iteration calculation in order to couple the solutions of the fluid dynamic equations to

Fig. 1 Temperature oscillations during the coupling iterations in the explicit-implicit method: 75%-bell nozzle, AR = 140, H/O propellant, Chamber pressure = 3.43 Mpa, $r^* = 0.068$ m

Fig. 2 Coupling iteration counts and temperature distributions along the nozzle axis in the explicit-implicit method

those of the species conservation equations. Although this iteration converges rapidly at low temperatures, we often suffer from its ill convergency in the near equilibrium region, as shown in Figures 1 and 2. This is because the energy source term K appearing in the energy equation (4) is excessively sensitive to the variations in the species mass fractions for high temperature near equilibrium conditions.

Because of this ill convergency of the coupling iteration, we cannot regard the explicit-implicit method as a sufficiently stable one. Thus, in order to obtain high computational efficiency, the scheme should be noniterative. This is possible if the both equations of the fluid dynamic and the species conservation are integrated simultaneously by an implicit scheme.

4. SECOND ORDER IMPLICIT FINITE-DIFFERENCE METHOD

4.1 Transformation of the Governing Equations

Since the interior points in this analysis are to be treated by a fixed grid technique, it is

convenient to transform the physical (x, r) plane to a rectangular (ξ, η) plane, as illustrated in Figure 3. The following coordinate transformation is employed.

$$\left. \begin{aligned} \xi &= x \\ \eta &= \frac{r}{r_w} \end{aligned} \right\} \quad (20)$$

where $r_w(x)$ represents the nozzle wall ordinate. Applying this transformation to equations (1) to (5) yields the final form of governing equations as

$$\frac{\partial y_i}{\partial \xi} = f_i, \quad i = 1, \dots, N \quad (21)$$

where

$$y_1 = u, y_2 = v, y_3 = P, y_4 = T, y_{4+j} = C_j, j = 1, \dots, N_s$$

and

$$f_1 = \frac{r_w'}{r_w} \eta u_\eta + \frac{1}{r_w(u^2 - a^2)} \left\{ -uvu_\eta + a^2 \left(v_\eta + \frac{v}{\eta} \right) + \frac{a^2 v}{\gamma} P_\eta - r_w K \right\} \quad (22-a)$$

$$f_2 = \frac{r_w'}{r_w} \eta v_\eta - \frac{1}{r_w u} \left\{ v v_\eta + \frac{a^2}{\gamma} P_\eta \right\} \quad (22-b)$$

Fig. 3 Physical and computational plane

$$f_3 = \frac{r_w'}{r_w} \eta P_\eta + \frac{1}{r_w(u^2 - a^2)} \{ \gamma v u_\eta - \gamma u (v_\eta + \frac{v}{\eta}) - uv P_\eta + \frac{\gamma u r_w}{a^2} K \} \quad f_1 = \frac{1}{r_w(u^2 - a^2)} \{ 2a^2 v_\eta - r_w K \} \quad (23-a)$$

$$- uv P_\eta + \frac{\gamma u r_w}{a^2} K \} \quad (22-c) \quad f_2 = 0 \quad (23-b)$$

$$f_4 = \frac{r_w'}{r_w} \eta T_\eta - \frac{v}{r_w u} T_\eta + \frac{a^2}{C_p r_w (u^2 - a^2)} \{ v u_\eta - u (v_\eta + \frac{v}{\eta}) - \frac{a^2 v}{\gamma u} P_\eta + \frac{r_w u}{a^2} [\gamma S_1 + (\frac{a^2}{u^2} - \gamma) S_2] \} \quad f_3 = \frac{1}{r_w(u^2 - a^2)} \{ -2 \gamma u v_\eta + \frac{\gamma u r_w}{a^2} K \} \quad (23-c)$$

$$+ (\frac{a^2}{u^2} - \gamma) S_2 \} \quad (22-d) \quad f_4 = \frac{a^2}{C_p r_w (u^2 - a^2)} \{ -2 u v_\eta + \frac{r_w u}{a^2} [\gamma S_1 + (\frac{a^2}{u^2} - \gamma) S_2] \} \quad (23-d)$$

$$f_{4+j} = \frac{r_w'}{r_w} \eta C_{j\eta} - \frac{1}{r_w u} \{ v C_{j\eta} - r_w \frac{\omega_j}{\rho} \}, \quad f_{4+j} = \frac{1}{u} \frac{\omega_j}{\rho}, \quad j = 1, \dots, N_s \quad (23-e)$$

$$j = 1, \dots, N_s \quad (22-e)$$

On the axis of symmetry, these equations are written as

The subscript η denotes the differentiation with respect to η .

4.2 Implicit Finite-Difference Scheme

When a second-order implicit difference approximation is applied to the ξ derivative in equation (21), we obtain

$$\Delta y_i^{(n+1)} = \frac{\Delta \xi^{(n+1)}}{2} [f_i^{(n)} + f_i^{(n+1)}] + O(\Delta \xi^3) \quad (24)$$

where

$$\Delta y_i^{(n+1)} = y_i^{(n+1)} - y_i^{(n)},$$

$$\Delta \xi^{(n+1)} = \xi^{(n+1)} - \xi^{(n)} \quad (25)$$

and the superscript n refers to a finite difference step for ξ .

As the functions $f_i^{(n+1)}$ ($i = 1, \dots, N$) include the unknowns $y_i^{(n+1)}$ ($i = 1, \dots, N$) implicitly, we need to consider the linearization of $f_i^{(n+1)}$ in $y_i^{(n+1)}$ so as to make the scheme noniterative. This linearization can be obtained using a local Taylor expansion, regarding f_i as a function of ξ , y_j and $y_{j\eta}$ ($j = 1, \dots, N$). Thus we can write

$$f_i^{(n+1)} = f_i^{(n)} + \left[\frac{\partial f_i}{\partial \xi} \right]^{(n)} \Delta \xi^{(n+1)} + \sum_{j=1}^N \left[\frac{\partial f_i}{\partial y_j} \right]^{(n)} \Delta y_j^{(n+1)} + \sum_{j=1}^N \left[\frac{\partial f_i}{\partial y_{j\eta}} \right]^{(n)} \Delta y_{j\eta}^{(n+1)} + O(\Delta \xi^2) \quad (26)$$

In this linearization procedure, however, the derivative terms with respect to η , $\Delta y_{j\eta}^{(n+1)}$ ($= y_{j\eta}^{(n+1)} - y_{j\eta}^{(n)}$), require an additional consideration. One of the methods to handle these terms is to approximate them by appropriate difference quotients such as

$$\Delta y_{j\eta}^{(n+1)} = (\Delta y_{j, m+1}^{(n+1)} - \Delta y_{j, m-1}^{(n+1)}) / 2 \Delta \eta \quad (27)$$

where m is the index of a radial point in the finite-difference grid. Inserting equation (26) with equation (27) into equation (24), the equations to be solved are reduced to the block-tridiagonal system of equations for each axial plane.

$$\begin{aligned} & \frac{\Delta \xi^{(n+1)}}{2} \sum_{j=1}^N \left[\frac{\partial f_i}{\partial y_{j\eta}} \right]^{(n)} \Delta y_{j, m-1}^{(n+1)} \\ & + 2 \Delta \eta \sum_{j=1}^N \left\{ \delta_{ij} - \frac{\Delta \xi^{(n+1)}}{2} \left[\frac{\partial f_i}{\partial y_j} \right]^{(n)} \right\} \Delta y_{j, m}^{(n+1)} \\ & - \frac{\Delta \xi^{(n+1)}}{2} \sum_{j=1}^N \left[\frac{\partial f_i}{\partial y_{j\eta}} \right]^{(n)} \Delta y_{j, m+1}^{(n+1)} \\ & = 2 \Delta \eta \Delta \xi^{(n+1)} \left\{ f_{i, m}^{(n)} + \frac{\Delta \xi^{(n+1)}}{2} \left[\frac{\partial f_i}{\partial \xi} \right]^{(n)} \right\} \end{aligned} \quad (28)$$

where δ_{ij} is the Kronecker delta. This implicit treatment is similar to the scheme of Warming and Beam¹³⁾ which is used to solve the time-dependent Navier-Stokes equations.

Another method to evaluate the terms $\Delta y_{j\eta}^{(n+1)}$ in equation (26) is possible if these terms are treated explicitly, assuming that these terms are independent of the unstable property in the calculation for the near-equilibrium flow region. Namely,

$$\Delta y_{j\eta}^{(n+1)} = \left[\frac{\partial y_{j\eta}}{\partial \xi} \right]^{(n)} \Delta \xi^{(n+1)} + O(\Delta \xi^2) \quad (29)$$

Thus, inserting equations (29) and (26) into equation (24) and neglecting the third-order terms, the equations are reduced to the following linear system of equations of order N at each grid point.

$$\begin{aligned} & \sum_{j=1}^N \left\{ \delta_{ij} - \frac{\Delta \xi^{(n+1)}}{2} \left[\frac{\partial f_i}{\partial y_j} \right]^{(n)} \right\} \Delta y_j^{(n+1)} \\ & = \Delta \xi^{(n+1)} \left\{ f_{i, m}^{(n)} + \frac{\Delta \xi^{(n+1)}}{2} \left[\frac{\partial f_i}{\partial \xi} \right]^{(n)} \right. \\ & \quad \left. + \frac{\Delta \xi^{(n+1)}}{2} \sum_{j=1}^N \left[\frac{\partial f_i}{\partial y_{j\eta}} \right]^{(n)} f_{j\eta}^{(n)} \right\} \end{aligned} \quad (30)$$

Of these two treatments of the terms $\Delta y_{j\eta}^{(n+1)}$, we chose the latter. One of the reasons is the simplicity of the explicit treatment. Only known points $(n, m-1)$, (n, m) and $(n, m+1)$ are required to calculate the unknown point $(n+1, m)$ in the explicit treatment.

By contrast, the implicit treatment of $\Delta y_{j\eta}^{(n+1)}$ requires the information from points $(n+1, m-1)$ and $(n+1, m+1)$, which are unknowns, and thus the block-tridiagonal system of equations, (28), is constructed. Therefore, the explicit treatment is simpler and requires less computer storage than the implicit treatment. This merit is further enhanced when the number of chemical species taking part in a problem becomes large.

Another reason to choose the explicit treatment of $\Delta y_{j\eta}^{(n+1)}$ comes from the consideration of computational efficiency, which will be discussed later.

4.3 Boundary Conditions

The boundary conditions along the nozzle wall can be obtained using characteristics equations. The following characteristics equations are derived from equations (1) to (5).

(a) Along streamlines,

$$\frac{dr}{dx} = \tan \theta \quad (31)$$

$$\frac{1}{2} d(V^2) + \frac{\alpha^2}{\gamma} dP = 0 \quad (32)$$

$$\frac{\gamma-1}{\gamma} dP - \frac{dT}{T} = \frac{B}{\cos \theta} dx \quad (33)$$

$$dC_i = \frac{\omega_i}{\rho V \cos \theta} dx \quad (34)$$

(b) Along left running characteristics,

$$\frac{dr}{dx} = \tan(\theta + \alpha) \quad (35)$$

$$dP = G \left\{ \left(A - \frac{\sin \theta}{r} \right) F dr - d\theta \right\} \quad (36)$$

where

$$\left. \begin{aligned} B &= (\gamma - 1) \frac{\gamma}{\rho a^2 V} \sum_{i=1}^{N_s} \omega_i h_i \\ A &= \frac{\gamma}{\rho a^2 V} \sum_{i=1}^{N_s} \omega_i \frac{\bar{R}}{W_i} T - B \\ F &= \cos \theta - \sin \theta \cot(\theta + \alpha) \\ G &= \frac{\gamma}{\sin \alpha \cos \alpha} \end{aligned} \right\} \quad (37)$$

Fig. 4 Grid points used in the equation for the wall boundary conditions

In Figure 4, points 1, 2 and 3 are known points and point 5 is the unknown point to be computed. Values at point 4 are determined by the interpolation among points 1, 2 and 3. Using these notations for each point, the difference forms of equations (31) to (36) are reduced to

$$V_5^2 = V_1^2 - (2RT)_{15} \{ P_4 - P_1 + D_{45} \lambda (x_5 - x_4) - G_{45} (\theta_5 - \theta_4) \} \quad (38)$$

$$P_5 = P_4 + D_{45} \lambda (x_5 - x_4) - G_{45} (\theta_5 - \theta_4) \quad (39)$$

$$T_5 = T_1 + \left[\frac{\gamma-1}{\gamma} T \right]_{15} \{ P_4 - P_1 + D_{45} \lambda (x_5 - x_4) - G_{45} (\theta_5 - \theta_4) \} - \left[\frac{TB}{\cos \theta} \right]_{15} (x_5 - x_1) \quad (40)$$

$$C_{i5} = C_{i1} + \left(\frac{\omega_i}{\rho V \cos \theta} \right)_{15} (x_5 - x_1) \quad (41)$$

where

$$D_{45} = G_{45} \left[A_{45} - \left(\frac{\sin \theta}{\gamma} \right)_{45} \right] F_{45} \quad (42)$$

$$\lambda = \tan(\theta + \alpha)_{45} \quad (43)$$

Subscripts 15 and 45 represent the average value between points 1 and 5 and points 4 and 5, respectively.

It is desired that, as in the treatment for the interior points, the above equations are solved in the form of a linear algebraic equation system for the unknowns of V_5^2 , P_5 , T_5 and C_{i5} ($i = 1, \dots, N_s$). In order to get such a system of equations, the above equations must be expressed by these unknowns explicitly. Again, we use the Taylor expansion. For instance, the terms E_{15} and E_{45} are

$$E_{15} = \frac{1}{2}(E_1 + E_5) = E_1 + \frac{1}{2} \left[\left[\frac{\partial E}{\partial \ell} \right]_1 \Delta \ell_{15} + \sum_{i=1}^{N-1} \left[\frac{\partial E}{\partial z_i} \right]_1 (z_{i5} - z_{i1}) \right] \quad (44)$$

$$E_{45} = \frac{1}{2}(E_4 + E_5) = E_4 + \frac{1}{2} \left[\left[\frac{\partial E}{\partial \ell} \right]_4 \Delta \ell_{45} + \sum_{i=1}^{N-1} \left[\frac{\partial E}{\partial z_i} \right]_4 (z_{i5} - z_{i4}) \right] \quad (45)$$

where

$$z_1 = V^2, z_2 = P, z_3 = T \text{ and } z_{3+i} = C_i$$

By these treatments, all terms of the right-hand side of equations (38) to (41) are expressed explicitly for V_5^2 , P_5 , T_5 and C_{i5} . However, there arises another problem because the nonlinear terms such as z_{i5}^2 and $z_{i5}z_{j5}$ appear. These nonlinear terms are linearized using Morreti's linearization method²⁾ as,

$$z_{i5} z_{j5} = z_{i5} z_{j1} + z_{i1} z_{j5} - z_{i1} z_{j1} \quad (46)$$

This linearization, thus, reduces the equations to the linear algebraic equation system for V_5^2 , P_5 , T_5 and C_{i5} .

The value of λ in equation (43) and the values at point 4 are iteratively determined. This iteration easily converges in two or three counts independent of the chemical reactions.

4.4 Initial Conditions

It is necessary to construct an initial data line suitable for the calculation of the flow field in

the supersonic domain. For the case of a conventional rocket nozzle, this can be given by the calculations of the flow fields of the combustion chamber and the nozzle throat. The flow field of the combustion chamber can be well approximated by the assumption of the one-dimensional flow, and the computer programs^{14), 7)} for the one-dimensional equilibrium and nonequilibrium flows are available. The result of this one-dimensional calculation is used to construct tables of properties (ρ , V , T , C_i) as a function of pressure. These tables span the nozzle throat region and are used to compute an average expansion coefficient.

$$\gamma_e = \ell n \left(\frac{p_\ell}{p_1} \right) / \ell n \left(\frac{\rho_\ell}{\rho_1} \right) \quad (47)$$

where the subscripts 1 and ℓ refer to the first and last table entries, respectively.

Using the above expansion coefficient and the throat geometry, the transonic flow field is calculated using the method of Kliegel and Levine.¹⁵⁾ The two-dimensional supersonic flow calculation is then started from the constant Mach line whose Mach number is slightly greater than one. The details for starting the finite-difference calculation from the initial line is found in reference 16.

5. RESULTS

5.1 Operational Counts

It is desirable to estimate the computational efficiency of the proposed scheme and other schemes. In calculations using an implicit scheme, most of the computational time is consumed in solving large order algebraic equation systems. Therefore, the computational efficiency may be made clear by investigating the arithmetic operational counts¹⁷⁾ required in the calculation of a system equation constructed for each scheme.

The comparison is made for the following three schemes, the proposed scheme, the explicit-implicit scheme and the full implicit scheme. In the following discussion, we consider the

operational counts only for the calculation of the system equation, and other arithmetic operations are neglected.

Denoting the number of the chemical species by N_s , the total number of unknowns equal $N_s + 4$. We also denote the total mesh number of radial direction by M .

(A) The proposed scheme

A system equation of the order $N_s + 4$ is constructed at each grid point in this scheme and can be solved using the Gauss elimination method. Thus the operational count for each grid point is¹⁷⁾

$$\frac{1}{3} (N_s + 4)^3 + (N_s + 4)^2 - \frac{1}{3} (N_s + 4) \quad \text{ops.} \quad (48)$$

(B) The explicit-implicit scheme

As the fluid dynamic equations are solved by the explicit method, we neglect the operational counts required for the calculation of this explicit part of the scheme. The species conservation equations are solved implicitly constructing at each grid point a system equation of the order N_s . Thus the operational count for this is¹⁷⁾

$$\frac{1}{3} N_s^3 + N_s^2 - \frac{1}{3} N_s \quad \text{ops.}$$

However, this scheme needs iterations to couple the solutions of fluid dynamic equations to those of species conservation equations. Thus the above operational count is multiplied by the number of iterations, I , in order to get the real count per grid point.

$$I \left(\frac{1}{3} N_s^3 + N_s^2 - \frac{1}{3} N_s \right) \quad \text{ops.} \quad (49)$$

(C) Full implicit scheme

As the radial derivative terms are handled implicitly in equation (26), a block-tridiagonal system of equations with each block having dimensions $(N_s + 4) \times (N_s + 4)$, is constructed at each axial plane. The operational count of this block tridiagonal system is then,¹⁷⁾

$$(3M - 2)[(N_s + 4)^3 + (N_s + 4)^2] \quad \text{ops.}$$

and the count for a grid point is

$$\left(3 - \frac{2}{M}\right) [(N_s + 4)^3 + (N_s + 4)^2] \quad \text{ops.} \quad (50)$$

Figure 5 shows these counts as a function of a number of chemical species, N_s , considered in a problem. Line A indicates the counts of the proposed method, and line C, which is about ten times as large a count as line A, the count of the full implicit method. Although the unconditionally stable property of the method indicated by line C make it possible to adopt a larger ξ -step size, this size can not be more than ten times the step size of the proposed scheme due to the accuracy requirement in practical problems. For instance, the total number of axial steps required in a calculation of the conventional bell-shaped rocket nozzle flow is approximately one hundred for the proposed scheme

Fig. 5 Operational counts required for solving the linear algebraic equation system constructed in each scheme: A = proposed scheme, B = explicit-implicit scheme, C = full implicit scheme

with twenty radial meshes. Thus, in order to get more computational efficiency in the full implicit method than the proposed scheme gives, the number of axial steps must be less than ten. This number of steps can not be expected to resolve the nozzle flow field in a reasonable accuracy.

Line B indicates the counts needed in the explicit-implicit method. The iteration number I required in the practical calculation is about three to ten as shown in Figure 2. Thus the operational count of line B ($I = 3$ or 10) becomes greater than the line of the proposed scheme.

These considerations, along with the operational counts of the system equations, clearly show the advantages of the proposed scheme in computational time.

5.2 Computational Results and CPU Times

In Figure 6 and 7, computational results are shown for a bell-shaped rocket nozzle. The accuracy of the proposed scheme was checked by comparing the pressure distributions along the

nozzle wall with experimental results¹⁸⁾ (Figure 7), as well as with those other numerical methods as to nonreactive and reactive flows.

Numerical stability was checked by computational experiments, and it was confirmed that the CFL condition is the stability limit.

The computational times required in the proposed scheme and the explicit-implicit scheme¹⁰⁾ for the calculation of the flow field of a practical rocket nozzle are compared in Figure 8. Hydrogen-oxygen propellant was assumed and the six chemical species were taken into account for a H-O system. Additionally, in order to examine the effect of the number of species on computational time, assumed argon-like nonreactive gases, whose molecular weights are equal to argon species, were added to the propellant.

By this figure, it is well demonstrated that the proposed scheme has high computational efficiency, especially for problems with a large number of species.

Fig. 6 Constant Mach number lines in a bell nozzle

Fig. 7 Pressure distribution along the nozzle wall: 75%-bell nozzle and 15° conical nozzle, AR = 140, H/O propellant, Chamber pressure = 3.43 Mpa, $r^* = 0.014$ m

Fig. 8 CPU times required in the proposed scheme and explicit-implicit method¹⁰⁾ for a calculation of 75%-bell nozzle: AR = 140, Hydrogen, oxygen and argon-like nonreactive gases, Chamber pressure = 3.43 Mpa, $r^* = 0.068$ m (FACOM M-160F Computer)

6. CONCLUSIONS

An implicit, noniterative method has been developed to solve the equations of chemically nonequilibrium flows in the axisymmetric supersonic nozzle. The main features of the proposed method are as follows. All equations are solved simultaneously at each point by handling the axial derivative terms implicitly, which make the scheme unconditionally stable with respect to the chemical rates. The radial derivatives are evaluated explicitly, so that the required computer storage is greatly reduced compared to the full implicit method. The computational efficiency of the proposed scheme was investigated by evaluating the arithmetic operational counts required for the solution of a linear algebraic equation system, as well as comparing the CPU times. It was shown that the proposed scheme greatly improves the computational efficiency for the nonequilibrium flow problem with a large number of chemical species.

Although the present study is confined to the supersonic flow field, it may be applied to subsonic-transonic flow problems with chemical reactions, by combining it with a time-dependent method. The time-dependent method requires much computational time and a very large amount of computer storage. Thus, much greater advantages of the proposed scheme can be expected in those reacting gas flow problems.

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