Efficient Calculation of Chemically Reacting Flow

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Abstract

A SEMI-IMPLICIT finite-volume formulation is used to study flow with chemical reactions. In this formulation, the source terms resulting from the chemical reaction are treated implicitly and the resulting system of partial differential equations is sovled using two time-stepping schemes. The first is based on the Runge-Kutta method and the second on an Adams predictor-corrector method. Results show that improvements in computational efficiency depend to a large extent on the manner in which the source term is treated. Furthermore, analysis and computation indicate that the Runge-Kutta method is more efficient than the Adams methods for these systems of differential equations. Finally, an adaptive time-stepping scheme is developed to study problems involving shock ignition. Calculations for a hydrogen air system agree well with other methods.

Contents

This work is part of recent efforts[1,2] designed to explore the use of semi-implicit computational schemes as a basis for developing efficient algorithms to calculate reacting flows. In these schemes, the terms responsible for the stiffness, which are the source terms resulting from the finite reaction rates, are treated implicitly; all others are treated explicitly.

Treating stiff terms implicitly is an idea advanced by Gear[3] in developing efficient algorithms for the integration of stiff ordinary differential equations. When the idea is applied to a system of partial differential equations, the net result is the multiplication of terms involving time derivatives by a preconditioning matrix. If one is interested in obtaining steady-state solutions, then use of the exact form of the preconditioning matrix is not necessary. There is always a good possibility that a simpler version of the preconditioning matrix may speed convergence to the steady-state solution.

The governing equations, with the source terms treated implicitly, can be written as[4]

$$S^n\frac{\partial U}{\partial t} = -\left(\frac{\partial E}{\partial x}+\frac{\partial F}{\partial y}\right)^n + H^n, \quad S = 1-\frac{\partial H}{\partial U}\Delta t \tag{1}$$

were superscript n refers to the n^{th} time level. The source term H depends on the temperature T and the densities of the various species ρf_i with f_i, the mass fraction of species i, satisfying the relation,

$$\Sigma f_i = 1 \tag{2}$$

The results presented here are based on a hydrogen/air global model developed in Ref. 5. The reacting species are H, OH, H_2, O_2, and H_2O with N_2 being an inert constituent. Thus, for a one-dimensional flow, the matrix S appearing in Eq. (1) is a 6×6. The exact calculation of S, which is referred to as scheme I, is rather expensive because T is not one of the variables making up U. Because of this, two simplifications of scheme I were investigated. Both involve modification of S and, as such, do not affect the accuracy of the steady-state solution. The first simplification, to be referred to as scheme II, entails calculating $\partial H/\partial U$ while keeping T constant. Thus, for the purpose of calculating $\partial H/\partial U$, $H=H(\rho,\rho f_i)$, with the f_i related by Eq. (2). Note that the dependance of H on ρ is a consequence of using Eq. (2) to eliminate one of the conservation of species equations. In this scheme, the order of S remains the same, but the calculation of its elements is greatly simplified.

Further simplications of scheme II is obtained by removing the dependance of H on ρ by replacing Eq. (2) with the fourth conservation of species equation. In this case, $H=H(\rho f_i)$ and the resulting matrix is 4×4. This is referred to as scheme III. A comparison of CPU times required by each of the above schemes is given in Table 1. It is seen that use of scheme III results in 50% reduction in computer time.

Another objective of this work is to examine various time stepping schemes. Runge-Kutta methods have proved to be rather popular after the demonstration by Jameson et al.[6] that such methods are efficient for the solution of the Euler equa-

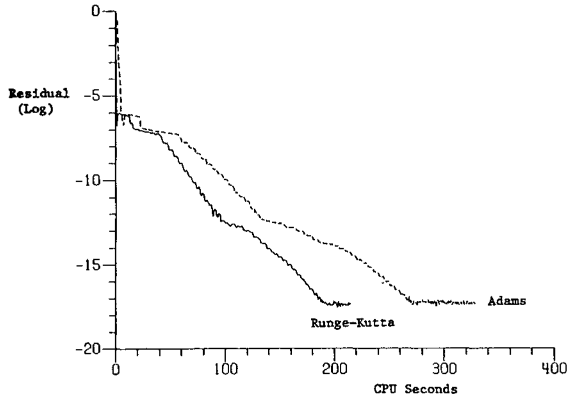

Fig. 1 Comparison of the residual histories for the two time-stepping schemes.

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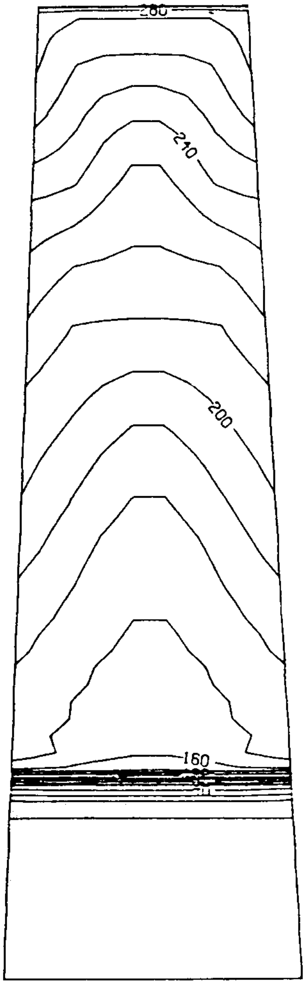

Fig. 2 Water concentration contours (contours interval is 0.10×10^{-2}).

Table 1 CPU times for various preconditioning schemes

Scheme	Relative CPU time
I	1.00
II	0.82
III	0.50

tions. The limiting CFL number for a four-step method is $2\sqrt{2}$. Examination of the Adams predictor-corrector methods[7] indicate that such methods are competitive with the Runge-Kutta methods for the solution of ordinary differential equations. Based on representative computations, it is seen from Fig. 1, which shows a typical residual plot as a function of CPU time, that calculations based on the Runge-Kutta method are more efficient than those based on the Adams method.

The traditional Runge-Kutta method[6] proved inadequate when used to calculate problems involving shock ignition. The scheme employed here captures shocks. The oscillations that accompany strong shock formations interacting with large chemical source terms were often found to cause some of the concentrations to become negative. Rather than select the time step by a requirement that limits changes in mass fraction by a certain percentage, the full gas dynamic time step was used after about 25 time steps. This was found to often cause some of the mass fractions to become negative and, as such, resulted in the premature termination of the calculations. The adaptive scheme employed here checks the signs of the updated mass fractions and, if all are positive, the remaining variables are updated and the integration is continued. Otherwise, the time step is halved and the calculations are repeated. For most results involving shock ignition, one to two halvings were needed while the shock was forming. Thus, the scheme allows the use of the full gas dynamic time step most of the time which contributes to the overall efficiency of the algorithm.

The approach developed here was used to study shock ignition in two-dimensional nozzles. Figure 2 shows a typical contour of H_2O concentration. Here, the inlet Mach number is 2. Notice that the expansion wave emanating from the corner of the inlet results in a higher temperature and accordingly, a higher rate of combustion toward the centerline.

Conclusions

The results presented here suggest that a semi-implicit integration scheme employing an adaptive time-stepping Runge-Kutta method is a viable approach for the calculation of reacting flows in the presence of strong shocks. Further, simplification of the preconditioning matrix resulting from the semi-implicit formulation can accelerate convergence to steady state without affecting the accuracy of the steady-state solution.

Acknowledgment

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