Improved Flux-Split Algorithm Applied to Hypersonic Flows in Chemical Equilibrium

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Abstract

A UNIQUE coupling technique is developed that maintains stability in an explicit, fully coupled finite-rate code while allowing a relatively high time step. The method is incorporated into an explicit finite-difference shock capturing algorithm and applied to hypersonic flows in near-thermochemical equilibrium. Numerical results are compared against ballistic range and flight data as well as against computations performed by a loosely coupled equilibrium code.

Contents

In general, there are two different approaches to coupling real-gas chemistry to the conservation equations of gasdynamics. The first method loosely couples the gasdynamic equations to an equilibrium chemistry package. The chemistry is not updated every time step. The second approach fully couples the global conservation equations to a set of species mass conservation equations that include source terms representing the production of species from finite-rate chemical reactions.

The addition of species mass conservation equations makes the equation set "stiff." If an explicit method is used, small time steps are required to maintain stability. The use of implicit methods relieves these time step restrictions, but requires the filling and inversion of large and complex block tridiagonal matrices, which can be memory and CPU intensive.

The purpose of this work is to propose a method that allows an explicit finite-rate algorithm to use a relatively high time step, and to compare numerical results from the fully coupled algorithm with those generated using a loosely coupled technique for test problems where experimental data exists. These test problems are in flow regimes in near-thermochemical equilibrium.

The gasdynamic solver used in this study uses the explicit Euler time march scheme to solve the two-dimensional/axisymmetric thin-layer Navier Stokes equations. Van Leer flux vector splitting,[1] was used to difference the inviscid fluxes.

Loosely Coupled Approach

Two different coupling methods were used. In the first, the gasdynamics was loosely coupled to a Gibbs free-energy minimization chemistry package.[2] The equilibrium state of the gas at each node point was determined by minimizing the Gibbs free-energy subject to conservation of mass, change, and static enthalpy. Pressure and static enthalpy, held constant through the minimization process, were obtained from the gasdynamics and supplied to the chemistry package. The chemical state of the gas was updated every 25 or 50 time steps.

Fully Coupled Approach

The second approach fully coupled the global conservation equation to a series of species mass conservation equations. Finite-rate codes are generally used to compute nonequilibrium flows but can be applied to flows in near-chemical equilibrium as well, and this is a good test of the stability of a finite-rate algorithm.

Seven species, N, N_2, O, O_2, NO, NO^+, e^-, and twenty-one chemical reactions were considered in this study. The forward and backward reaction rates were obtained from Park.[3]

The problem with including species conservation equations in the equation set is that source terms can sometimes be large relative to the flux terms, causing nonphysical species densities, such as $\rho_i > \rho$ or $\rho_i < 0$. For example, when the temperature is high, such as behind the shock when the shock is moving off the body, the magnitude of the source terms will be large, reflecting the gas's tendency to dissociate. As the temperature relaxes and approaches its steady state value, the magnitude of the species density updates diminishes.

Large source terms cause the equation set to be stiff. However, if in the initial high temperature stage the magnitude of the species density updates could be controlled by scaling them, the algorithm could maintain stability until the temperature has relaxed to a point where the controls would no longer be necessary. It would also be desirable to maintain the trends of the chemistry. For instance, if the code wanted to produce twice as much atomic oxygen as atomic nitrogen at some point, this should still be the case after the species density updates were scaled.

Relating change in mass fraction $\delta\gamma_i$ to change in species density $\delta\rho_i$,

$$\delta(\rho_i) = \delta(\gamma_i \rho) = \gamma_i \delta\rho + \rho \delta\gamma_i \tag{1}$$

or

$$\delta\gamma_i = (\delta\rho_i - \gamma_i \delta\rho)/\rho \tag{2}$$

a scheme was devised to update the species densities that circumvent the stiffness associated with the explicit formulation. The method maintains stability even when very large source terms are present. The procedure is as follows.

1) Obtain the changes in species density $\delta\rho_i$ by solving the species conservation equations. The species mass fluxes are split exactly like the global mass flux, except ρ_i is used instead of ρ.

2) Calculate the changes in species mass fraction $\delta\gamma_i$ from Eq. (2). Note that for consistency in Eq. (2), the ρ in the denominator is the updated value $\rho^{n+1} = \rho^n + \delta\rho$ obtained from solving the global mass conservation equation, and the γ_i in the numerator is γ_i^n.

3) Find the maximum $\delta\gamma_i$, and if its magnitude is greater

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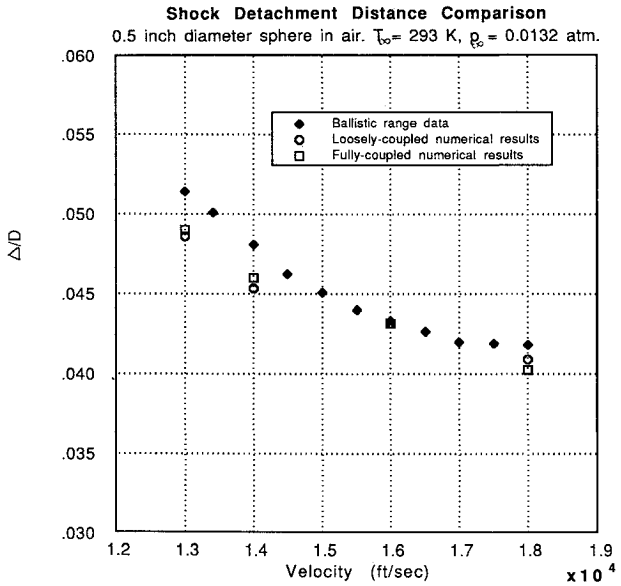

Fig. 1 Shock standoff comparison.

than a prescribed tolerance, scale the γ_i's

$$\delta\gamma_i = \frac{\delta\gamma_i}{|\delta\gamma_{\max}|} * \text{tol} \tag{3}$$

The value tol is the maximum amount any species mass fraction is permitted to change per time step. A typical value of tol is 0.01 This scaling also preserves the relative magnitudes of the $\delta\gamma_i$'s.

4) Update the mass fractions

$$\gamma_i^{n+1} = \gamma_i^n + \delta\gamma_i \tag{4}$$

5) Update the species densities

$$\rho_i^{n+1} = \gamma_i^{n+1}\rho^{n+1} \tag{5}$$

The updated species densities are then used to calculate a new temperature and pressure.

This process limits the rate at which the gas can dissociate and ionize and prevents wild swings in mass fractions and temperature. The gas gradually and stably relaxes to its steady-state composition and temperature. The explicit code can be run at global time steps corresponding to CFL numbers of 0.5 to 0.9, comparable to those possible with a perfect gas code.

Results

An effort was made to compare numerical results generated using the fully coupled method with those computed using the loosely coupled method and against experimental data.

The first experiment involved measurement of shock detachment distances on spheres.[4] The sphere diameter was 0.5 in., the ambient air pressure was 10 mm Hg, and the freestream temperature was 293 K. Test velocities range from 13,000 to 18,000 ft/s. A plot of normalized shock standoff vs freestream velocity is shown in Fig. 1. The two coupling approaches predicted very similar shock standoff distances in good agreement with the experimental results.

The next case concerned flight data, the RAMC II flight experiment. The RAMC II vehicle, launched in 1968, was a 15 cm nose radius 9 deg half angle cone with an overall length of 130 cm. One of the quantities inferred from measurements taken was peak electron density along the body at several altitudes along its trajectory.[5]

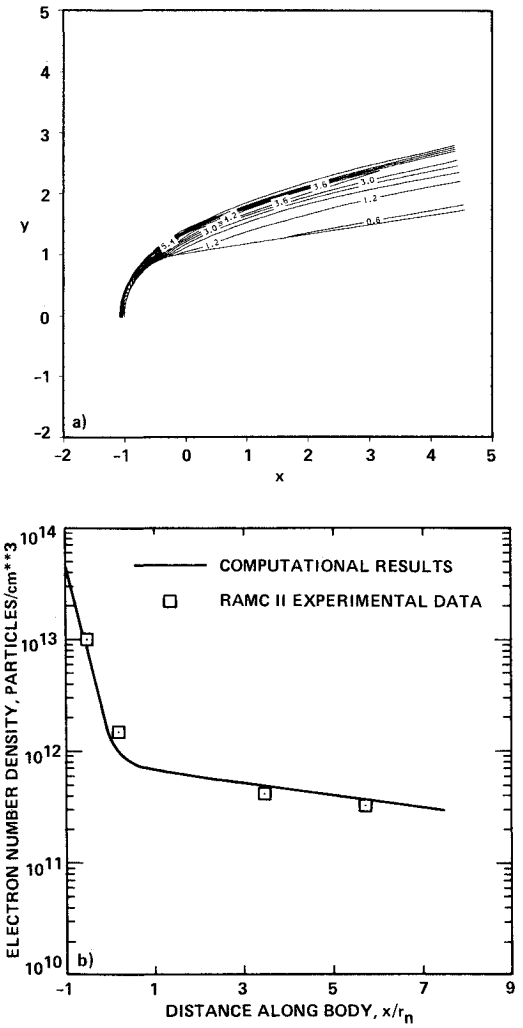

Fig. 2 RAMC II flight data. a) Computed normalized density countours, ρ/ρ_∞. b) Measured and calculated electron number density.

Figure 2a shows the flowfield generated by the finite rate algorithm at freestream conditions corresponding to an altitude of 61 km. This altitude was chosen because the flowfield would be in near-thermochemical equilibrum. Freestream temperature and pressure were 252 K and 13.3 Pa. The wall temperature in the numerical computations was held fixed at 1500 K. Figure 2b shows experimental and calculated peak electron density along the body. The correlation between the two is excellent.

References

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