## Time-Dependent Solutions of Nonequilibrium Airflow past a Blunt Body

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## Theme

THIS paper presents a finite-difference technique that can be used to calculate an inviscid, supersonic, reacting flow of multicomponent mixtures past a blunt body at an angle of attack. The calculation is carried out by a two-step Lax-Wendroff scheme that advances the solution in time until the steady-state solution results. Boundaries of the shock layer are calculated from a new procedure. The efficiency of the technique is improved by using two distinct time increments.

## **Contents**

The primary concerns in the numerical study of the flowfield are the accuracy of the predicted results, the efficiency, and the ease of application of the calculation procedure. The consideration of chemical and physical processes, coupled with the fluid-dynamic equations, makes the choice of a calculation procedure even more stringent. The time-dependent technique that has been developed in the past several years probably represents the most advanced tool in the flowfield calculations. It has been shown for an ideal gas that this technique is superior in many ways to the steady techniques: the method of integral relations and the inverse matching techniques. The subsequent application of a time-dependent technique to reacting blunt-body problems is therefore logical in view of its success with nonreacting flow problems. After reviewing previous analyses, however, it appears that although valuable knowledge has been accumulated in the application of the time-dependent technique, none of them have the potential to solve a three-dimensional angle-of-attack problem with the realistic gas model. The calculation of the three-dimensional nonequilibrium flowfield was attempted in Ref. 1, where a sharp-shock procedure was applied to a binary dissociating gas. The sharp-shock procedure is considered to be more efficient than the shock-capturing procedure developed in Ref. 2 for a similar gas model. However, Ref. 1 still used a very involved calculation procedure for flow properties within the shock layer and on the boundaries, making the consideration of a multicomponent mixture impractical. An additional difficulty is that numerical instability would occur in integrating the species conservation equations if the time increment is determined from the usual CFL condition. Reference 3 and later analyses tried to circumvent this difficulty by using a time increment determined from the relaxation time of chemical reactions for the integration of all governing equations. Because the chemical relaxation time is generally of one or two orders of magnitude less in comparison to the CFL time, a large amount of machine time is required to reach the steady-state solution. A combination of the time-dependent and steady procedures was then used in Ref. 4 to solve a two-dimensional flowfield. Unfortunately, extension to an angle-of-attack case is a rather tedious task. The more efficient calculation procedure described here can be used to calculate three-dimensional nonequilibrium blunt-body flowfields of multicomponent mixtures.

Governing equations. This system of equations has the following form

$$d\rho/dt + \rho \operatorname{div}\vec{u} = 0 \tag{1}$$

$$d\vec{u}/dt + 1/\rho \operatorname{grad} p = 0 \tag{2}$$

$$\frac{dT}{dt} + \frac{p}{c_v \rho} \operatorname{div} \vec{u} + \sum_{i=1}^{l} \omega_i e_i / c_v = 0$$
 (3)

$$dc_i/dt = \omega_i \qquad (i = 1, 2, ..., l) \tag{4}$$

$$p = \rho RT \sum_{i=1}^{l} \frac{c_i}{M_{wi}} \tag{5}$$

Here  $\vec{u}$ , p,  $\rho$ , and T are velocity, pressure, density, and temperature for the mixture; R is the universal gas constant,  $c_v$  is the specific heat at constant volume,  $c_i$ ,  $M_{wi}$ ,  $e_i$ , are the mass concentration, molecular weight, and specific internal energy of the ith species;  $\omega_i$  is the production of the ith species as a result of chemical reaction. The governing equations (1–5) are the usual conservation equations along with an equation of state.

Equations (1-5) are transformed from the spherical polar coordinate system on which the equations are written to a new coordinate system that requires the shock and the body to be parallel. The shock layer after transformation is called the computation region. The time derivatives of dependent variables are then used to advance the solution. The CFL value is used for Eqs. (1) and (2), while the reaction relaxation time is used for Eqs. (3) and (4). Numerical experiments have been conducted to justify the simultaneous use of two time increments. The asymptotic solution can be obtained for all the dependent variables, and the convergence of the species concentration is about as fast as that of other flow properties.

Shock and Wall Boundaries. A new procedure treating both boundaries is described as follows: The shock fitting is carried out for each time step by matching the finite-difference solution with the Rankine-Hugoniot relations. The finite-difference solution is obtained using a one-side difference formula to replace the space derivatives in the direction normal to the shock. Shock speed, among other quantities, is determined from the shock-fitting procedure and then used to update the shock position and the computation region. The shock speed is also used as a measure of the steadiness of the solution since a stationary shock is to be obtained as the solution marching toward the steady state. Note that in the calculation of shock, frozen flow is assumed.

On the wall no matching process between the finitedifference solution and the wall conditions is needed. Instead, the dependent variables in Eqs. (1-3) are obtained at the wall by the one-side Lax scheme. The boundary condition that

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requires the wall be a streamline is applied to the velocity by adjusting the components so that the normal component to the wall is zero. Since the wall is assumed to be noncatalytic, integration of Eq. (4) is not performed.

The procedure used is essentially a first-order scheme in time and space. An artificial viscosity term is introduced by the finite-difference formulation to Eqs. (1-4). The first-order accurate solution, however, is improved by imposing the exact boundary conditions to the solution. The accuracy of the result is, therefore, not measurable in a mathematical sense. A unified two-step scheme can be applied, but it is less efficient than the present procedure because two shock fittings are involved for each time step.

Numerical results. The first test case was a sphere at freestream conditions used in Ref. 5. The computed shock position, temperature, and density profiles along the stagnation line were in satisfactory agreement with the results in Ref. 5. Variation of flow properties were noted from the use of different sets of rate constants. However, the shock position and the pressure distribution on the wall were insensitive to the values of the rate constants. The finitedifference solution was obtained with five points in the radial direction and 10 points in the angular direction. Twenty minutes of computational time on a UNIVAC 1108 were required for a 300-time-step calculation. The shock speed had decreased to a near-stationary value of 1% of the freestream speed. The changes in species concentration as well as in other flow properties between two successful steps at the end of the calculation were not discernible. This test case was recalculated using one time increment given by the relaxation time. The calculation took more than 2000 time steps to reach a steadiness of solution equivalent to the solution obtained by using two time increments. Furthermore, the difference between these two solutions in species concentration was within 6%.

The second test case was a 20° half-angle cone with an ellipsoid nose at an angle of attack of 20°. The calculation procedure for boundaries was checked out for an ideal gas model using a mesh of  $(7 \times 10 \times 8)$  defined according to the spherical coordinate system  $(r,\theta,\phi)$ . The result was in excellent agreement with the one shown in Ref. 1, in which the method of characteristics was used to calculate the two boundaries. However, the application of this new procedure

to a very large angle-of-attack problem should be less reliable because the velocity component in the meridional plane is simply determined from the finite-difference solution. Unlike the other two components, a boundary condition is not available to correct the finite-difference results. The nonequilibrium calculation was made through 300 time steps. The maximum shock speed was one-tenth of the freestream, or roughly, the accuracy of the results was within 10% of the steady solution. Characteristics of the flowfield, namely the shock position, and the NO profile along the stagnation line were reasonable. There is no further confirmation of the validity of this procedure since comparable results are not available.

Conclusion. A finite-difference calculation procedure for chemical reacting blunt-body flows is discussed in this paper. The treatment of boundaries of the shock layer is found to be efficient and accurate. The idea of using distinct time increments to advance flow variables simultaneously is workable and leads to a meaningful steady-state solution. From the proposed procedure, a computer program has been written to execute the test cases. The machine running time for a typical nonequilibrium calculation at an angle of attack is several orders of magnitude less than that required by other procedures. The application of this procedure has demonstrated that sufficient accuracy in flow properties can be obtained for engineering applications with no more than 10 grid points in each of the space dimensions.

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