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Implicit Flux-Split Algorithm to Calculate Hypersonic Flowfields in Chemical Equilibrium

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Introduction

THE aeroassisted orbital transfer vehicle (AOTV) and the national aerospace plane will be required to maneuver at hypersonic velocities in the upper atmosphere in flow regimes where the ideal gas assumption does not apply. The design of these vehicles will depend on a new generation of numerical algorithms that combine the gasdynamic equations of computational fluid dynamics with equilibrium and nonequilibrium chemical reactions. The first step in developing a hypersonic computational fluid dynamics capability is a solid equilibrium code, one that is efficient and stable.

In recent years, a number of attempts have been made to simulate real-gas flowfields about blunt bodies.[1-3] This study presents an implicit, shock-capturing algorithm for calculating hypersonic equilibrium flow over blunt bodies. The fluxes are diferenced using first-order Steger-Warming[4] flux vector splitting. The equilibrium chemistry package is based on the Gibbs free energy minimization technique of Gordon and McBride.[5]

The present algorithm has shown itself to be robust and efficient. The techniques used are easy to understand and allow the code to be written in a modular, straightforward manner. Modifications and extensions are easily implemented. The code has proved its ability to capture strong shocks about blunt bodies at hypersonic velocities.

Governing Equations

The Euler equations for two-dimensional or axisymmetric perfect gas flow without external forces can be expressed in conservation law form in generalized coordinates[6] as

$$\frac{\partial Q}{\partial t}+\frac{\partial F}{\partial \xi}+\frac{\partial G}{\partial \eta}+rH=0 \tag{1}$$

with

$$Q=J^{-1}\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ e\end{bmatrix} \qquad F=J^{-1}\begin{bmatrix}\rho U\\ \rho uU+\xi_x p\\ \rho vU+\xi_y p\\ (e+p)U\end{bmatrix}$$

$$G=J^{-1}\begin{bmatrix}\rho V\\ \rho uV+\eta_x p\\ \rho vV+\eta_y p\\ (e+p)V\end{bmatrix} \qquad H=\frac{J^{-1}}{y}\begin{bmatrix}\rho v\\ \rho uv\\ \rho v^2\\ (e+p)v\end{bmatrix}$$

It is necessary to relate the pressure to the flow variables. The parameter β is introduced and defined as the ratio of static enthalpy to internal energy. For an ideal gas, β equals the ratio of specific heats, γ. Expressing the internal energy in terms of the flow variables and the static enthalpy in terms of β, p, and ρ yields the desired equation of state:

$$p=(\beta-1)[e-\tfrac{1}{2}\rho(u^2+v^2)] \tag{2}$$

Method

The basic form of the algorithm is the Beam and Warming approximate factorization algorithm[7]

$$(I+\Delta t\delta_\xi A^n)[I+\Delta t(\delta_\eta B^n+rC^n)]\delta Q^n$$
$$=-\Delta t(\delta_\xi F^n+\delta_\eta G^n+rH^n) \tag{3}$$

The spatial derivatives are differenced using an upwind technique: that of Steger-Warming flux vector splitting.[4] The first-order flux-split technique is naturally stable and easy to code. Strong shocks can be captured without artificial dissipation terms or flux limiters. For viscous flows, first-order differencing is too dissipative to resolve the boundary layer accurately, but for inviscid flow calculations this dissipative nature is not as big a concern. Proper selection of the grid and the use of solution grid adaption techniques minimize any inaccuracies and shock smearing caused by the first-order method. Accurate results were obtained for a Mach 20 hemisphere test problem using the first-order method.

Steger-Warming flux vector splitting is based on the fact that the Euler equations are homogenous of degree one, such that $F=AQ$ and $G=BQ$. The flux vector F is split into positive and negative components:

$$F=F^+ +F^- =A^+Q+A^-Q \tag{4}$$

$$A^+=S_A\Lambda_A^+S_A^{-1} \qquad A^-=S_A\Lambda_A^-S_A^{-1} \tag{5}$$

The matrices Λ_A^+ and Λ_A^- contain the positive and negative eigenvalues of A, respectively, and S_A is the eigenvector matrix of A. The matrices G and B are similarly split. From domain of dependence and linear stability considerations, backward-difference approximations are used for the positive fluxes and positive-flux Jacobians and forward-difference approximations are used for the negative fluxes and negative-flux Jacobians.

Boundary Conditions

Along the body surface, the tangent Cartesian velocity components are found by setting V equal to zero and extrapolating U from the interior.[6] The freestream total enthalpy, $(e+p)/\rho$, is assumed constant along the body. This assumption is acceptable for steady-state calculations.

One additional parameter, for instance pressure, is necessary to determine the flow quantities along the wall boundary. The normal momentum equation can be used to determine this pressure. It is generally written in nonconservative form.[6] It was desired to use an impulsive starting procedure with the

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algorithm, but stability problems arise when the nonconservative form is used with an impulsive start. This stability problem disappears if the normal momentum equation is evaluated in its conservation law form:

$$\eta_x\left(\frac{\rho uU}{J}+\frac{\xi_x p}{J}\right)_\xi+\eta_y\left(\frac{\rho vU}{J}+\frac{\xi_y p}{J}\right)_\xi$$
$$+\eta_x\left(\frac{\rho uV}{J}+\frac{\eta_x p}{J}\right)_\eta+\eta_y\left(\frac{\rho vV}{J}+\frac{\eta_y p}{J}\right)_\eta=0 \qquad (6)$$

This results in a scalar tridiagonal that can be solved for the pressure at the body surface.

Chemistry Package

The chemistry package is based on the method of Gordon and McBride.[5] The equilibrium state of the gas at each node point is determined by minimizing the Gibbs free energy, subject to conservation of mass, charge, and static enthalpy. Both pressure and static enthalpy are held constant throughout the chemistry process.

The minimization is performed using Lagrange multipliers. A descent Newton-Raphson method solves for updated values of species mole fraction, mixture molar mass, and temperature. This is an iterative process, continued until the system converges. The minimization uses values of enthalpy, entropy, and specific heat for each species obtained from polynomial curve fits to the JANAF[8] thermochemical data.

Values of pressure and static enthalpy are obtained from the conservation variables and β and supplied to the chemistry package. The chemistry returns updated values of mixture molar mass, temperature, and β. The value of β is held fixed between chemistry updates, generally for 15 or 25 steps. Holding β constant is equivalent to saying that β does not vary with the conservation variables. It has been shown that β is a slow function of the conservation variables, but for steady-state calculations the constant β assumption is acceptable.

Adaptive Grid

The solution adaptive-grid technique of Nakahashi and Deiwert[9] was used to align the grid lines with the shock and to cluster lines in regions of strong gradients. Details of the adaptive-grid technique are given in Ref. 9 and will not be discussed here.

Results

The code was tested by computing Mach 20 flow over an axisymmetric hemisphere. Freestream conditions corresponded to an altitude of 20 km. The chemistry was updated every 15 gasdynamic steps. Results generated by the current algorithm could be compared against those of Lyubimov and Rusanov.[10]

An equispaced grid having 32 streamwise and 32 radial points was adapted using Nakahashi and Deiwert's code. Figure 1 shows the normalized temperature plot using the adapted grid for the Mach 20 calculation. The L2 norm of the density residual for the hemisphere calculation is shown in Fig. 2. The spikes in the residual plot occur at 15 step intervals and coincide with when the chemistry is updated. After a certain point, the spikes become large and oscillate about a constant value. This reflects a certain disparity when the shock location stabilizes between the chemistry package and the gasdynamic algorithm. This type of behavior is typical of decoupled methods, where the gasdynamic and chemistry codes exist as separate entities.

Table 1 compares numerical results along the stagnation line found in the current study with those from Ref. 10. Values of temperature, normalized pressure, normalized density, and species mole fractions are compared at the body, the shock, and the midpoint between the body and shock. Agreement is generally within 5%. The values obtained using the current algorithm also agree with those found at the same conditions by Balakrishnan et al.[2]

The code was then used to calculate equilibrium flowfields over more practical configurations. Figure 3 shows inviscid equilibrium flow over an axisymmetric AOTV forebody at Mach 20 with freestream conditions corresponding to 20 km.

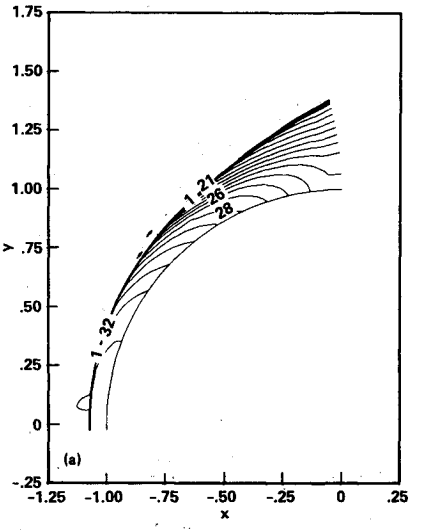


Fig. 1 Hemisphere, Mach 20, normalized temperature.

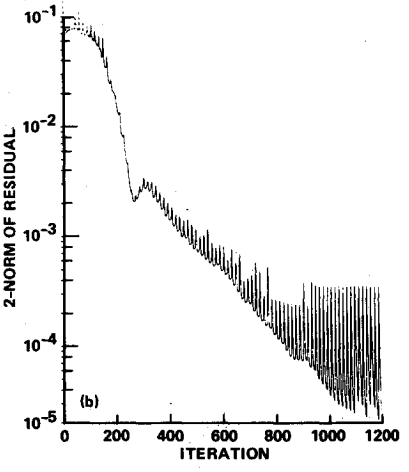


Fig. 2 Residual plot.

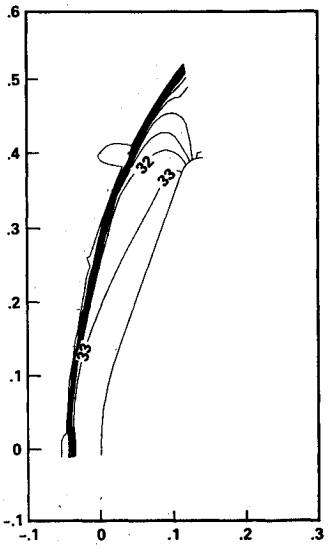
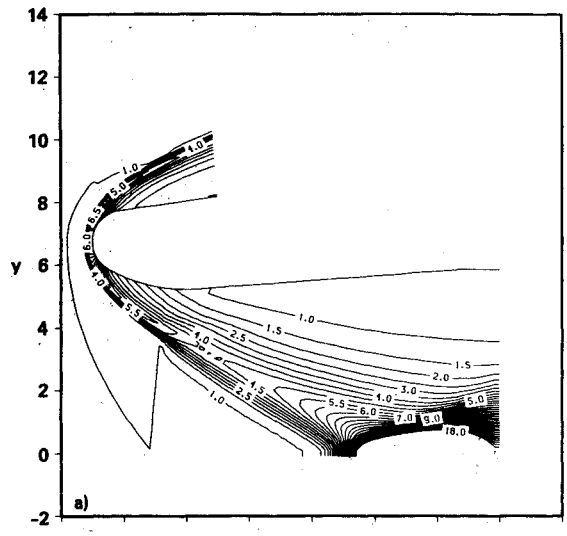


Fig. 3 AOTV forebody, Mach 20, normalized temperature.

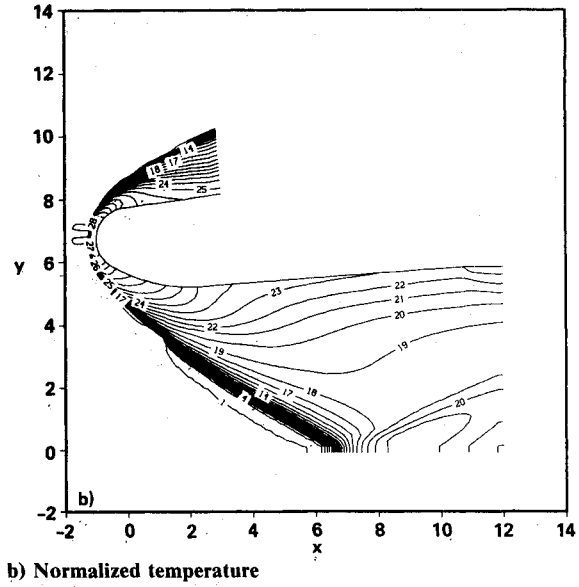
Table 1 Comparison of results (Mach 20, 20 km)

	Normalized distance from wall r_n[a]					
	0.0		0.50		1.0	
	Present	Ref. 18	Present	Ref. 18	Present	Ref. 18
$\frac{p}{p_\infty}$	533.4	536.9	527.4	532.3	506.6	511.7
$\frac{\rho}{\rho_\infty}$	11.91	11.85	11.86	11.76	11.40	11.37
$T(K)$	7283	7395	7252	7388	7243	7357
Mole fraction						
O	0.2951	0.2933	0.2957	0.2928	0.2958	0.2933
O_2	1.089-3	9.265-4	1.123-3	9.232-4	1.091-3	9.232-4
N	0.1967	0.2003	0.1915	0.1996	0.1931	0.1970
N_2	0.4851	0.4776	0.4894	0.4780	0.4881	0.4801
NO	2.133-2	2.070-2	2.143-2	2.065-2	2.106-2	2.057-2
e^-	3.927-4	3.945-4	3.821-4	3.921-4	3.828-4	3.840-4

[a] $r_n = 0$ at the wall; $r_n = 1$ at the shock.



a) Normalized density



b) Normalized temperature

Fig. 4 Hypersonic inlet, Mach 20.

The temperature along much of the forebody surface is in excess of 7000 K. Figure 4 shows equilibrium flow through a hypersonic inlet at the same conditions. This problem was chosen to demonstrate the code's ability to compute internal as well as external flows. Only the upper half of the axisymmetric inlet is shown. Some interesting flow phenomenon is apparent, including a Mach stem and a reflected shock. No significant problems were encountered when the code was applied to these more complex configurations.

Conclusions

The objective of this work was to develop an algorithm that could accurately predict inviscid, equilibrium, high Mach number flows. That goal has been achieved. The method has proved its ability to capture strong shocks. Solutions for a generic axisymmetric hemisphere at Mach 20 compare well with previously published results. The code has shown its ability to be applied to both internal and external hypersonic flows over a variety on configurations.

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Deforming Grid Method Applied to the Inverse Problem of Heat Conduction

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Nomenclature

c = heat capacity of the material
h = heat-transfer coefficient
k = thermal conductivity
L = thickness of material

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