AIAA JOURNAL
Vol. 31, No. 5, May 1993

Hypersonic Nonequilibrium Flow Computations Using the Roe Flux-Difference Split Scheme

Eswar Josyula,* Datta Gaitonde,† and Joseph S. Shang‡
Flight Dynamics Directorate, Wright-Patterson Air Force Base, Ohio 45433

Abstract

THE Roe flux difference splitting scheme is investigated for accuracy in simulating hypersonic reacting flows. The extension of the Roe scheme to include the finite rate chemical kinetic equations follows the approach of Grossman and Cinnella. Formal second-order accuracy is obtained by employing the monotonic upstream schemes for conservation laws (MUSCL) approach in conjunction with the minmod limiter to degenerate the solution to first-order accuracy in the vicinity of strong shock waves. The full Navier-Stokes equations are solved with finite rate chemistry for the flow past an axisymmetric blunt body at zero incidence at several Mach numbers. The vibrational energy is assumed to be in thermodynamic equilibrium with the other internal energy modes. The air mixture is assumed to consist of the five species O_2, O, N_2, N, and NO. The surface heat transfer predicted by this scheme is validated for flows with Mach numbers 15.3 and 16.34 when compared with classical theory and experimental results. Both catalytic and noncatalytic wall boundary conditions are used. The entropy correction parameter, necessary to enforce the entropy condition in Roe's scheme, is found to be a simple and effective means to control numerical error due to the degenerated eigenvalue structure in the stagnation region, thus suppressing the numerical bulge or "carbuncle" phenomenon.

Nomenclature

D	= arc length along cylinder surface
M_∞	= freestream Mach number
Rey_∞	= freestream Reynolds number based on nose radius
R_n	= nose radius
T_∞	= freestream temperature
η	= distance along stagnation streamline
Θ	= body angle

Contents

Recent advances in the development of flux-split schemes have had a remarkable influence on the computation of hypersonic flows. This paper focuses on the Roe's approximate Riemann solver for computing the dissociated flow past a blunt body. A well-known problem of Roe's algorithm is the deficiency in enforcing the entropy condition. Following the approach of Harten,[1] the eigenvalues of the flux Jacobian are modified ("cutoff") when they are below some small threshold. However, the parameter controlling the magnitude of this cutoff must be carefully selected. One formulation is described by Riedelbauch and Brenner,[2] who computed several flows in chemical and thermal equilibrium with the "upwind" total variation diminishing (TVD) scheme by utilizing Roe's approximate Riemann solver to determine the state at the computational interfaces. However, the effect of this entropy correction on the physics of high-temperature flows in chemical nonequilibrium has not been studied and was one of the objectives of the investigation reported in Ref. 3. The effects of entropy cutoff ($0.01 \leq \tilde{\delta} \leq 0.5$) on surface heat transfer and pressures were investigated and found to be negligible beyond a required minimum for the flow conditions and the grid selected. The magnitude of cutoff necessary to obtain nonanomalous solutions was higher for finer grids. This paper presents results of surface heat transfer and species mass-concentrations in the shock-layer for nonquilibrium hypersonic flow, considering the entropy correction reported in Ref. 3.

It is the purpose of this paper to study the Roe flux-difference split scheme for modeling the inviscid terms of the governing equations for a viscous flow in chemical nonequilibrium past an axisymmetric blunt body. The approach of Grossman and Cinnella[4] for treating the inviscid fluxes according to the Roe scheme is used in the present study. The upper limit temperature for the present analysis is restricted to 9000 K and the maximum altitude considered is 42 km, for the purpose of validating the present numerical scheme with experimental and theoretical results. Since the objective of this paper is to study the ability of the numerical scheme to predict surface heat transfer, which is mainly influenced by the thermochemical properties near the surface, ionization and radiation of the atomic species are neglected. Simplifying assumptions are also made for the transport properties by considering Sutherland's law for computing the viscosity of the gas. Details of the governing equations and the numerical scheme, including the entropy correction parameter, are as given in Ref. 3.

The surface heat transfer prediction by the present scheme is validated for a flow past a blunt body at Mach 16.34, for which experimental results were obtained in a shock tunnel by Holden et al.[5] The algorithm is also validated for the surface heat transfer for a Mach 15.3 flow in chemical nonequilibrium, for which theoretical[6] results are available for purpose of comparison. The Roe scheme is implemented on a grid with 50 points in the streamwise direction and 45 points in thenormal direction. The computation is performed in local time-stepping mode with a Courant-Friedrich-Lewy (CFL) number of 0.9.

Iterative convergence is monitored by examining the L2 Norm of the residual and the surface heat transfer over several characteristic times. The criterion of convergence is met after the normalized residual drops more than eight orders of magnitude. Convergence also implies that the change in surface heat transfer does not change more than 1% between two consecutive solutions of one time unit apart.

The flowfield is discussed for results presented in the following sections to demonstrate the ability of the numerical scheme to predict the surface heat transfer and mass concentrations in the shock-layer for chemically reacting flows. Discussion of the entropy correction parameter and a grid resolution study were presented in Ref. 3.

Presented as Paper 91-1700 at the AIAA 22nd Fluid and Plasmadynamics Conference, Honolulu, HI, June 24-26, 1991; received Aug. 27, 1991; synoptic received Aug. 24, 1992; accepted for publication Sept. 9, 1992. Full paper available from AIAA Library, 555 W. 57th St., New York, NY 10019.

*Aerospace Engineer, Wright Laboratory. Member AIAA.
†Visiting Scientist, Wright Laboratory. Member AIAA.
‡Senior Scientist, Wright Laboratory. Associate Fellow AIAA.

Mach 16.34 Case

The surface heat transfer prediction of the present scheme is validated with the experimental results of Holden et al.[5] for the following flow conditions: $M_\infty = 16.34$, cylinder radius = 0.0381 m, $T_\infty = 52.2$ K, and $T_{wall} = 294.4$ K. For the simulated flow conditions, since the chemical reaction rate is much slower than the flow time scale, the flowfield exhibits frozen flow characteristics. The perfect gas computation is also performed to show this negligible chemical nonequilibrium in the flowfield.

Figure 1 shows the comparison of heat transfer distribution for both perfect and reacting gas computations with experimental observations of Holden et al.[5] The heat transfer values are within the experimental scatter and show excellent agreement. The perfect gas and reacting gas comparison shows very little difference because the relatively low temperatures after the shock wave compression lead to negligible degrees of dissociation.

Mach 15.3 Case

A second case is presented for the following conditions: $M_\infty = 15.3$, cylinder radius = 0.00635 m, $T_\infty = 293$ K, and $T_{wall} = 1200$ K. The computation is made for both noncatalytic and fully catalytic wall boundary conditions. The computed surface heat transfer results are validated with theoretical predictions.

Figure 2 is a comparison of species mass-concentrations for O_2, O, and NO along the stagnation streamline for a noncatalytic and a fully catalytic wall at Mach 15.3. The concentrations for the noncatalytic wall do not show any recombination at the surface. The results for the noncatalytic wall boundary condition match the trends obtained by Candler's computation[7] for the same set of flow conditions. Because of the complete recombination of atoms at the surface, the concentrations of O and NO are zero at the surface for the fully catalytic wall. The peak concentrations of O and NO within the shock-layer, however, do not show much variation compared to those for a noncatalytic wall.

Figure 3 compares the surface heat transfer for perfect gas and reacting gas with both noncatalytic and fully catalytic wall boundary conditions. The stagnation point heat transfer for the fully catalytic wall compares well with the theoretical prediction of Detra et al.[6] The heat transfer prediction for a noncatalytic wall is about 40% less than that for a perfect gas. The contribution of diffusion heat flux is zero due to the specification of a noncatalytic wall. Thus, the surface heat transfer is made up entirely of conduction. Since dissociation is endothermic, the temperature is reduced for the reacting gas, and the corresponding heat transfer is lower than that of the perfect gas. However, for the flow with the fully catalytic wall boundary condition the contribution of diffusion flux raises the heat transfer over that of the noncatalytic wall and is nearly equal to the heat transfer as predicted by the perfect gas.

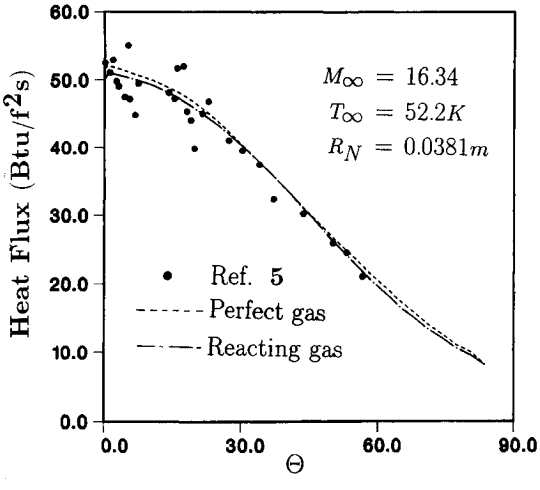

Fig. 1 Validation of surface heat transfer distribution in low enthalpy flow.

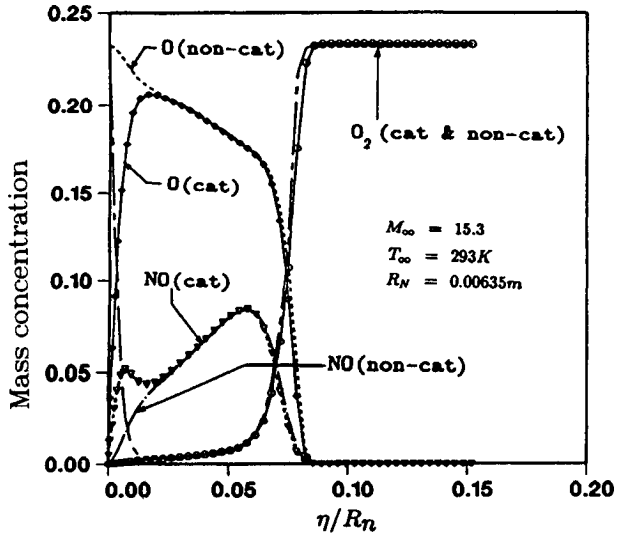

Fig. 2 Comparison of mass-concentration along stagnation streamline for a noncatalytic and a fully catalytic wall.

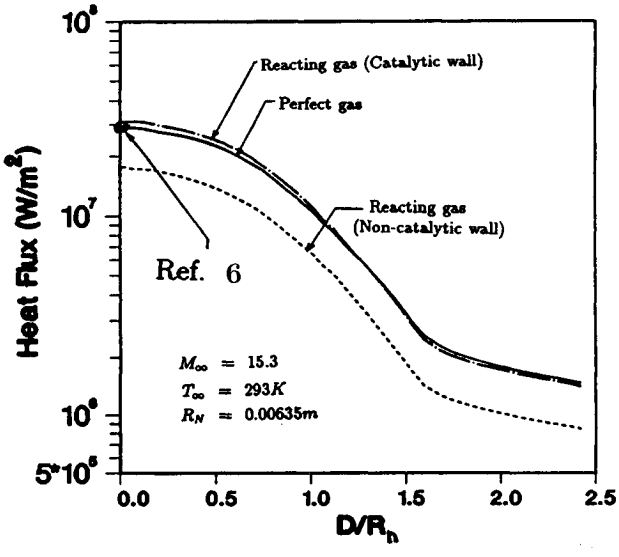

Fig. 3 Comparison of surface heat transfer.

References

[1]Harten, A., "High Resolution Schemes for Hyperbolic Conservation Laws," *Journal of Computational Physics,* Vol. 49, No. 3, 1983, pp. 357-393.

[2]Riedelbauch, R., and Brenner, G., "Numerical Simulation of Laminar Hypersonic Flow Past Blunt Bodies Including High Temperature Effects," AIAA Paper 90-1492, June 1990.

[3]Josyula, E., Gaitonde, D., and Shang, J. S., "Nonequilibrium Hypersonic Flow Solutions Using the Roe Flux-Difference Split Scheme," AIAA Paper 91-1700, June 1991.

[4]Grossman, B., and Cinnella, P., "Flux-Split Algorithms for Flows with Non-equilibrium Chemistry and Vibrational Relaxation," *Journal of Computational Physics,* Vol. 88, No. 1, 1990, pp. 131-168.

[5]Holden, M. S., Wieting, A. R., Moselle, J. R., and Glass, C., "Studies of Aerothermal Loads Generated in Regions of Shock/Shock Interaction in Hypersonic Flow," AIAA Paper 88-0477, Jan. 1988.

[6]Detra, R. W., Kemp, N. H., and Riddell, F. R., "Addendum to Heat Transfer to Satellite Vehicles Re-entering the Atmosphere," *Jet Propulsion,* Vol. 27, No. 12, Dec. 1957, pp. 1256, 1257.

[7]Candler, G. V., "The Computation of Weakly Ionized Hypersonic Flows in Thermochemical Nonequilibrium," Ph.D. Dissertation, Stanford Univ., Stanford, CA, 1988.