CHAPTER VI

SUMMARY AND CONCLUSIONS

VI.1 Summary

In this dissertation a numerical technique for solving the governing equations of a hypersonic flow has been presented. Using this algorithm, we may study gases that behave in a non-ideal manner with chemical reaction, thermal excitation, and ionization allowed to occur. With such a description of the gas we are able to treat a flowfield that is characterized by multiple temperatures and variable concentrations of different chemical species. The thermal modes are linked together using finite-rate excitation mechanisms and the composition of the gas is determined by the use of chemical rate equations. The equation set that describes such a flowfield was derived for an n species gas with m diatomic species. The chemical source terms and thermal excitation mechanisms were discussed and, where necessary, new ones were derived.

A numerical method to solve the above equation set with seven chemical species, four of which diatomic, and one ionic, was developed. This technique was based on an algorithm proposed by MacCormack (1985). It has several positive features. In particular, it is fully implicit, uses flux-splitting, solves the equations in a fully coupled fashion, and employs Gauss-Seidel line-relaxation. Using a numerical method that is fully implicit allows time steps to be taken that are many orders of magnitude greater than the fluid, chemical, or thermal time scales. Thus the rate of convergence to a steady-state is not hindered appreciably by the degree of reaction or thermal excitation of the gas. This is important for highly reactive flows because the relaxation time scales can be far smaller than time steps that would yield a solution in a reasonable amount of computer time. The inviscid fluxes are differenced according to the direction of information travel, which allows subsonic and supersonic regions to be computed without the addition of artificial numerical damping. A non-dissipative form of flux-splitting was used except in regions of large pressure gradients. This enables strong bow shock waves to be captured and correct boundary layer profiles to be obtained. Solving the equation set in a fully coupled manner allows the modifications of the thermodynamic state of the gas due to reaction and thermal excitation to directly

influence the fluid dynamics, and *vice versa*. This also helps maintain numerical stability of the method for large time steps. Finally, the use of Gauss-Seidel line-relaxation reduces the computational cost of using an implicit method. An approximate inverse of the very large implicit matrix is obtained which is accurate enough to maintain numerical stability for large time steps.

The numerical algorithm has one main drawback. It is computationally intensive and requires 5.7 msec of CPU time per time step per grid point on a Cray X-MP. A typical solution converges in about 500 iterations, which for the grids used in this study, takes about one and a half CPU hours on the Cray. This is a significant, though not inordinate, amount of computer time[1].

This numerical method was then applied to a series of test cases in which the computed results were compared to experimental data. The comparison of shock detachments on spheres and cones and electron number densities on a sphere-cone with experiment were excellent for all cases. While this does not represent a validation of the numerical method for arbitrary conditions, it does verify that the physical model is adequate for wide range of hypersonic flows and that the numerical method is functioning correctly.

The computational technique was applied to a proposed Aeroassisted Orbital Transfer Vehicle at two flight conditions. The resulting flowfields were used to compute the radiative emission from the gas and to determine the radiative heating. The results from these computations agree with other researchers' published data in at least a qualitative sense. The affect of thermo-chemical nonequilibrium on the flowfield was made evident in the high altitude case.

VI.2 Conclusions

The results from the computations have demonstrated several features of the numerical method, the physical model of high temperature air, and the physics of hypersonic flows. We can make the following specific conclusions about each of these aspects.

The implicit computational technique has been shown to be capable of obtaining a converged solution for large (in this case, fifteen) equation sets. The presence of large mass

[1] The computer time could be reduced by further vectorizing the program.

and energy source terms do not cause numerical difficulties. Also the numerically "stiff"[2] nature of these hypersonic flows due to rapid reactions and thermal excitation does not appreciably hinder the rate of convergence to a steady-state. The number of time steps required to achieve a steady-state increases by an order of magnitude in going from a perfect gas to a reacting flow, whereas the "stiffness" may increase by typically six orders of magnitude.

From the results, we can make several conclusions about the physical model that was developed for high temperature air. First, it yields correct shock standoff distances for the test cases computed. This is a relatively sensitive measure of the way the model approximates the bulk physics of the flow because the standoff is sensitive to the temperature and density in the shock layer. The model accurately reproduces the electron number densities on the sphere-cone case presented. This is also sensitive to the quality of the model because the number of electrons in the flow is directly determined by the translational temperature and the density at any point. The results presented using a quasi-steady-state assumption make it clear that nonequilibrium has a strong effect on the amount of reaction products predicted on the afterbody of the experiment. Finally, the computed radiative emission from the flow agrees with previously published results. The degree of radiation is strongly dependent on the vibrational and electronic state of the gas, which helps confirm the ability of the numerical method to predict such multi-temperature flows.

The results indicate several things about the physics of hypersonic flows and the requirements of a numerical method in predicting the aerothermodynamics of hypersonic vehicles. The flowfields that envelop a hypersonic vehicle are highly reactive and thermally excited. These processes occur at finite rates, which when coupled with the large convection speeds, results in a state of thermo-chemical nonequilibrium for much of the flight regimes of several proposed hypersonic vehicles. The importance of including chemical nonequilibrium in the analysis was demonstrated by the results of the computations for the RAM-C II test. It was shown that the predicted electron number densities on the afterbody of the vehicle for the high altitude case is four orders of magnitude in error if the ion producing reaction is assumed to be in equilibrium. The effect of thermal

[2] "Stiffness" refers to the ratio between the maximum and minimum time scales of the problem. This ratio is large for a "stiff" problem.

nonequilibrium on the flowfield is large because of the use of the two temperature model for the determination of the chemical reaction rates. This influences the degree of reaction of the flowfield, the shock standoff distance, and the temperature distribution. An analysis that does not include thermal nonequilibrium will tend to over-estimate the reaction rates, which causes a diminished shock standoff distance and an overly low temperature distribution.

A second conclusion about the flow features is that in many of these flows there are significant amounts of atomic species in the boundary layer and directly in contact with the wall. This is a result of two things, namely the nonequilibrium nature of the flow and the assumed non-catalytic wall. Many of the reactants are convected to the wall before they can recombine. This tends to lower the heat transfer to the wall because some of the total energy is absorbed by the heat of formation of the reactants. If the wall is non-catalytic, then less energy may be convected to the wall. This effect has ramifications in the design of hypersonic vehicles. If a significant portion of the free-stream energy can be converted to chemical energy, which does not contribute to heating the wall, then the heat shielding can be reduced.

The results also indicate that a model that uses only one vibrational temperature is adequate to describe the vibrational state of air. However, this assumption is not good in the case of a gas that is made up of chemical species having widely different vibrational relaxation rates. results also show that including a separate electron translational temperature is important in the representation of the flows discussed in this work. The electron temperature tends to rise faster than the the vibrational temperature behind the shock wave, and then lag it nearer the wall. This results in a state of nonequilibrium between these energy modes and an assumption that they are the same is probably not accurate. Rotational nonequilibrium may have significant influence on a hypersonic flow in a rarified regime. This is indicated by the nature of the thermal state of the gas behind the shock wave at high altitude where a large degree of thermal nonequilibrium exists.

VI.3 Future Research

There are two main directions in which further research is needed in this area. Improvements in the physical modeling of the high temperature physics must be made to

build confidence in this analysis technique. Secondly, the numerical method needs to be strengthened in some areas and extended in others.

The current physical model of the gas has several deficiencies. The model for vibrational relaxation needs to be improved because of the strong influence of the vibrational state of the gas in the entire flowfield. The current model has not been proven at high temperatures and this model is particularly suspect in regions of expansion where the vibrationally excited molecules are becoming de-excited. This needs to be explored by computing and performing experiments on wake regions of hypersonic vehicles and perhaps rocket plumes. Further work needs to be done to develop a better electron-vibration coupling model than the one presented in this work. Catalytic wall conditions need to be included so that a more accurate prediction of the heat transfer can be made and an analysis of its effect on the flowfield can be performed. The number of chemical species that represents reacting air could be increased from the current seven to include more ionic species. This would allow calculations to be performed in higher temperature flows where there is more appreciable ionization. And finally, a technique for coupling radiation to the flowfield calculation would be a useful addition for the extension of the model to highly radiative flows.

The numerical method should be extended in several ways. First, the cost of making the computations should be reduced by making the algorithm stable for larger time steps and by reducing the computer time required for each iteration. A second useful and straight-forward addition would be to make the numerical method second-order accurate in space. Also an adaptive grid algorithm should be coupled to the solution procedure to allow selective refinement of the grid. This would improve the efficiency of the method by concentrating grid points where they are needed. The numerical solution procedure is general enough that, with some modifications, it could be applied to a wide range of other problems, such as combustion processes, as well as to other hypersonic flows. As such, it shows promise for extension and refinement.