CHAPTER IV

THE COMPARISON OF COMPUTATIONS TO EXPERIMENT

IV.1 Introduction

In this chapter we will compare the computed results from the numerical method to existing experimental evidence. There are few experimental results available in the hypersonic regime for which the numerical method was developed. We require a high free-stream velocity and a combination of body geometry and free-stream density that results in relaxation rates that cause thermo-chemical nonequilibrium to be present. While these conditions exist for many full-scale vehicles, there are few experimental facilities that can produce a state of thermo-chemical nonequilibrium. Consequently there are only a small number of experiments that produce conditions of interest and measure quantities that are useful in verifying the accuracy of the numerical method. In this chapter, a relative measure of the degree of nonequilibrium present in the gas is developed and then the computational results are compared to experiment.

IV.2 The Degree of Nonequilibrium

All high-speed gas flows are out of thermo-chemical equilibrium to a certain extent. However, for the cases where the chemical and thermal relaxation time scales are much less than the fluid time scales we can assume that the gas is in equilibrium. And for conditions where the relaxation rates are much greater than the fluid time scales, a frozen-flow assumption is applicable. Between these two limits there is a continuum of degrees of thermo-chemical nonequilibrium which may be quantified in the following manner.

If we consider the species mass convection equation (2.3.1) for a steady-state condition, we have

$$\frac{\partial}{\partial x_j}\left(\rho_s u_{sj}\right) = w_s. \tag{4.2.1}$$

We may non-dimensionalize this equation with the free-stream conditions and the nose radius as

$$\begin{aligned} \frac{r_n}{\rho_\infty u_\infty}\frac{\partial}{\partial x_j}\big(\rho_s u_{sj}\big) &= \frac{r_n w_s}{\rho_\infty u_\infty}, \\ \frac{\partial}{\partial \bar{x}_j}\big(\bar{\rho}_s \bar{u}_{sj}\big) &= \frac{r_n w_s}{\rho_\infty u_\infty} = \Psi. \end{aligned} \tag{4.2.2}$$

The non-dimensional quantity, Ψ, may be thought of as the ratio of the fluid time scale to the chemical time scale, or conversely as the ratio of the chemical reaction rates to the fluid motion rates. For the case of chemical equilibrium, we will have infinite chemical rates or $\Psi \to \infty$, and for frozen-flow case where the fluid rates are much larger than the chemical rates, $\Psi \to 0$. For conditions between these two limits, the flow is in chemical nonequilibrium. It should be noted that Ψ is a relative measure and as such can only be used to compare conditions of different flows.

A more useful form of the parameter Ψ may be derived by considering the primary reaction that occurs in high-temperature air flows, which is the dissociation of diatomic oxygen by collisions with diatomic oxygen and nitrogen. In this case we have

$$w_s = w_{\mathrm{O}_2} = k_f \rho_{\mathrm{O}_2}\Big(\frac{\rho_{\mathrm{O}_2}}{M_{\mathrm{O}_2}} + \frac{\rho_{\mathrm{N}_2}}{M_{\mathrm{N}_2}}\Big) = k_f \rho_{\mathrm{O}_2}\frac{\rho}{M}. \tag{4.2.3}$$

If we substitute expression (2.8.4), $k_f = CT^\eta \exp(-\theta_{\mathrm{O}_2}/T)$, and use the hypersonic limit for the density change across the shock, we have[1]

$$\begin{aligned} \Psi_{\mathrm{O}_2} &= K T_{\mathrm{shk}}^{-1} \exp(-59500/T_{\mathrm{shk}})\frac{\rho_\infty r_n}{u_\infty}, \\ K &= c_{\mathrm{O}_2}\Big(\frac{\gamma+1}{\gamma-1}\Big)^2 \frac{C}{M} \simeq 7\times 10^{15}\ (\mathrm{m^3\,K/kg\,s}), \end{aligned} \tag{4.2.4}$$

where we have substituted the values of the constants that were used in the computations. The post-shock temperature[2], T_{shk}, can be approximated using the hypersonic shock relation

[1] See Appendix A, Table A.5, Reaction 2, for the constants.

[2] We have assumed that the peak reaction rate occurs immediately behind the normal shock wave, and for simplicity that the reaction is governed by the translational temperature only.

$$T_{\rm shk} \simeq \frac{2\gamma(\gamma-1)}{(\gamma+1)^2}\mathcal{M}_\infty^2 T_\infty. \tag{4.2.5}$$

Alternatively, we can write the Ψ_{O_2} in terms of the Reynolds number (based on the nose radius) as

$$\Psi_{O_2} \simeq K T_{\rm shk}^{-1} \exp(-59500/T_{\rm shk}) \frac{Re\,\mu_\infty}{u_\infty^2}. \tag{4.2.6}$$

We will see that the relative value of the reactivity of the gas, Ψ_{O_2}, gives a direct indication of the degree of nonequilibrium of the flow.

IV.3 Comparison of Shock Detachment Distances on Spheres

In the early 1960s a set of experiments was performed at the Naval Ordnance Laboratory in which spheres were fired into air at hypervelocities (Lobb (1964)). The results are presented as shock detachment distances on the stagnation streamline for a wide range of flight conditions. Also Schlieren photographs of the sphere in flight at two different conditions are given. We will compare the computed shock wave location to the experimental result for these two cases. The shock standoff distance is a sensitive measure of the accuracy of the numerical method because it is directly influenced by the density distribution between the shock wave and the body surface, which is affected by the degree of reaction and thermal excitation of the gas.

The two test cases considered are at widely varying conditions ranging from essentially frozen-flow to a nonequilibrium case. The test conditions and the reactivity, Ψ_{O_2}, are presented below in Table 4.1. For each case the wall temperature was fixed at 1000 K and the wall was assumed to be non-catalytic. Results for both cases were obtained using the seven-species reacting air technique and with a perfect gas Navier-Stokes algorithm.

Table 4.1 Conditions for Test Cases 1 and 2.

	Case 1.	Case 2.
T_∞ (K)	293	293
u_∞ (m/s)	2440	5280
p_∞ (N/m^2)	1330	664
$\mathcal{M}_\infty$	7.10	15.3
Ψ_{O_2}	8.8×10^{-5}	62

Because of the large discrepancy in the free-stream velocity between these two cases, there is a very large difference (six orders of magnitude) in the reactivity of the gas. We will see that in the first case the flowfield is frozen, namely that the reaction rates are much smaller than the flow rates, and therefore a perfect gas assumption is accurate in this regime. However, the second case is one where thermo-chemical nonequilibrium exists.

IV.3.1 Test Case 1.

Figure 4.1 is a plot of the 35×50 grid that was used in the calculations for Case 1; a similar grid was used for Case 2. The next figure is a plot of the shock wave standoff distance for the first test case. There are two numerical results, one using the nonequilibrium seven-species technique and a second using a standard perfect gas Navier-Stokes algorithm. The shock detachment derived from the computational results was determined by locating the maximum density gradient outside the boundary layer. This criterion was chosen because the Schlieren shadowgraph is sensitive to density gradients. We should also note that the experimental error in the determination of the shock location was between 5 and 10 percent. There is a very good agreement between both of the computed results and the experiment for the three experimental shock locations plotted. We see that based on the shock detachment, the gas acts essentially as a perfect gas within the flowfield. Further evidence of this behavior is given in the next two figures. The mass concentrations of the primary chemical species on the stagnation streamline are plotted in Figure 4.3 and the temperatures are plotted in Figure 4.4. The first of these figures shows that there is essentially no chemical reaction of the gas and the second indicates that the gas is only slightly vibrationally excited. Thus a perfect gas assumption would be a good one in this case. This also indicates that when the reactivity is on the order of 10^{-4} the flow is frozen.

The next four figures are two-dimensional contour plots of some of the relevant flow variables for this test case. Figure 4.5 is a contour plot of the Mach number in the flowfield. It clearly shows the bow shock wave, the sonic line, and the acceleration of the gas as it expands around the shoulder of the sphere. The next figure is a contour plot of the per cent mass concentration of diatomic oxygen. We see that there is a very small degree of dissociation of the gas in the entire flowfield as indicated by Figure 4.3. Figure 4.7 is a plot of the translational-rotational temperature for Case 1. We see that

its peak occurs at the nose and falls off rapidly on the shoulder of the body. Thus as expected, T is governed primarily by the geometry of the body. However, if we consider Figure 4.8, which is a contour plot of the vibrational temperature of nitrogen, we see that it has a very different distribution. Most obviously, the peak vibrational temperature is lower than the peak translational-rotational temperature by about 1300 K. Also the peak $T_{v\mathrm{N}_2}$ occurs in the thermal boundary layer in a similar fashion to that shown in Figure 4.4. The vibrational temperature is higher than the translational-rotational temperature near the wall for $x/r_n > 1$. This is caused by the convection of the vibrationally excited gas from the nose region to the shoulder of the body before it has a chance to cool. However, as mentioned above, the translational-rotational temperature falls rapidly due to the expansion of the flow and a state of thermal nonequilibrium results.

IV.3.2 Test Case 2.

The reactivity of Case 2 is much larger than the previous case and as such we would expect that the perfect gas assumption would be inaccurate. We see that this is the case by plotting the shock standoff distance resulting from the seven-species and perfect gas numerical methods against the experimental data as in Figure 4.9. Again we see a very good comparison with experiment for the reacting gas solution, however the perfect gas results are severely (37%) in error. The decrease in the shock detachment distance from the first case to the second is caused by the high degree of chemical reaction in Case 2. This results in a higher density ratio across the shock and therefore a smaller standoff.

The degree of reaction and thermal excitation is evident from the next two figures which are plots of the molar concentrations and temperatures on the stagnation streamline. Figure 4.10 shows that there is a very large degree of reaction with the diatomic oxygen almost completely dissociated. The dissociation of diatomic nitrogen does not go to completion, because this reaction has a larger activation energy. There is a small amount of ions produced in this case. The recombination of the monatomic species near the wall are caused by the cooled wall which results in a cool thermal boundary layer and a large density near the wall. This tends to drive the reactions backward, absorbing the monatomic species. Figure 4.11 shows three of the six temperatures on the stagnation streamline. We see that the peak temperature is much higher for this case than for the

previous one, with a peak temperature of nearly 12,000 K. There is significant thermal excitation, but the three temperatures plotted do not equilibrate except in the thermal boundary layer. The other three vibrational temperatures were not plotted because they are very similar to $T_{v\mathrm{N}_2}$ due to the strong vibration-vibration coupling. This will be discussed further for other test cases where more thermal excitation occurs. These two plots indicate that when Ψ_{O_2} is about 60 there is significant chemical reaction and thermal excitation.

Figure 4.12 is a contour plot of the Mach number for the second test case and is similar in character to the previous case. However, if we consider the next figure, we see that there is a significant degree of dissociation of oxygen throughout the flowfield for this case. The region near the wall is completely devoid of O_2. Figure 4.14 is a plot of the contours of percent diatomic nitrogen mass concentration. It shows that there is appreciable dissociation of N_2 in the nose region, but significantly less in the afterbody region. This plot also indicates a typical nature of a chemical nonequilibrium flow. There is a large degree of a reaction in the high temperature gas near the stagnation point. This gas is convected around the body and slowly recombines in the cool shoulder region. Thus we have N_2 mass concentrations of about 75% in much of this part of the flowfield. If we had assumed that the gas was in chemical equilibrium, the numerical method would have predicted that essentially no dissociated nitrogen would be present in this region.

The next three figures are contour plots of the three temperatures plotted in Figure 4.11. As we saw in this figure there is significant thermal excitation of the vibrational and electron translational modes of the gas on the stagnation streamline. These figures demonstrate that this excitation occurs in much of the flowfield and is not just confined to the boundary layer as in Case 1. We also see that the excitation of the vibrational modes lags the translational-rotational modes as discussed previously. We can detect that the excitation of electron translational energy lags both the heavy-particle translational and vibrational energies. This is a result of the strong coupling of N_2 vibration with electrons. The heavy-particle translational modes excite the vibrational modes, which then excite the electron translational modes. The interplay between these energy modes will become stronger and more evident for the higher Mach number cases that will be considered below.

We can conclude from these two test cases that the numerical method gives us the

correct shock detachment for two disparate cases of hypersonic flow. The shock standoff distances agree within experimental error and grid resolution. This is not a validation of the algorithm, but it indicates that it correctly represents the bulk physics of the high temperature air for both cases.

IV.4 Comparison of Shock Detachment Distances on Cones

J. H. Spurk (1970) performed experiments on cones at high Mach numbers in pure diatomic oxygen in an expansion tube. He measured shock standoff distances using interferometry for two nonequilibrium cases. We will compare these experimental data to the results of the seven-species computation. The free-stream conditions for the experiments, which we call Cases 3 and 4, are given below. However, the free-stream is somewhat removed from equilibrium in each case. For the conditions of his first test case, Spurk postulates that the vibrational temperature of oxygen is somewhat higher than the free-stream translational temperature. And for the second case there is some free-stream reaction and a small degree of vibrational nonequilibrium. However, the degree of thermochemical nonequilibrium is not known accurately and, as such, the free-stream conditions are assumed to be those predicted by a thermal equilibrium assumption with no dissociation. Thus for both cases, we have set the free-stream concentrations of all species except diatomic oxygen to zero and we have let the vibrational temperature be in equilibrium with the translational temperature. The experimental error in the determination of the free-stream density and the shock detachment is nominally 20%.

Table 4.2 Conditions for Test Cases 3 and 4.

	Case 3.	Case 4.
θ_c (deg.)	45.0	34.9
T_∞ (K)	1250	1140
u_∞ (m/s)	6350	5710
p_∞ (N/m^2)	4810	5720
$\mathcal{M}_{n\infty}$	7.40	5.65
Ψ_{O_2}	322	35.9

The expression for the reactivity for these test cases must be modified slightly due to the conical geometry and the pure oxygen free-stream. If we base the characteristic

length on the total length of the conical surface and use the normal Mach number in the expression for the post-shock temperature, we have

$$\begin{aligned}\Psi_{O_2} &= \Big(\frac{\gamma+1}{\gamma-1}\Big)^2 \frac{C}{M_{O_2}} T_{\rm shk}^{-1} \exp(-59500/T_{\rm shk}) \frac{\rho_\infty L}{u_\infty}, \\ T_{\rm shk} &\simeq \frac{2\gamma(\gamma-1)}{(\gamma+1)^2} \mathcal{M}_{n\infty}^2 T_\infty.\end{aligned} \tag{4.4.1}$$

The values of the reactivity are not directly applicable to the previous cases, however they serve as an order of magnitude reference.

IV.4.1 Test Case 3.

The first of these cases that we will consider is that of a 45° cone, 25 mm long traveling at a Mach number of 9.41. Figures 4.18 and 19 are plots of the grid used to represent the body. The nose of the cone was blunted with a spherical nose to make the numerical method directly applicable. The nose radius is 1% of the total length of the cone and thus has little effect on the main flowfield. The shock wave standoff distance measured in the y direction from the surface of the cone to the shock is plotted in Figure 4.20 against the data of Spurk. There is a large amount of scatter in the experimental data, and the computational results fall near the center of its limits. The result of perfect gas cone theory is plotted and shows that the predicted shock standoff is 6.8 mm at $x = 25$ mm, which is over 100% in error. Also plotted are the equilibrium results of Spurk (1970) which fall about 50% below the experimental results. Thus this test case is one in which thermochemical nonequilibrium has a macroscopic affect on the flowfield. The good comparison is another support for the validity of the method.

Figure 4.21 is a plot of the computed surface pressure coefficient versus that predicted by ideal cone theory. As expected, *Cp* is large at the nose due to the blunted nose, but otherwise there is good agreement between the two results. We would not expect the pressure to be identical on the cone afterbody because the presence of nonequilibrium alters the shock wave angle, and consequently, the pressure ratio across the shock. The reacting gas analysis predicts that the shock is more oblique and this would result in a smaller pressure rise and a lower *Cp*, as demonstrated by this figure.

The reactivity of this case is high relative to the first two cases considered, but this

partly a result of having used the body length instead of the nose radius as a reference length. With this high reactivity we expect there to be appreciable reaction and thermal excitation. The next series of plots are designed to indicate the thermo-chemical state of the gas. They are plots of the mass concentrations and temperatures versus η, the normal distance from the cone, at three x locations. The stagnation streamline results, Figures 4.22 and 23, show that there is a large amount of O_2 dissociation (35%) and significant thermal nonequilibrium. This is the type of behavior that is expected on the stagnation streamline. Figures 4.24 and 25 are plots of the same quantities at $x = 1.2\,\text{mm}$. They show that there is also a large, though lesser, degree of reaction and thermal excitation. The post-shock temperature is lower in this case because the shock wave is oblique. The gas near the wall is approaching thermal equilibrium because it has been convected from the nose region and has had some time to equilibrate. This type of behavior is also evident in the next two figures which are at the point $x = 15.6\,\text{mm}$. The gas near the wall that has been in the shock layer for an appreciable time is highly reacted and thermally equilibrated. And the gas that has just passed through the shock wave is significantly out of thermo-chemical equilibrium. As a result, an analysis that did not include finite-rate chemical reactions and thermal excitation would be erroneous.

The next four figures are contour plots of the Mach number, the percent mass concentration of diatomic oxygen, the translational-rotational temperature, and the vibrational temperature of oxygen. In examining these plots, the most obvious thing to notice is that the shock layer is very thin, occupying a 3.4° wedge. This is approximately one-half as thick as 6.9° wedge that a perfect gas analysis would predict. Most of the shock layer is at a constant Mach number of 2.5 as shown in Figure 4.28. The next plot indicates the degree of reaction of the gas. Generally, the dissociation of the gas increases with increasing distance along the cone. This is a result of the nonequilibrium nature of the flowfield because the fluid that enters the shock layer near the nose has had sufficient time to react as it flows along the cone. The next two figures show the distribution of the two relevant temperatures in the flowfield. If we compare them, it is evident that the portion of the flowfield near the wall and downstream of the point $x \simeq 5\,\text{mm}$ is essentially equilibrated at a temperature of 5000 K. This is also a result of the gas having had sufficient dwell time in the shock layer to have equilibrated. Thus the gas in the conical flowfield is in

thermo-chemical nonequilibrium near the nose and the shock wave and is in approximate equilibrium in the proximity of the wall beyond about 5 mm from the nose.

IV.4.2 Test Case 4.

The second of test case of Spurk is a 34.9° half-angle cone travelling at a Mach number of 8.89. Again the body is represented with a spherically blunted nose and a conical afterbody on a 35×50 mesh as shown in Figure 4.32. The computed shock standoff distance is compared to the experimental results in the next figure. The predicted shock wave location falls within the experimental scatter for most of the cone length but is somewhat low for $x > 15$ mm. However, the computed results are within the stated 20% accuracy of the experiment and the possible nonequilibrium state of the free-stream may have an influence on the shock location. A perfect gas solution predicts a standoff of 3.4 mm at $x = 25$ mm, which is 24% larger than the experimental result. The perfect gas analysis is more accurate in this case than in the previous one because the flow is closer to being frozen and the degree of reaction and thermal excitation is much less. Figure 4.34 is a plot of the computed pressure coefficient plotted against the perfect gas cone theory result. As before, the computed *Cp* is high at the nose, and somewhat lower on the afterbody. This is expected for the same reasons mentioned in the 45° case.

Figures 4.35 and 36 show the mass concentrations and temperatures at $x = 1.8$ mm which corresponds approximately to the location used for Figures 4.24 and 25. We see that there is considerably less dissociation of oxygen and that the vibrational modes are significantly less excited. The gas has reacted near the wall only and much of the flow is chemically frozen. The gas is also significantly unreacted at the point $x = 18$ mm as shown in Figure 4.37. However, the vibrational temperature is approaching equilibrium with the translational temperature at this point as shown in the next figure. It also illustrates an interesting feature of this flow, in which there is a small peak in the translational temperature distribution near the wall. This is caused by a combination of factors, namely that the gas is heated because the no-slip condition at the wall results in a conversion of kinetic energy to thermal energy. However, the wall has a fixed temperature of a relatively cool 1000 K which forces the temperature to be drawn toward the wall temperature in the thermal boundary layer. The juxtaposition of these two mechanisms results in the

peak in the temperature distribution for this case. The previous conical flowfield did not demonstrate this behavior because more of the kinetic energy was removed from the gas as it passed through the stronger bow shock.

The next figures are contour plots of the same variables that were plotted for the 45° cone case. Figure 4.40 again shows that there is significantly less chemical reaction in this flowfield with most of the flow made up of about 90% diatomic oxygen. The next two plots show that there is also significant thermal nonequilibrium in much of the shock layer.

The results from these two test cases show good agreement with experiment for the shock wave detachment. These cases also demonstrate that even for a very simple geometry with one diatomic species, complicated physical phenomena occur at hypersonic speeds.

IV.5 Comparison to the RAM-C Flight Experiments

During the late 1960s three experimental probes were flown into the atmosphere at approximately satellite speed[3]. These probes, called the RAM-C tests, were sphere-cone configurations with a 0.1524 m nose radius, 9° cone half-angle, and a total length of 1.295 m. They were instrumented to measure electron number densities in the flowfield. The second test, RAM-C II, is of particular interest because no ablation products were produced. This probe had a beryllium heat-sink nose cap and a Teflon coated afterbody. Electron number densities were measured at four axial locations using microwave reflectometers and in the boundary layer using an electrostatic rake.

Computations were performed to replicate the RAM-C II tests at altitudes of 61, 71, and 81 kilometers. This altitude range approximately spans a region of near thermo-chemical equilibrium at 61 km to strong nonequilibrium at 81 km. The wall temperature was fixed at 1500 K which is an approximation to the unknown experimental wall temperature. The wall was assumed to be fully non-catalytic which is also an approximation to the RAM-C II test. In each case the free-stream velocity was 7650 m/s. The corresponding free-stream conditions for each of these three test cases are given in Table 4.3 below. In each case the free-stream was composed of 79% N_2, 21% O_2, and trace amounts of the other constituents.

[3] See Akey and Cross (1970), Granthan (1970), and Jones and Cross (1972).

Table 4.3 Conditions for RAM-C II Test Cases.

	Case 5.	Case 6.	Case 7.
H (km)	61	71	81
T_∞ (K)	254	216	181
R_e	19500	6280	1590
$\mathcal{M}_\infty$	23.9	25.9	28.3
Ψ_{O_2}	172	48.2	10.5

The computations were performed on body-fitted meshes with 35 points axially along the sphere-cone and 50 points in the flowfield normal to the body. Figure 4.43 shows a typical mesh used for one of the test cases.

IV.5.1 Comparison of Electron Number Densities

The computed results are first compared to the peak electron number density measured axially along the body at each altitude. As an additional demonstration of the influence of a nonequilibrium assumption on the flowfield, the results from the seven-species reacting gas will be compared to those from a five-species nonequilibrium reacting flow program. This solution technique is identical to the seven-species method, except that the ionization reaction[4] and the species NO^+ and e^- are not included. However, by making a so-called quasi-steady-state assumption, we can use this solution to predict the number of electrons present in the flowfield. This process is outlined below.

If we assume that the reaction that produces electrons is in equilibrium everywhere in the flowfield we obtain the expression

$$\frac{k_{f_6}}{k_{b_6}} = \frac{N_{NO^+} N_e}{N_N N_O} = K_{eq_6}. \tag{4.5.1}$$

But the number density of the ions is equal to that of the electrons and we know the number density of the atomic species N and O. The backward rate constant is a function of $T_{v_{NO^+}}$ and T_e which are not calculated with the five-species model. Due to the strong energy coupling, we assume that these two temperatures are equal to the vibrational temperature of N_2. Thus,

[4] Reaction 6 in equation (2.8.1).

$$
\begin{aligned}
N_e^2 &= N_{\mathrm{N}} N_{\mathrm{O}} \frac{k_{f_6}(T)}{k_{b_6}(T_{v_{\mathrm{N}_2}})} \\
&= N_{\mathrm{N}} N_{\mathrm{O}} k_{f_6}(T) \frac{K_{\mathrm{eq}_6}(T_{v_{\mathrm{N}_2}})}{k_{f_6}(T_{v_{\mathrm{N}_2}})}.
\end{aligned}
\tag{4.5.2}
$$

Using equation (2.8.4), we have

$$
N_e^2 = N_{\mathrm{N}} N_{\mathrm{O}} \Big(\frac{T}{T_{v_{\mathrm{N}_2}}} \Big)^{\eta_6} \exp\Big(\frac{\theta_6}{T_{v_{\mathrm{N}_2}}} - \frac{\theta_6}{T} \Big) K_{\mathrm{eq}_6}(T_{v_{\mathrm{N}_2}}). \tag{4.5.3}
$$

This allows us to approximate the number density of the electrons using the five-species approach which does not include any ionized species. The quasi-steady-state assumption only relies on the electron producing reaction being in equilibrium at the local thermo-chemical state of the gas. Thus results obtained with it will be more accurate than those computed using a pure equilibrium approach where all of the reactions and thermal excitation are assumed to be equilibrated.

The computed peak electron number density results from the seven-species nonequilibrium technique and the five-species nonequilibrium method with the quasi-steady-state assumption plotted against x/r_n in Figures 4.44 to 46. The full seven-species nonequilibrium results show an excellent agreement with the flight test data, but the five-species plus quasi-steady-state results are significantly in error, especially in the high altitude case. The electron number density is highest at the nose and falls off rapidly around the shoulder of the body. However, there are a significant number of electrons frozen in the flow due to the relatively slow recombination reaction of the electrons. This is most pronounced in the highest altitude case due to the rarified free-stream conditions and resulting low reaction rates. The results that rely on the equilibration of the ionization reaction do not capture this effect, and as a result over-predict the recombination rate and under-predict the number of electrons in the afterbody flowfield. If an equilibrium analysis had been used in this case, the predicted electron concentrations would be even more erroneous than the five-species results.

Figure 4.47 compares the computed results using the seven-species model to the measured electron number density near the body surface at $x/r_n = 8.10$ for altitudes of 71 km and 81 km. The results are approximately the right magnitude but do not show the correct

behavior near the wall. This problem is likely caused by the uncertainty in wall boundary conditions. The surface of the probe was probably catalytic for the electron-ion recombination reaction and thus would cause a lessening of the electron number density near the wall. This wall effect is not currently included in the calculations. Alternatively, the fixed-wall temperature used in the calculations may be too high which would produce an excessive number of electrons near the wall.

The next several sections will be devoted to a discussion of each of the three cases that were computed for the RAM-C II configuration. The results will be compared and contrasted to examine the effects of altitude. A detailed consideration of the 71 km case is given to show some more of the details of this flowfield.

IV.5.2 Test Case 5: RAM-C II at 61 km

The low altitude or relatively high density conditions of the flow for this case yield a high reactivity and thus we would expect a high degree of chemical reaction and thermal excitation. This is evident in Figures 4.48 and 49 which are plots of mass concentration and temperatures on the stagnation streamline. The diatomic oxygen is destroyed rapidly and a maximum of about 50% of the nitrogen dissociates. The effect of the cooled wall is evident in the behavior of nitrogen concentration near the wall where a significant recombination occurs. There is a significant production of nitric oxide just behind the shock where it reaches a 10% concentration. But it also dissociates rapidly so that there is almost none in the wall region. The mass concentration of the ion, NO^+, is so low that it does not appear on the figure; in this case its maximum concentration is 0.164%.

Figure 4.49 shows that for this case, there is significant thermal nonequilibrium behind the shock wave and near thermal equilibrium for the portion of the flowfield near the wall. We can speculate that the behavior of the electron temperature is a result of two excitation mechanisms. Its initial rise behind the shock is a result of translation-electron energy exchanges due to the high translational temperature. The second, slower rise occurs because of the strong coupling between the relatively high vibrational energy of nitrogen and the electron translational modes.

The next two plots, Figures 4.50 and 51 show the same quantities at the point where the sphere and the cone join. At this location the flow is supersonic except in the boundary

layer and the gas that originated at the nose has expanded around the sphere causing the translational temperature to drop. As a result, the gas is less reactive, however a significant amount of the reaction products from the nose are frozen in the flow as shown in Figure 4.50. The oxygen in the wall region is still fully dissociated and the nitrogen is appreciably reacted. The next figure shows that the gas is relatively cool with a peak translational-rotational temperature of 9000 K. The vibrational temperature is higher than the translational temperature near the wall. This is a result of the vibrational translational energy being frozen in the gas as it is swept around the shoulder of the body. There was evidence of this form of thermal nonequilibrium in Case 2, but it is more pronounced here.

IV.5.3 Test Case 6: RAM-C II at 71 km

The computed flowfield for the RAM-C II flight vehicle at conditions corresponding to 71 km are discussed in this section. The state of the gas is examined at several axial locations on the body and through the use of contour plots.

The first plot, Figure 4.52 is a comparison of the surface pressure coefficient, $Cp = (p - p_\infty)/\frac{1}{2}\rho_\infty u_\infty^2$, on the sphere-cone with that predicted by perfect gas cone theory for a 9° cone. The computed results are much higher on the blunt nose, as expected, and asymptote to the theoretical value on the afterbody. On the stagnation streamline, the mass concentration distribution has a similar form to the previous case as shown in Figure 4.53. However, because of the lower density and consequently, lower reactivity, the gas reacts more slowly and to a lesser extent in this case. The next figure is a plot of the molar concentration of the constituents on the stagnation streamline. Several things are apparent from this plot. First, the molar concentrations of the electrons and the ions are identical because the diffusion velocities for each of these species are the same. Thus there is no force to drive them apart. This effect would not be observed if there were more than one ionic species in the flowfield. Secondly, we should note that there are reactants at the point $\eta/r_n = 0.14$, which is not evident from the previous plot. The next figure is a plot of three temperatures on the stagnation streamline. The point of the initial temperature rise is at $\eta/r_n = 0.125$, thus there are reactants ahead of the thermal shock. The only way that these constituents may reach the free-stream is by diffusive fluxes across the shock wave. The mass concentration gradient is very strong at this point, thus the diffusive velocity

would be large and some portion of the reactants produced in the shock layer move ahead of the shock wave.

The temperature plot, Figure 4.55, also shows that there is a significant amount of thermal nonequilibrium throughout the entire stagnation region. The translation-rotational temperature reaches a peak of 25,000 K and the vibrational temperature of nitrogen peaks at 11,000 K. The electron temperature rises rapidly in the shock wave and then rises slowly in the near-wall region. From this it appears that the translational modes of the heavy particles are responsible for the initial excitation of the electron translational modes. The electron-vibration coupling is unimportant until the vibrational modes have been excited. Figure 4.56 is a plot of the four vibrational temperatures on the stagnation streamline. We see that they are all similar in magnitude and distribution, however the excitation of the vibrational energy of NO and NO^+ occurs ahead of the other two molecules. It is not clear what causes this effect, except that diffusion of excited NO and NO^+ molecules from downstream may result in a higher vibrational level at the upstream locations. The vibration-vibration coupling causes the different vibrational temperatures to approximately equilibrate with each other for most of the flowfield. Because of this effect, it would appear that a single vibrational temperature would be adequate to describe this flow. However, there may be gases where different molecules may have radically different relaxation rates than the rest of the gas and the single vibrational temperature approximation would break down.

The next plot shows the distribution of density along the stagnation streamline. For these flight conditions the boundary layer is distinct and separate from the shock layer, so that there is not a merged shock-boundary layer. However, for this case the density rise across the shock wave occurs over an appreciable distance. This smearing of the shock is due in part to the numerical method, but it also is a result of the rarified free-stream. A comparison with Figure 4.55 shows that there is an appreciable distance (approximately 2% of the nose radius) between the rise in the density and temperature in the shock wave.

Figures 4.58 and 59 are plots of the mass concentration and temperatures normal to the body at the sphere-cone juncture. Most of the reacted gas is near the wall because it originated in the nose region. The dissociation of oxygen occurs more slowly than in the stagnation streamline case and the nitrogen is significantly less dissociated. There is a

large degree of thermal nonequilibrium near the shock wave, however the gas near the wall is close to translational-vibrational equilibrium. We observe the over-shoot of vibrational temperature as in the lower altitude case. The electron temperature is essentially constant at this location. Further along the body, at $x/r_n = 8.1$, we have a different distribution of species and temperature, as shown in Figures 4.60 and 61. The reaction is confined to a region near the body and there are significantly fewer products at this point. The gas in the near-wall region is still over 7000 K because it is heated by the no-slip wall condition. The vibrational temperature is about 3000 K cooler in this area. The electron temperature is higher than the translational-rotational temperature for a small portion of the flowfield. This is likely a result of diffusion of high temperature electrons away from the wall. If we examine Figure 4.62, which is a plot of the molar concentration at this location, we see that the concentration gradients are relatively steep, which would tend to drive the reactants outward. This would account for the elevated electron temperature near the shock wave.

The next figures are contour plots of the computed RAM-C II flowfield at the 71 km conditions. The first, Figure 4.63, is a contour plot of the Mach number and shows the bow shock wave. Within this shock layer, there is significant chemical reaction as is evident from the next two figures which are plots of the percent mass concentration of N_2 and O_2. We can see the basic nature of the flowfield from these plots, namely that the gas reacts strongly in the nose region, and then is swept around the body and recombines slowly. A fairly large portion of the flowfield is devoid of diatomic oxygen as shown in Figure 4.65. The logarithm of the electron number density, $\log N_e$, is plotted in the next figure. This plot corresponds directly to the peak electron number density *vs.* axial location plotted in Figure 4.45. There is a peak in the electron number density about one-third of the way between the wall and the shock wave. The decrease in the number of electrons with x is also evident from this plot. The next three figures are contour plots of the translational-rotational, nitrogen vibrational, and electron temperatures, respectively. The vibrational and electron temperatures remain lower than the translational temperature for almost the entire flowfield. Most of the flow over the afterbody is at a translational temperature of 6000 K. Much of the flowfield has an electron temperature of about 4000 K.

IV.5.4 Test Case 7: RAM-C II at 81 km

The results from the last test case, that of the RAM-C II vehicle at 81 km, are presented in this section. The free-stream conditions are such that the gas is much less reactive than the lower altitudes as is shown in Figure 4.70, which is a plot of the mass concentration on the stagnation streamline. The reactions occur very slowly so that they have not reached completion by the time the gas reaches the wall. The equilibrium concentration of diatomic oxygen would be essentially zero, however there is appreciable diatomic oxygen in the entire flowfield. The temperature rise through the shock wave occurs over a significant portion of the flowfield as seen in Figure 4.71. The nitrogen vibrational and electron temperatures are much lower than the translational temperature along the entire stagnation streamline. The next figure is a plot of the density distribution on the stagnation streamline and it shows that there is no discontinuous shock wave under these rarified flight conditions. The density rise through the shock is nearly indistinguishable from the rise in the boundary layer and thus we have a merged shock-boundary layer. Figures 4.73 and 74 are plots of the mass concentrations and temperatures at the sphere-cone juncture. Again we see little chemical reaction and a large degree of thermal nonequilibrium.

The free-stream conditions for this case are more rarified than for any of the other test cases computed. The Knudsen number based on the free-stream conditions and the nose radius for this case is 0.025. Thus this flow is in the transitional regime where the assumptions associated with the continuum approach become suspect. The numerical method is able to achieve a solution, but the wall boundary conditions and the treatment of the shock wave are possibly inadequate. Further research needs to be done in this area to determine the limits of the continuum approach.

IV.6 Conclusions From the Test Cases

The numerical method has been compared to seven different test cases under very different flow conditions. The cases ranged between the almost non-reactive case of the half-inch sphere traveling at a Mach number of 7.1 to the highly reactive case of the RAM-C II sphere-cone at an altitude of 61 km. In each case the numerical method was able to predict the experimental evidence, either shock standoff distances or electron number densities, to within the experimental uncertainty. The excellent shock wave detachment comparison indicates that the basic physics of the high temperature air are represented

correctly. The replication of the RAM-C II flight experiment data for electron number density shows that this particular detail of the flow is also accurately modeled. These results support the use of many of the physical models that were discussed in Chapter II, but this is not conclusive evidence that they are correct. These comparisons do not validate all aspects of the physical models used in the calculations and the numerical method itself. A great deal more testing is required in conjunction with experiments that produce high quality data of other flowfield quantities.

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