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THE COMPUTATION OF THERMO-CHEMICAL NONEQUILIBRIUM HYPERSONIC FLOWS

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Several conceptual designs for vehicles that would fly in the atmosphere at hypersonic speeds have been developed recently. For the proposed flight conditions the air in the shock layer that envelops the body is at a sufficiently high temperature to cause chemical reaction, vibrational excitation, and ionization. However, these processes occur at finite rates which, when coupled with large convection speeds, cause the gas to be removed from thermo-chemical equilibrium. This non-ideal behavior affects the aerothermal loading on the vehicle and has ramifications in its design.

A numerical method to solve the equations that describe these types of flows in two dimensions has been developed. The state of the gas is represented with seven chemical species, a separate vibrational temperature for each diatomic species, an electron translational temperature, and a mass-averaged translational-rotational temperature for the heavy-particles. The equations for this gas model are solved numerically in a fully coupled fashion using an implicit finite volume time-marching technique. Gauss-Seidel line-relaxation is used to reduce the cost of the solution and flux-dependent differencing is employed to maintain stability.

The numerical method has been tested against several experiments. The calculated bow shock wave detachment on a sphere and two cones was compared to those measured in ground testing facilities. The computed peak electron number density on a sphere-cone was compared to that measured in a flight test. In each case the results from the numerical method were in excellent agreement with experiment. The technique has been used to predict the aerothermal loads on an Aeroassisted Orbital Transfer Vehicle including radiative heating. These results indicate that the current physical model of high temperature air is appropriate and that the numerical algorithm is capable of treating this class of flows.

Research Objectives

- Study flows with thermo-chemical nonequilibrium
  - multiple temperatures: $T \neq T_v \neq T_e$
  - chemical state not in equilibrium at local e, ρ
- Primary application to blunt re-entry vehicles in air
  - other nonequilibrium problems are possible, *e.g.* NASP
  - could be used with other gases, *e.g.* H_2 – Air
  - steady-state
  - two-dimensional or axisymmetric
  - laminar
- Demonstrate feasibility of numerical solutions to reacting flows
  - stiff equations
  - large source terms

Justifications

- Proposed hypersonic vehicles:
  - AOTV/AFE
  - NASP
  - Mission to Mars
- Ground-based testing is difficult
- Nonequilibrium effects important:
  - force coefficients
  - convective and radiative heating
- Study high-temperature air physics:
  - effects of thermo-chemical nonequilibrium
  - develop new modeling techniques

Technical Approach – Thermodynamic Model

- Translational-rotational equilibrium assumed
- One vibrational temperature for each diatomic species
- Electron-electronic temperature
    - free-electron and electronic temperatures equal
- Model finite-rate energy transfer modes

Technical Approach – Conservation Equations

- Governing equations in two dimensions:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = W$$

- For a gas with n species, m diatomic:

$$U = \left(\rho_1,\ \rho_2,\ \ldots,\ \rho_n,\ \rho u,\ \rho v,\ E_{v_1},\ \ldots,\ E_{v_m},\ E_e,\ E\right)^T$$

Technical Approach – Equations of State

- Pressure and temperature:

$$T = \frac{1}{\rho c_v}\Big(E - \sum_{s=1}^{m} E_{v_s} - E_e - \frac{1}{2}\rho(u^2 + v^2) - \sum_{s=1}^{n} \rho_s h_s^\circ - \sum_{s\neq e}^{n} \rho_s e_{\mathrm{el}\,s}\Big),$$

$$p = \sum_{s\neq e}^{n} \frac{\rho_s}{M_s} RT + p_e, \qquad c_v = \sum_{s\neq e}^{n} \frac{\rho_s}{\rho} c_{v_s}.$$

- Electron pressure and temperature:

$$T_e = \frac{1}{\rho_e c_{ve}}\big(E_e - \frac{1}{2}\rho_e(u^2 + v^2)\big), \qquad p_e = \rho_e \frac{R}{M_e} T_e.$$

- Vibrational temperature:

$$E_{v_s} = \rho_s \frac{R}{M_s} \frac{\theta_{vs}}{e^{\theta_{vs}/T_{vs}} - 1}.$$

Technical Approach – Chemical Model

- Air is modeled with seven species:

$$N_2,\ O_2,\ NO,\ NO^+,\ N,\ O,\ \text{and}\ e^-.$$

- Possible reactions:

$$\begin{aligned}
N_2 + M &\rightleftharpoons 2N + M \\
O_2 + M &\rightleftharpoons 2O + M \\
NO + M &\rightleftharpoons N + O + M \\
N_2 + O &\rightleftharpoons NO + N \\
NO + O &\rightleftharpoons O_2 + N \\
N + O &\rightleftharpoons NO^+ + e^-,
\end{aligned}$$

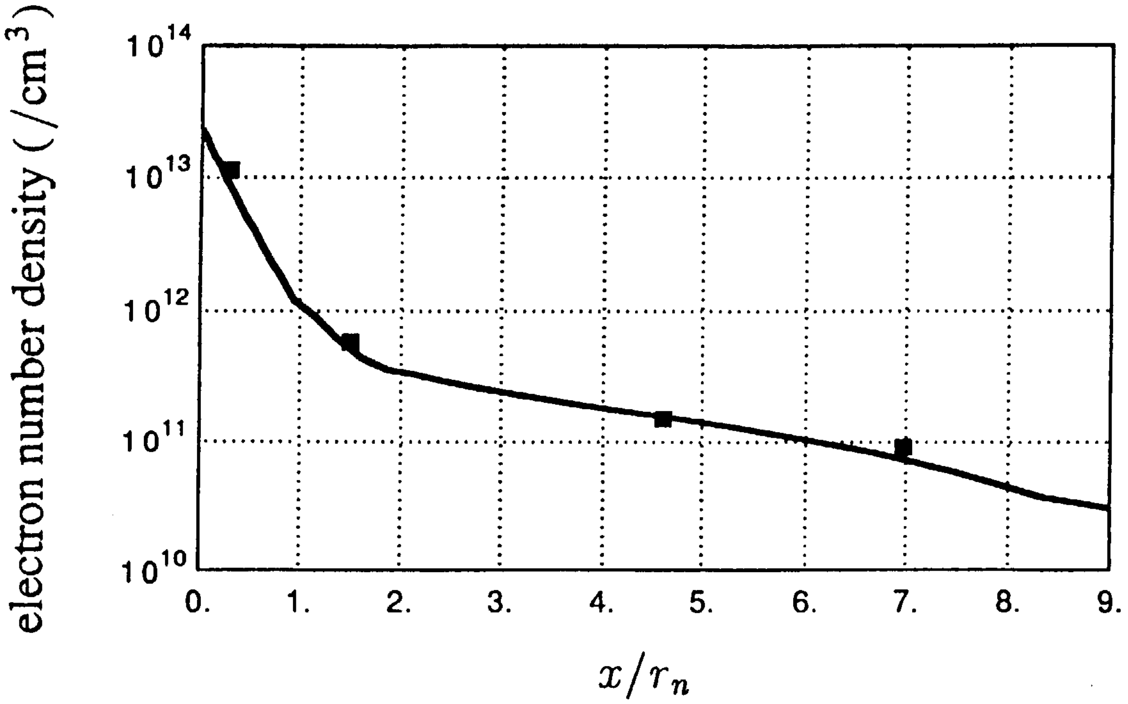
  - use two-temperature reaction rate (TT_v) model of Park

Technical Approach – Numerical Algorithm

- Equations solved in fully coupled fashion:
  - nonequilibrium directly influences solution
- Gauss-Seidel line-relaxation technique of MacCormack (1985)
- Fully implicit:
  - large time steps for rapid convergence
  - rapid reactions do not slow convergence appreciably
  - many computations required per time step
- Gauss-Seidel line-relaxation reduces cost of implicit method
- Flux-splitting:
  - stability in subsonic and supersonic regions
  - capture bow shock wave

Validation – Peak Electon Number Density

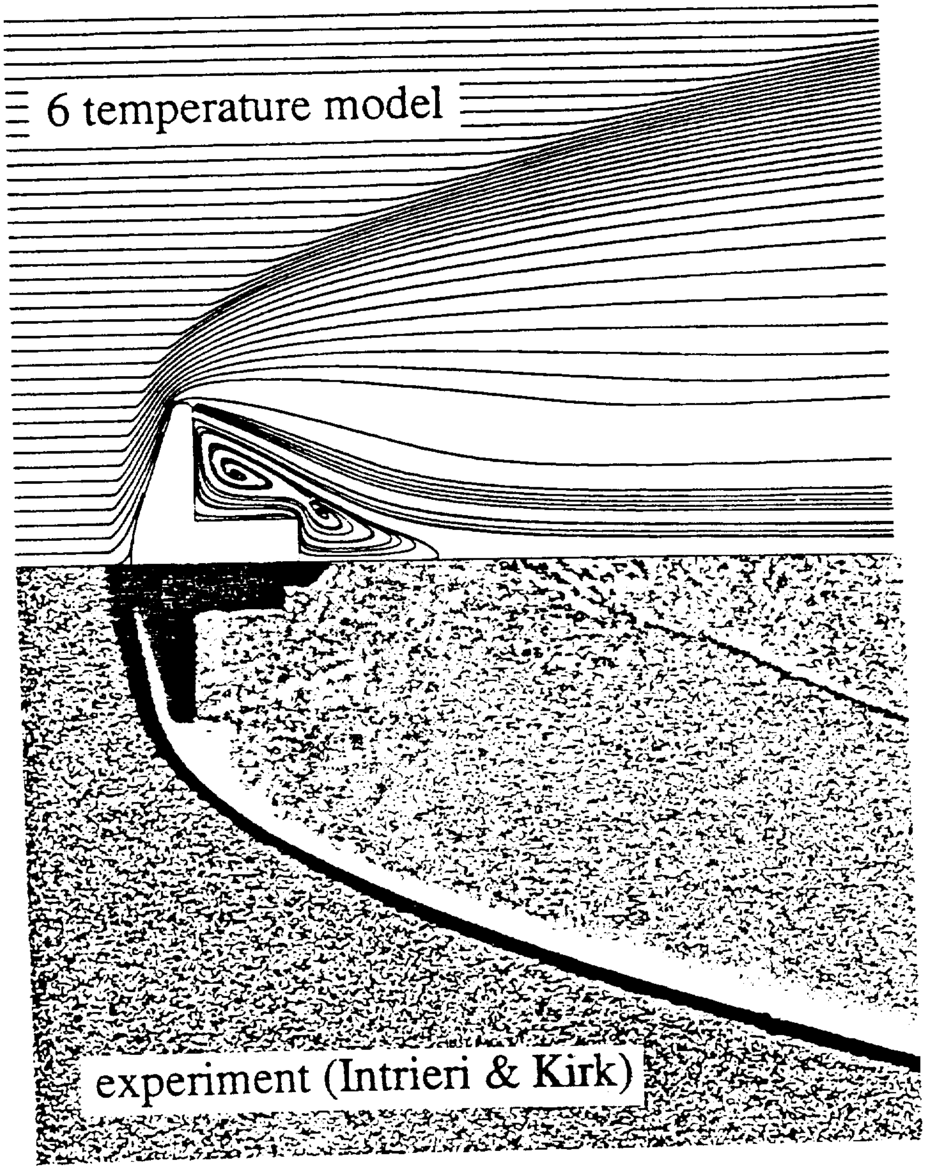
- Sphere–9° Cone in air. $u_\infty = 7.65\,\mathrm{km/s}$, $\mathcal{M}=25.9$, $Re = 6280$.



Results – Axisymmetric AOTV

- Shadowgraph of an axisymmetric AOTV model in air.

  $u_\infty = 4.02\,\mathrm{km/s}$, $\mathcal{M}_\infty = 11.6$, $Re = 343000$, $\psi = 180$.



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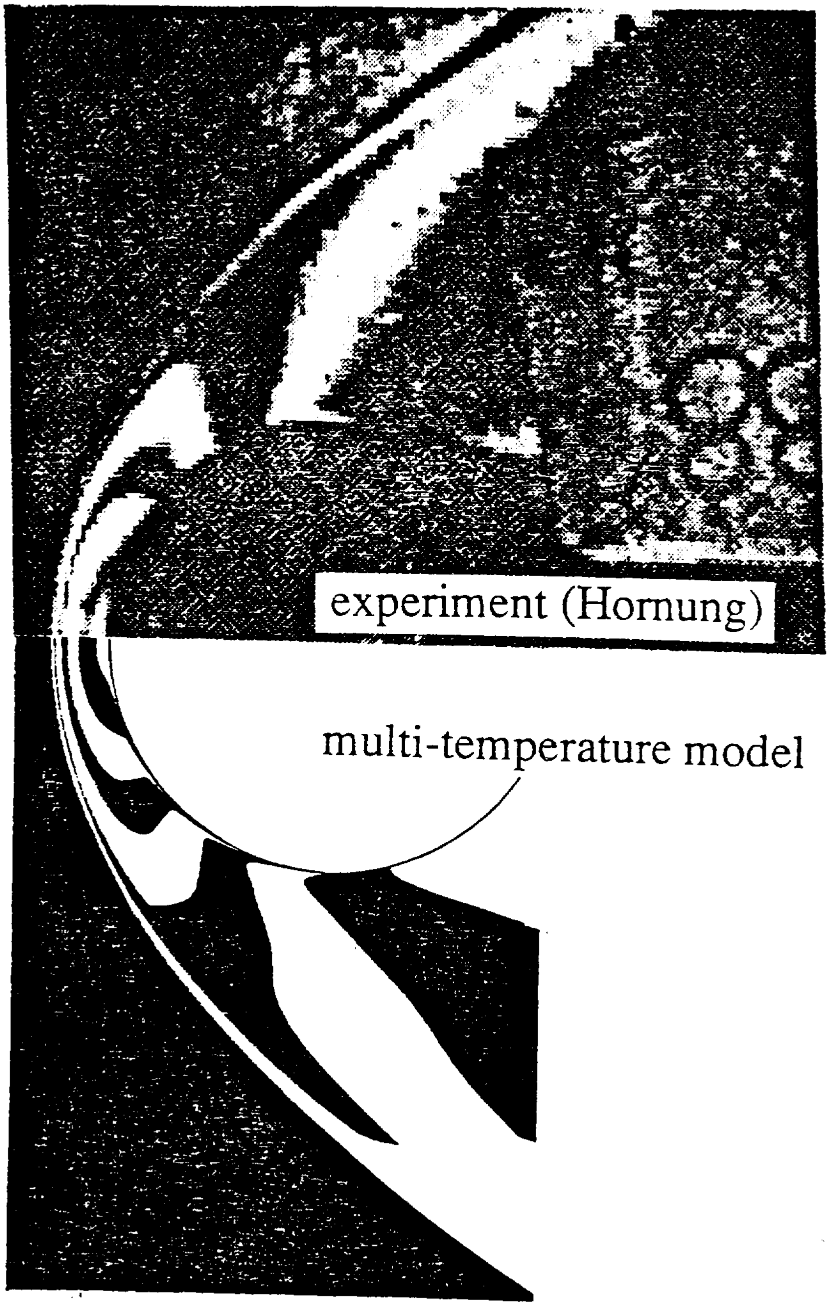
Results – Cylinder

- Interferogram of 2 inch diameter cylinder in N_2 and N.
  $u_\infty = 5.59\,\mathrm{km/s}$, $\mathcal{M}_\infty = 6.1$, $Re = 12000$, $\psi = 5.5$.



Status of Computer Code

- Current status:
  - basically a research code
  - not vectorized (26 mflops on Cray X-MP)
  - code being used outside of Ames
  - typical solution takes 1.5 hours of Cray X-MP CPU
- Near-term improvements:
  - vectorized version
  - more efficient physical modelling
  - anticipate factor of 5 speedup
  - other gas models

Conclusions

- Algorithm for thermo-chemical nonequilibrium flow developed:
    - seven species, six temperatures
    - complete viscous terms (binary diffusion, laminar)
    - implicit numerical method
    - fully coupled equation set
    - results compared to experiment
- Future work:
    - three-dimensions
    - better models for high temperature air
    - larger degree of ionization