THE COMPUTATION OF WEAKLY IONIZED HYPERSONIC FLOWS IN THERMO-CHEMICAL NONEQUILIBRIUM

A DISSERTATION
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FOR THE DEGREE OF
DOCTOR OF PHILOSOPHY

By
Graham V. Candler
June 1988

I certify that I have read this thesis and in my opinion it is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.

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Stanford University, 1988

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.

In this dissertation, the differential equations that describe a hypersonic thermo-chemical nonequilibrium flowfield are derived. A numerical method to solve these equations in two dimensions is discussed and results for some test cases are presented. 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 was then 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.

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Roman Symbols

a	Speed of sound, see (C.8).
$\tilde{a}$	Modified speed of sound, see (C.14).
$a_+,\ a_-$	Modified speeds of sound, see (C.16).
A_{im}	Constants for use in equilibrium reaction constant, see (A.1).
A_{sr}	Constant used in Millikan and White vibrational relaxation model, see (2.7.3).
$A_s,\ B_s,\ C_s$	Constants used in Blottner viscosity model, see (2.6.3).
$A',\ B'$	Jacobians of F' and G', see (3.3.3).
$A'_+,\ A'_-$	Flux-split Jacobians of F'.
$B'_+,\ B'_-$	Flux-split Jacobians of G'.
$\hat{A},\ \hat{B}, \ldots \hat{E}$	Block matrices defined in (3.4.2).
c_s	Mass concentration of species s, $\quad c_s = \rho_s/\rho$.
$\mathrm{c_s}$	Thermal speed of species s, see (2.7.7).
c_p	Mass-averaged specific heat at constant pressure.
c_v	Mass-averaged specific heat at constant volume.
c_{vs}	Translational-rotational specific heat at constant volume of species s.
$c_{v\mathrm{tr}\,s}$	Translational specific heat at constant volume of species s.
$c_{v\mathrm{rot}\,s}$	Rotational specific heat at constant volume of species s.
$c_{v\mathrm{vib}\,s}$	Vibrational specific heat at constant volume of species s.
C	Jacobian of W with respect to U.
$C_A,\ C_{A'}$	Jacobians used in diagonalization of A', see (3.3.7).
C_{f_m}	Constant for use in the Arrhenius form of reaction rates, see (2.8.4).
$\mathcal{D}$	Diffusion coefficient of uncharged species.
$\mathcal{D}_s$	Diffusion coefficient of species s.
d	Dimensionality of the problem.
d_s	Molecular diameter of species s.
e	Electron charge.
e^-	Symbol used to denote electrons.
e_e	Electron translational energy per unit mass.
$e_{\mathrm{el}\,s}$	Electronic energy of species s per unit mass, see (2.5.8).
e_{vs}	Vibrational energy per unit mass of species s.
$e^*_{vs}(T)$	Vibrational energy per unit mass of species s at the local T.
E	Total energy per unit volume.

$\mathbf{E}$	Block matrix for the use in implicit boundary condition treatment, see (3.5.5).
E_e	Electron translational energy per unit volume.
E_{vs}	Vibrational energy per unit volume of species s.
E_s	Total energy per unit volume of species s.
$\tilde{E}_i$	Electric field in the i direction.
$F,\ G$	Flux vectors in the x and y directions.
$F',\ G'$	Rotated flux vectors in the ξ and η directions, see (3.2.8).
$F'_{\mathrm{I}},\ F'_{\mathrm{v}}$	Inviscid and viscous components of F'.
$G'_{\mathrm{I}},\ G'_{\mathrm{v}}$	Inviscid and viscous components of G'.
g_{is}	Degeneracy of electronic states for state i of species s, see (2.5.8).
h_s	Enthalpy per unit mass of species s, see (2.5.7).
h_s°	Heat of formation of species s.
$i,\ j$	Indices used for vector components and also to denote grid points.
$IL,\ JL$	Size of grid in the ξ and η directions.
k	Boltzmann constant.
k_{f_m}	Forward reaction rate of reaction m, see (2.8.4).
k_{b_m}	Backward reaction rate of reaction m, see (2.8.4).
K	Generic constant.
K_{eq_m}	Equilibrium constant of reaction m, see (2.8.4).
Kn	Knudsen number.
l	Reaction number.
$\mathcal{L}e$	Lewis number, see (2.6.7).
m	Number of diatomic species or reaction number.
M	Mass-averaged atomic weight.
$\mathcal{M}$	Mach number.
M_s	Atomic weight of species s.
M_η	Matrix used in the implicit treatment of the viscous terms, see (3.3.21).
n	Number of species or time level of computation.
N	Jacobian used in the implicit viscous terms, see (3.3.23).
N_2	Symbol used for diatomic nitrogen.
N	Symbol used for atomic nitrogen.
NO	Symbol used for nitric oxide.
NO^+	Symbol used for ionized nitric oxide.
N_s	Number density of species s,
$\hat{N}$	Avogadro's number.
O_2	Symbol used for diatomic oxygen.
O	Symbol used for atomic nitrogen.

p	Pressure.
p_s	Species s partial pressure.
P_{si}	Momentum transfer rate of species s in direction i.
P_{sr}	Probability of vibration energy transfer, see (2.7.13).
q_j	Translational-rotational heat conduction in direction j.
q_{ej}	Electron translational heat conduction in direction j.
q_{tj}	Total heat conduction in direction j.
q_{vsj}	Vibrational heat conduction of species s in direction j.
Q_s	Generic energy transfer rate of species s.
Q_{vs}	Vibrational energy transfer rate of species s.
$Q_{e-v\,s}$	Electron-vibration energy transfer rate of species s.
Q_{T-e}	Translation-electron energy transfer rate.
$Q_{T-v\,s}$	Translation-vibration energy transfer rate of species s.
$Q_{v-v\,s}$	Vibration-vibration energy transfer rate of species s.
r_n	Nose radius.
R	Gas constant.
$\mathcal{R}$	Reaction, see (2.8.2).
R_A	Rotation matrix.
Re	Reynolds number based on nose radius or total length.
Re_x	Local Reynolds number.
R_s	Gas constant of species s.
$\bar{R}$	Mass-averaged gas constant.
RHS	Right hand side of equation, see (3.5.5).
$s'_{ix},\ s'_{iy}$	Direction cosines of surface $i+\frac{1}{2}, j$ in the x and y directions, see (B.5).
$s'_{jx},\ s'_{jy}$	Direction cosines of surface $i, j+\frac{1}{2}$ in the x and y directions, see (B.5).
S	Jacobian of V with respect to U.
S_s	Exponent for use in the diffusion model of vibrational relaxation, see (2.7.6).
t	Time.
T	Translational-rotational temperature.
T_e	Electron translational temperature.
T_{vs}	Vibrational temperature of species s.
$\bar{T}$	Average temperature for use in reaction rates.
$\mathbf{T}$	Metric transformation matrix, see (B.1).
$u,\ v$	Mass-averaged velocity components in x and y direction.
u_j	Mass-averaged velocity vector.
u_{sj}	Species s velocity vector.
v_{sj}	Species s diffusion velocity vector.

$\mathrm{u}_s,\ \mathrm{v}_s$	Diffusion velocities of species s in x and y directions.
$u',\ v'$	Mass-averaged velocity components normal and tangential to a surface.
$\tilde{u}',\ \tilde{v}'$	Modified velocity components, see (C.7).
U	Vector of conserved quantities.
$V,\ \mathbf{V}$	Vectors of non-conserved variables.
w_s	Mass source term due to reaction of species s.
W	Source vector.
$x,\ y$	Cartesian coordinates.
x_j	Cartesian coordinate vector.
X_s	Molar concentration of species s.
Z_s	Charge number of species s.
Z_{sr}	Number of $s-r$ collisions per unit time.

Greek Symbols

$\bar{\gamma}$	Effective ratio of specific heats, see (C.10).
δ	Boundary layer thickness.
δ_{ij}	Kronecker symbol.
$\delta F_\mathrm{v},\ \delta G_\mathrm{v}$	Implicit changes in the Cartesian viscous fluxes.
$\delta F'_\mathrm{v},\ \delta G'_\mathrm{v}$	Implicit changes in the rotated viscous fluxes.
δU	Implicit change in the vector of conserved quantities.
Δt	Time step.
ΔU	Explicit change in the vector of conserved quantities.
ε_{vs}	Vibrational energy per particle of species s.
η_m	Constant for use in Arrhenius form of reaction rate for reaction m, see (2.8.4).
θ_c	Cone half-angle.
$\theta_{\mathrm{el}\,is}$	Electronic activation energy of state i for species s, see (2.5.8).
θ_m	Characteristic temperature of reaction for reaction m.
θ_s	Characteristic temperature for use in diffusive model of vibrational relaxation.
θ_{vs}	Characteristic temperature of vibration of species s.
κ	Conductivity of translational-rotational temperature.
κ_e	Conductivity of electron translational temperature.
κ_{vs}	Conductivity of vibrational temperature of species s.
λ	Second coefficient of viscosity.
$\Lambda_{A'}$	Diagonal matrix of convection speeds of characteristic variables for A'.

$\Lambda_{A'+},\ \Lambda_{A'-}$	Diagonal matrices of positive and negative convection speeds of characteristic variables for A'.
μ	Viscosity of mixture.
μ_s	Species viscosity.
$\xi,\ \eta$	General coordinate directions, ξ along the body and η normal to the body.
ρ	Density.
ρ_s	Density of species s.
σ_{sr}	Collision cross-section for species s and r. (Specific to the process.)
τ_{cs}	Collision limited vibrational relaxation rate of species s, see (2.7.7).
τ_{es}	Electron energy relaxation rate of species s, see(2.7.12).
τ_{ij}	Shear stress tensor, see (2.6.1).
τ_{sij}	Species shear stress tensor.
$\tau_{s_{\mathrm{L-T}}}$	Landau-Teller vibrational relaxation rate of species s, see(2.7.2).
τ_{vs}	Vibrational relaxation rate of species s, see (2.7.6).
ϕ_s	Parameter for use in Wilke mixing model, see (2.6.5).
Ψ	Reactivity of the gas, see (4.2.2).

Difference Operators

$$\frac{D_+ Z_{ij}}{\Delta\xi} \equiv Z_{i+1j} - Z_{ij} \qquad \frac{D_- Z_{ij}}{\Delta\xi} \equiv Z_{ij} - Z_{i-1j}$$

$$\frac{D_+ Z_{ij}}{\Delta\eta} \equiv Z_{ij+1} - Z_{ij} \qquad \frac{D_- Z_{ij}}{\Delta\eta} \equiv Z_{ij} - Z_{ij-1}$$

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