AE-512 Molecular Gas Dynamics

Final Project - Part 2

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Non-equilibrium flow behind the shock was computed. A MATLAB code was developed to:

1) Read the necessary input data
2) Compute the post-shock properties using the Rankine-Hugoniot relations.
3) Solve the non-equilibrium flow behind the shock

Brief description of the MATLAB subroutines

1) **FUN_read_species_data, FUN_read_electronic_data, FUN_get_reactions and FUN_get_stoichiometric_coefficients**: Read the necessary thermodynamic data related to the species, get all the necessary reactions for the kinetic model.
2) **FUN_mass2mole_frac, FUN_get_thermo_prop and FUN_get_mix_thermo_prop**: Utility functions for conversion of mass fraction to mole fraction and to calculate the thermodynamic properties of the given species or mixture at the given temperature and density.
3) **compute_rh_jump:** Calculate the post-shock properties using the Rankine-Hugoniot relations in an iterative manner.
4) **FUN_kinetics_solver:** Calculates the reaction rates and rate of production of each species for the species and vibrational energy source terms.
5) **FUN_get_vib_source_term:** computes the source term for the vibrational energy equation.
6) **FUN_get_Kp_eq_stat and FUN_total_partition_function:** Calculates the partition functions and equilibrium constant.
7) **ode_system and FUN_solve_1d_noneq_flow:** assemble the partial differential equations and solve them for the given x range.

The flow was assumed to be in Thermodynamic Non-Equilibrium. The freestream conditions used for the calculation of post-shock properties were:

Property	Value
P	5 Pa
T	200K
U	7000 m/s
Y_{N2}	1
Y_N	0

The post-shock properties were calculated using the Rankine-Hugoniot equations:

$$\rho_2 = \frac{M_{mix}P_2}{RT_2}$$

$$U_2 = \frac{\rho_1}{\rho_2}U_S$$

$$P_2 = P_1 + \rho_1 U_S^2 \left(1 - \frac{\rho_1}{\rho_2}\right)$$

$$T_2 = T_2 - \frac{H_2 - H_1 - \frac{1}{2}U_S^2 \left(1 - \left(\frac{\rho_1}{\rho_2}\right)^2\right)}{C_{p,2}}$$

These equations were iteratively solved until a convergence of 10^{-10} was reached. The post-shock properties were used as the initial conditions for the non-equilibrium flow solver. The vibrational temperature for the initial condition was taken to be equal to the freestream temperature(200K).

The governing equation for the steady one-dimensional non-equilibrium flow are:

$$\frac{d}{dx}\begin{pmatrix} \rho_s u \\ p + \rho u^2 \\ \rho u H \\ \rho u e_v \end{pmatrix} = \begin{pmatrix} \omega_s \\ 0 \\ 0 \\ \Omega_v \end{pmatrix}$$

The canonical forms of this equation was used in the 1d solver which are:

$$\frac{dy_i}{dx} = \frac{\omega_i}{\dot{m}}$$

$$\frac{du}{dx} = \frac{-\frac{uRTc_p}{\dot{m}}\sum_i \frac{\omega_i}{M_i} + \frac{Ru}{M_{mix}\dot{m}}\sum_i h_i(T)\omega_i}{\det(A)}$$
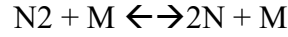
$$\frac{dT}{dx} = \frac{-\frac{1}{\dot{m}}\left(u^2 - \frac{RT}{M_{\text{mix}}}\right)\sum_i h_i(T)\omega_i + \frac{u^2 RT}{\dot{m}}\sum_i \frac{\omega_i}{M_i}}{\det(A)}$$

$$\frac{dT_V}{dx} = \frac{1}{\dot{m}c_{v,v}}\left(\Omega_V - \sum_m e_v^{(m)}\omega_m\right)$$

where,

$$\det(A) = u^2 c_p - \frac{R}{M_{\text{mix}}}\left(Tc_p + u^2\right)$$

For the kinetic solver, the equations used are:

$$N2 + M \longleftrightarrow 2N + M$$

Where M is the collision partner (M = N2 or N).

The forward and backward reaction rate constants were calculated using the Arrhenius equation and the equilibrium rate constant, calculated using the partition functions.

The preferential dissociation of molecules was modeled using the Park two-temperature model, $Tc = (TT_v)1/2$. In the kinetic model, Tc is the rate-controlling temperature, and T_v is the vibrational temperature.

For the vibrational energy source term, the contribution from the vibrational-translational relaxation was modeled using the Landau-Teller model, and the contribution from the reaction-induced vibrational energy was calculated using the production rates of molecular species and the vibro-electronic internal energies.

$$\Omega_V = \Omega_{vVT} + \Omega_{vreactions}$$

$$\Omega_{vVT} = \rho C_{v,v}(T - T_v)/\tau$$

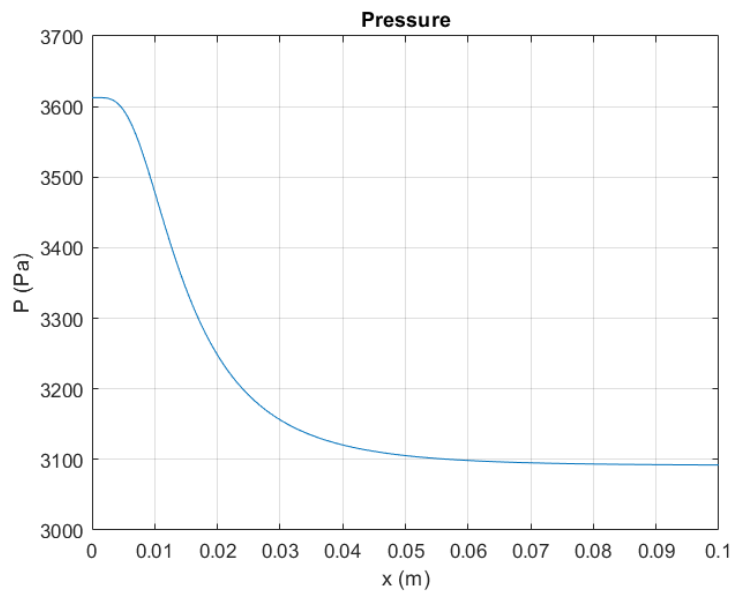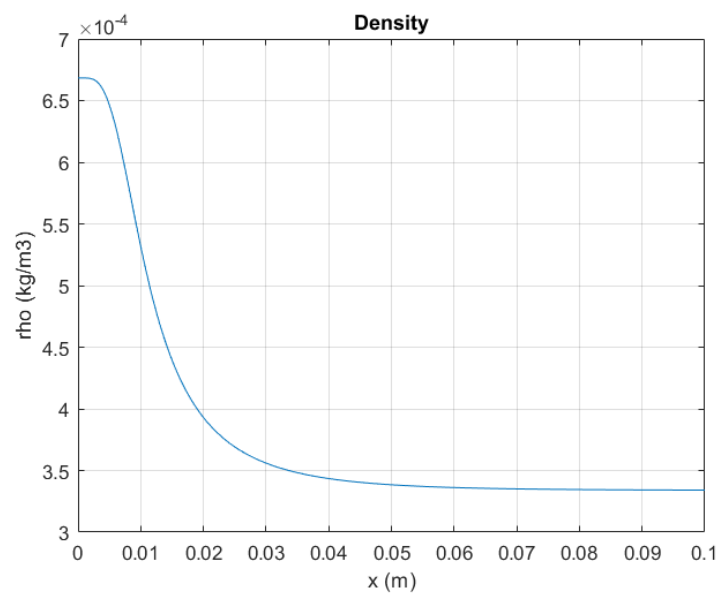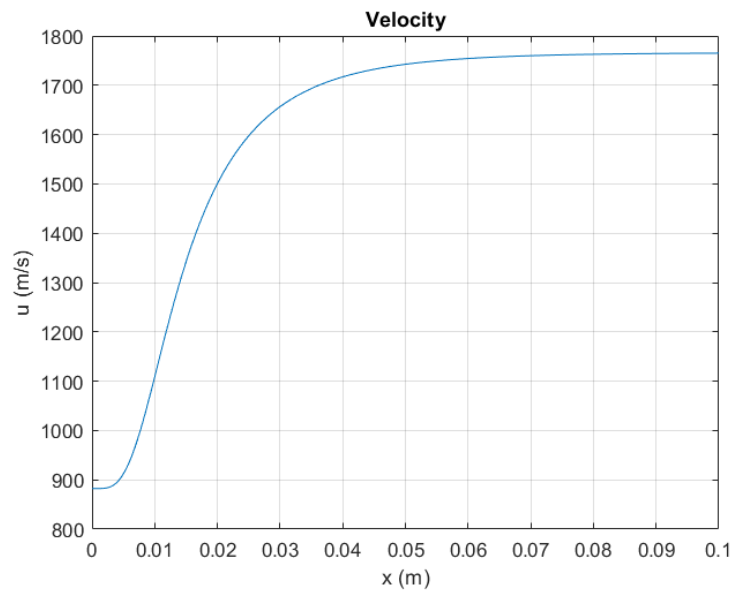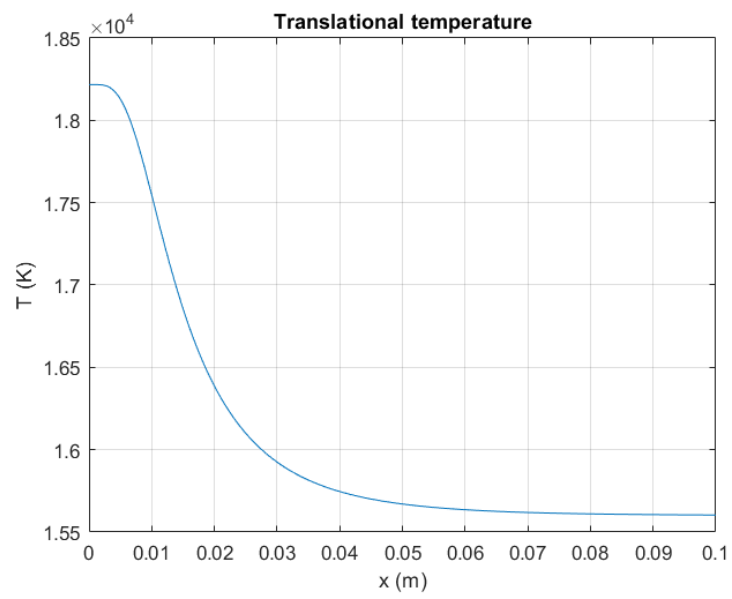$$\Omega_{vreactions} = \sum e_v^{(m)}\omega_m$$

Results

The post-shock conditions obtained from Rankine-Hugoniot relations are:

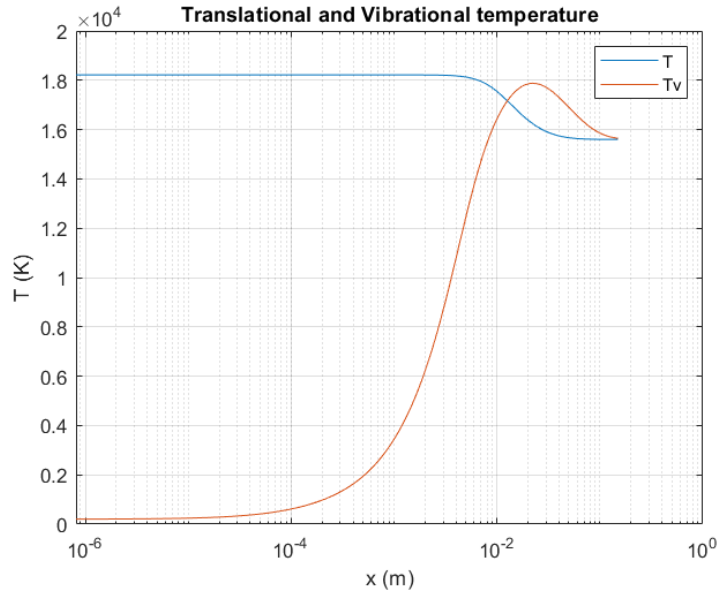| Property	Value
P	3612.74 Pa
T	18216.95K
U	882.42 m/s
Tv	200K
Y_{N2}	1
Y_N	0

The following graphs show the variation of Pressure, Velocity, Density, Mass fractions and Temperature with x.

Velocity

u (m/s) vs x (m)

Density

rho (kg/m3) vs x (m)

Mass Fractions

Translational temperature

Translational and Vibrational temperature

From the graphs, it was visible that, the properties vary smoothly after the shock jump, downstream of the shock. Due to the sudden increase in temperature across shock, the N2 starts to dissociate and tries to reach the equilibrium composition.

The vibrational energy levels are also excited which is seen by the rise in the vibrational temperature. A strong non-equilibrium exists near the shock, characterized by the large difference between the translational and the vibrational temperature. As the fluid moves downstream, it starts to reach thermodynamic equilibrium. The vibrational temperature increases until both vibrational and translational temperatures equalize.

A decrease in the translational energy leads to a decrease in pressure and hence a decrease in in density. This leads to an increase in the velocity due to mass conservation.

References

[1] Vincenti, W. G., and C. H. Kruger. "Physical gas dynamics, Kriger Pub." (1975).

[2] Park, Chul. "Assessment of two-temperature kinetic model for ionizing air." *Journal of thermophysics and heat transfer* 3.3 (1989): 233-244.

[3] Gnoffo, Peter A. *Conservation equations and physical models for hypersonic air flows in thermal and chemical nonequilibrium*. Vol. 2867. National Aeronautics and Space Administration, Office of Management, Scientific and Technical Information Division, 1989.

[4] Anderson, John David. *Hypersonic and high temperature gas dynamics*. Aiaa, 1989.