Thermochemical relaxation region behind a Shock Wave

An approach with the Mutation++ library

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Project for the course of Fundamentals of Hypersonic Flows

Contenuti

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Relaxation Behind a Shock Wave

Project Goal

The goal is to study the effect of thermochemical non equilibrium on the relaxation region behind a normal shock wave.

3 different models are studied

1. Thermochemical equilibrium, the shock wave is approximated by a step function, the relaxation region has zero thickness.
2. Thermodynamic equilibrium, the gas is assumed to be well described by 1 temperature, finite rate chemistry acts on the flow
3. Themochemical non-equilibrium, the internal vibrational degrees of freedom are not in equilibrium with the others. The two temperature approximation is used.

Models

Equilibrium

1. Initial conditions, Y_∞, M_∞, P_∞, T_∞
2. Solve the RH jump using the P.I.G gas jump as initial guess
3. No relaxation

Non-Equilibrium

1. Initial conditions, Y_∞, M_∞, P_∞, T_∞
2. Solve the RH jump using the P.I.G gas jump as initial guess and $Y_i = Y_{i\infty}$, $T_i^{(v)} = T_\infty$
3. Relax the flow by solving the Euler equations
4. More equations (than unknowns) are solved in order to check that the error is not large

Mutation++

The library

Mutation serves as a wide database for thermochemical data. Custom species, mixtures and reactions can also be added

The Core

1. All elements are stored in a xml file
2. Species can be built from elements. The internal DoF structure must be specified
3. Millikan-White data must be specified (for all vibrators and partners) in a VT.xml file

Mixtures

1. The species present, their default composition must be specified in a .xml
2. All possible reactions, along with Arrhenius parameters are specified in another xml file

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Governing Equations

The 1D steady Euler equations for a reacting mixture read

$$\frac{\partial}{\partial x}[\rho u] = 0$$

$$\frac{\partial}{\partial x}[\rho_i u] = \dot{\omega}_i(\rho_i, \rho e, \rho e^v)$$

$$\frac{\partial}{\partial x}[\rho u u + P(\rho_i, \rho e, \rho e^v)] = 0$$

$$\frac{\partial}{\partial x}[\frac{1}{2}\rho u^3 + \rho u e + u P(\rho_i, \rho e, \rho e^v)] = 0$$

$$\frac{\partial}{\partial x}[\rho u e^v] = \Omega_v(\rho_i, \rho e, \rho e^v)$$

$$e_i = e_i^{tr} + e_i^{int}$$

Variables

The primary variables are $\rho, \rho_i, \rho u, \rho e, \rho e^v$ but the solver will use P, Y_i, u, T, T_v. The mixture state can be specified by using $Y_i, (P, T, T_v)$

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$$\frac{\partial}{\partial x}[\rho u u + P(\rho_i, \rho e, \rho e^v)] = 0$$

$$\frac{\partial}{\partial x}[\frac{1}{2}\rho u^3 + ue + uP(\rho_i, \rho e, \rho e^v)] = 0$$

$$\frac{\partial}{\partial x}[\rho u e^v] = \Omega_v(\rho_i, \rho e, \rho e^v)$$

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The primary variables are $\rho, \rho_i, \rho u, \rho e, \rho e^v$ but the solver will use P, Y_i, u, T, T_v. The mixture state can be specified by using $Y_i, (P, T, T_v)$

Solution Procedure

All above equations have a the following structure

$$\frac{\partial}{\partial x}\mathbf{f}(P, Y_i, u, T, T_v) = \mathbf{s}(P, Y_i, u, T, T_v)$$

The computational domain is discretized following the Finite Volume fashion

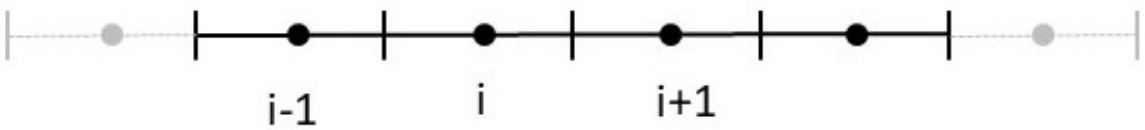

Figure: Computational Domain

All the problem unknowns are assumed to be constant over the computational cell. The boundary presents therefore a discontinuity

Solution Procedure

The equations are integrated

$$\int_{x_i}^{x_{i+1}} \frac{\partial \mathbf{f}}{\partial x} dx = \int_{x_i}^{x_{i+1}} \mathbf{s} dx$$

The following result is obtained

$$\mathbf{f}_{i+1} - \mathbf{f}_i = \frac{1}{2} h(\mathbf{s}_{i+1} + \mathbf{s}_i)$$

The above is a system of nonlinear equations that can be solved with standard methods.

Advantages and disadvantages of the chosen scheme

The previous work writes the problem in the following way, calling $\mathbf{u}$ the vector of solved variables

$$\hat{\mathbf{J}} \cdot \frac{\partial \mathbf{u}}{\partial x} = \mathbf{s}$$
$$\frac{\partial \mathbf{u}}{\partial x} = \hat{\mathbf{J}}^{-1} \cdot \mathbf{s}$$

Compared to this scheme the main advantage is that it avoids the construction and inversion of the jacobian (provided that this quantity is not required by the nonlinear solver).
The main disadvantage is that it is at most first order accurate in smooth regions.

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Introduction to Thermochemical models

As shown from the 1D steady Euler equations for a mixture, in order to get a solution, we need to model both the finite rate production of each species $\dot{\omega}_i(\rho_i, \rho e^t, \rho e^v)$ and the production term for vibrational internal energy $\Omega_v(\rho_i, \rho e^t, \rho e^v)$.

Internal Energy Levels

For what concerns the internal energy levels, we chose to model them according to the RRHO models, i.e.:

- Rotational = Rigid Rotator
- Vibrational = Harmonic Oscillator

Thermochemical properties

From the RRHO model

$$P = \rho\left(\sum_{i=0}^{N_s-1} Y_i R_i T^{rt} + Y_e R_e T^{ev} \right)$$

$$e = \sum_{i=0}^{N_s} Y_i \left(e_i^{tr} + e_i^{rot} + e_i^{ev} + \Delta e_i^f(T_{ref}) \right)$$

Mutation can also use the polynomial approximation for the specific heat. In this case

$$e = \sum_{i=0}^{N_s} Y_i \left(\int_{T_{ref}}^{T} C_v^i(T')dT' + \Delta e_i^f(T_{ref}) \right)$$

Transfer Properties

Using finite rate chemistry

$$\dot{\omega}_i = M_i \sum_{reactions} (\nu''_{ir} - \nu'_{ir})[K_{f,r} \prod_{species} n_i^{\nu'_{ir}} - K_{b,r} \prod_{species} n_i^{\nu''_{ir}}]$$

where:

$$K_{f,r}(T_{eff}) = C_f T_{eff}^{\eta_f} exp\left(-\frac{\Theta_D}{T_{eff}}\right), \qquad \text{Forward Coefficient}$$

$$K_{b,r}(T_{eff}) = \frac{K_{f,r}(T_{eff})}{K_{eq,r}(T_{eff})}, \qquad \text{Backward Coefficient}$$

$$K_{eq,r}(T_{eff}) = \left(\frac{p^o}{RT_{eff}}\right)^{\Delta\nu_r} exp\left(-\frac{\Delta G_r^o}{RT_{eff}}\right), \qquad \text{Equilibrium Coefficient}$$

$$T_{eff} = T_{rt}^{(q)} \cdot T_{ev}^{(1-q)}, \qquad \text{Park's Effective Temperature}$$

The vibrational relaxation source term reads

$$\Omega_v = \Omega_v^{VT} + \Omega_v^{CV}$$

$$\Omega_v^{VT} = \sum_{i=0}^{N_s} \rho_i \frac{e_i^v(T^{rt}) - e_i^v(T^{ev})}{\tau_i}$$

$$\Omega_v^{CV} = \sum_{i=0}^{N_s} \dot{\omega}_i e_i^{ev}$$

Coefficients τ_s are computed using the Millikan-White model.

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Studied Cases

Species

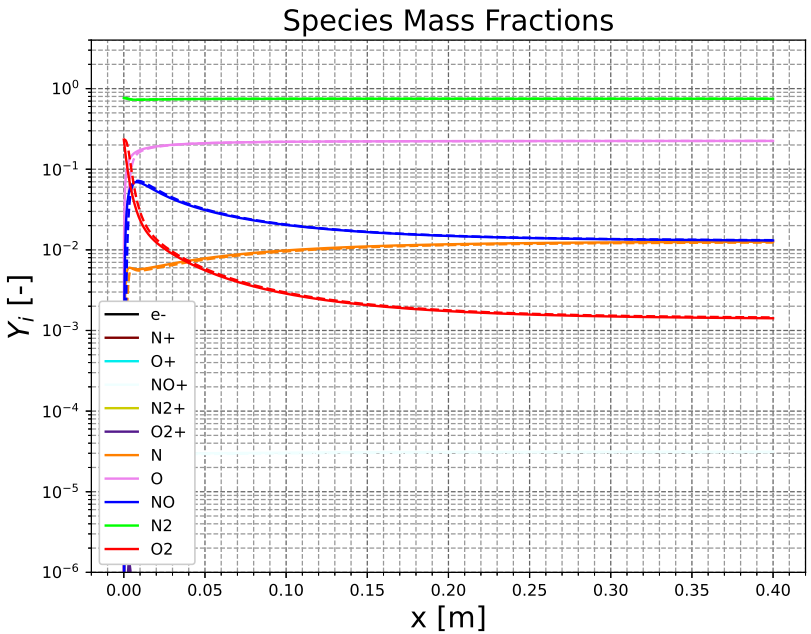
The species are O, N, NO, N2, O2, their relative positive ions and electrons

Case 1	
Variable	Value
M_∞	13.2 [-]
T_∞	268 [K]
P_∞	61 [Pa]

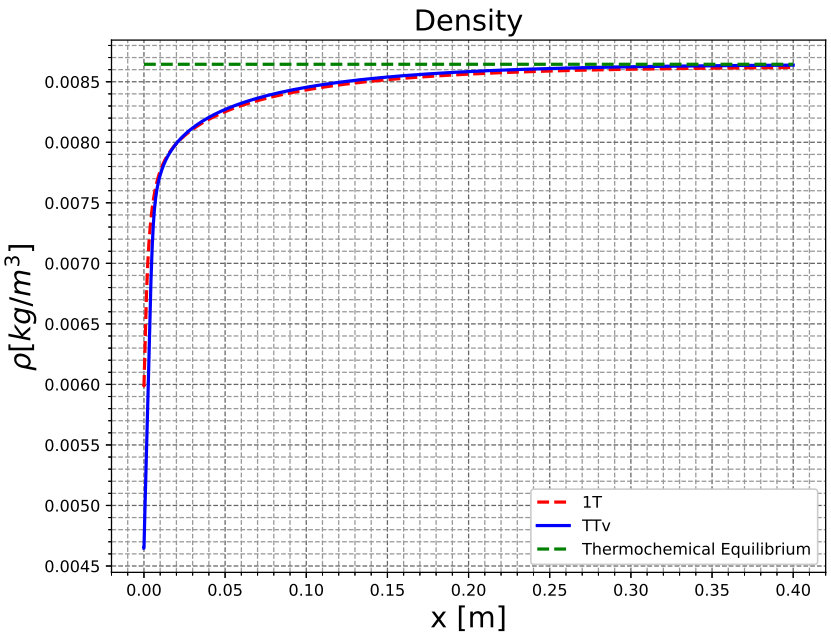
Case 2	
Variable	Value
M_∞	26.2 [-]
T_∞	227 [K]
P_∞	9.9 [Pa]

1. CASE 1, Low Hypersonic
2. CASE 2, High Hypersonic

Case 1, Part 1

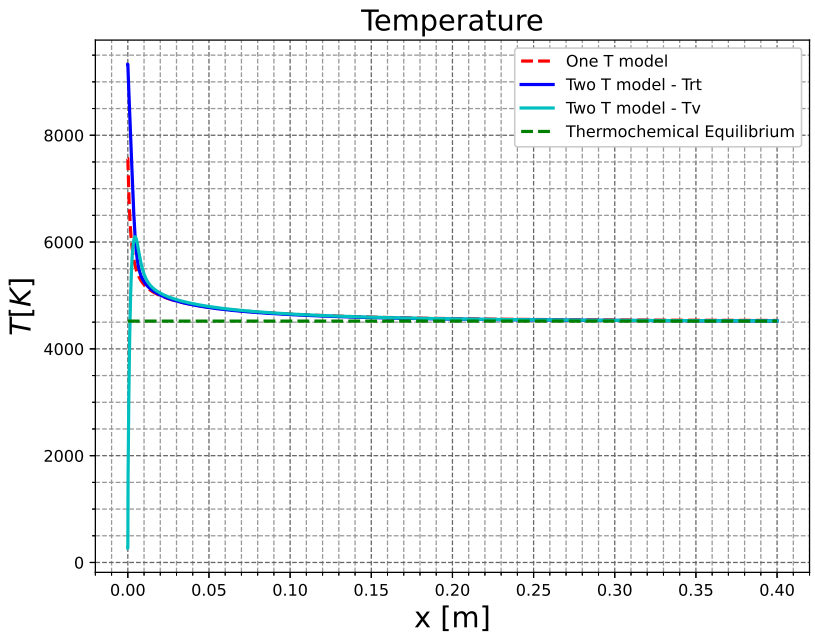


(a) Species

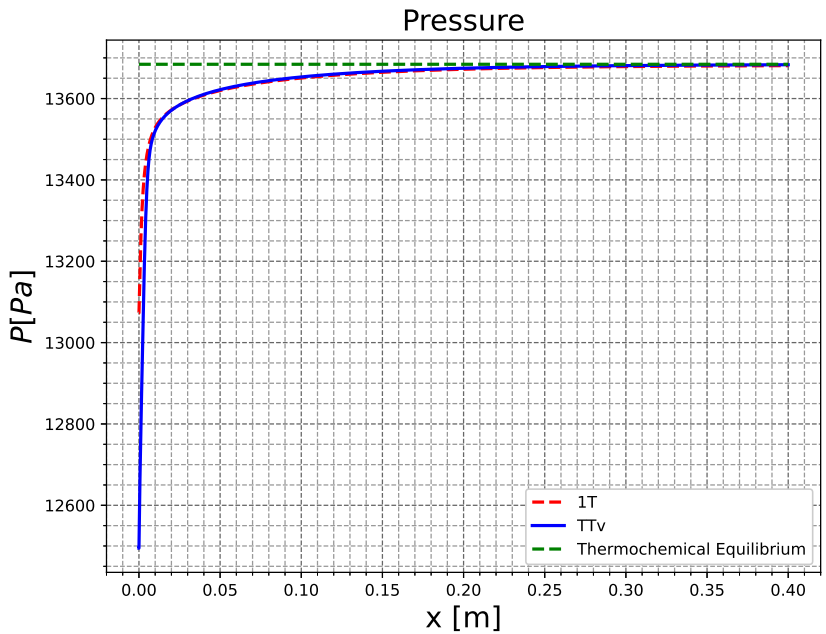


(b) Density

Case 1, Part 2



(a) Temperatures



(b) Pressure

Case 1, Comments

Post Shock	
Variable	Value
U	576 [m/s]
T	7567 [K]
P	13072 [Pa]

Equilibrium	
Variable	Value
U	400 [m/s]
T	4519 [K]
P	13674 [Pa]

1. Thermodynamic equilibrium happens before chemical equilibrium
2. No ions are generated
3. Molecular oxygen dissociates into atomic oxygen. The same happens for nitrogen but with a much lower yield
4. Nitric oxide appears in the mixture

5 species model

Because no ions appear in the reaction, a model with only 5 species is considered sufficient to model this particular case.

Species

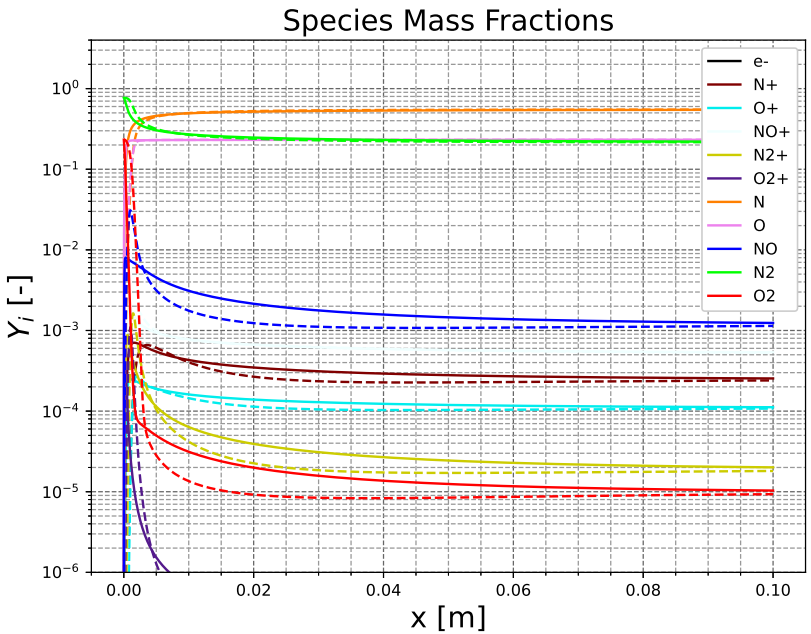
The species are O, N, NO, N2, O2

The following table shows the equilibrium values of the properties

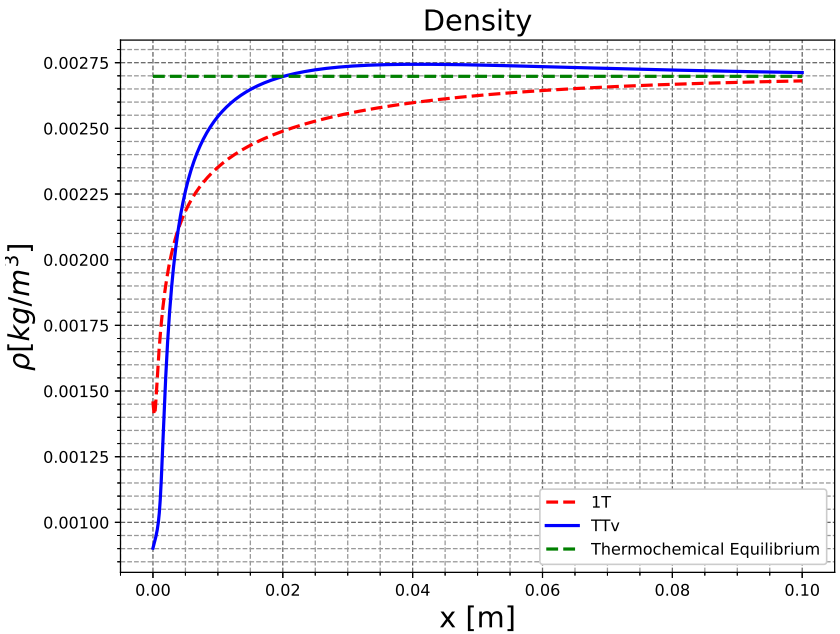
11 species	
Variable	Value
U	400 [m/s]
T	4519 [K]
P	13674 [Pa]

5 species	
Variable	Value
U	400 [m/s]
T	4520 [K]
P	13684 [Pa]

Case 2, Part 1

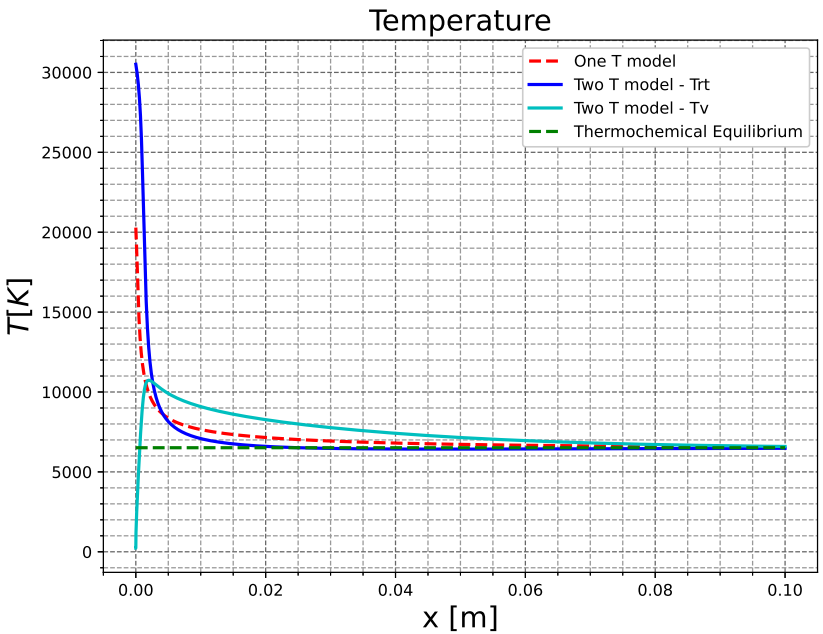


(a) Species

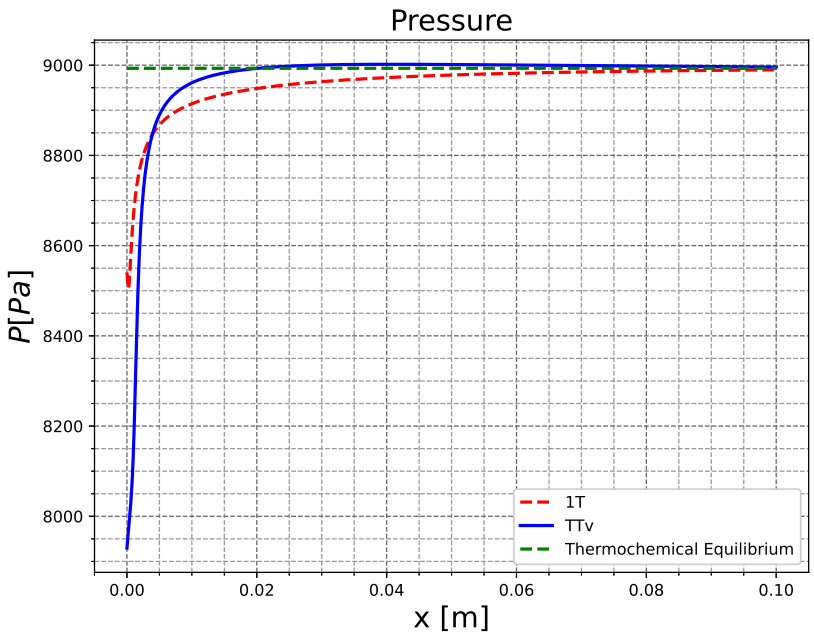


(b) Density

Case 2, Part 2



(a) Temperatures



(b) Pressure

Case 2, Comments

Post Shock	
Variable	Value
U	821 [m/s]
T	20289 [K]
P	8540 [Pa]

Equilibrium	
Variable	Value
U	444 [m/s]
T	6512 [K]
P	8993 [Pa]

1. Thermodynamic equilibrium happens with chemical equilibrium
2. In this case, all ions are present, except for O2+ which is present only at the beginning.

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Mars Atmosphere Composition

19 species model, 27 reactions. Park 1994: Journal of Thermophysics and Heat Transfer Vol. 8 No. 1

Species			
Name	Name	Name	Name
e-	C+	N+	O+
N2+	O2+	CN+	CO+
NO+	C	N	O
C2	N2	O2	CN
CO	NO	CO2	

Note

Carbon dioxide (95% composition) and molecular nitrogen (3% composition) make up almost 98% of the martian atmosphere. The rest is primarily composed of Argon but is not considered in this model.

Mars Atmosphere Model

NASA provides simple functional forms of $T(h)$ and $P(h)$

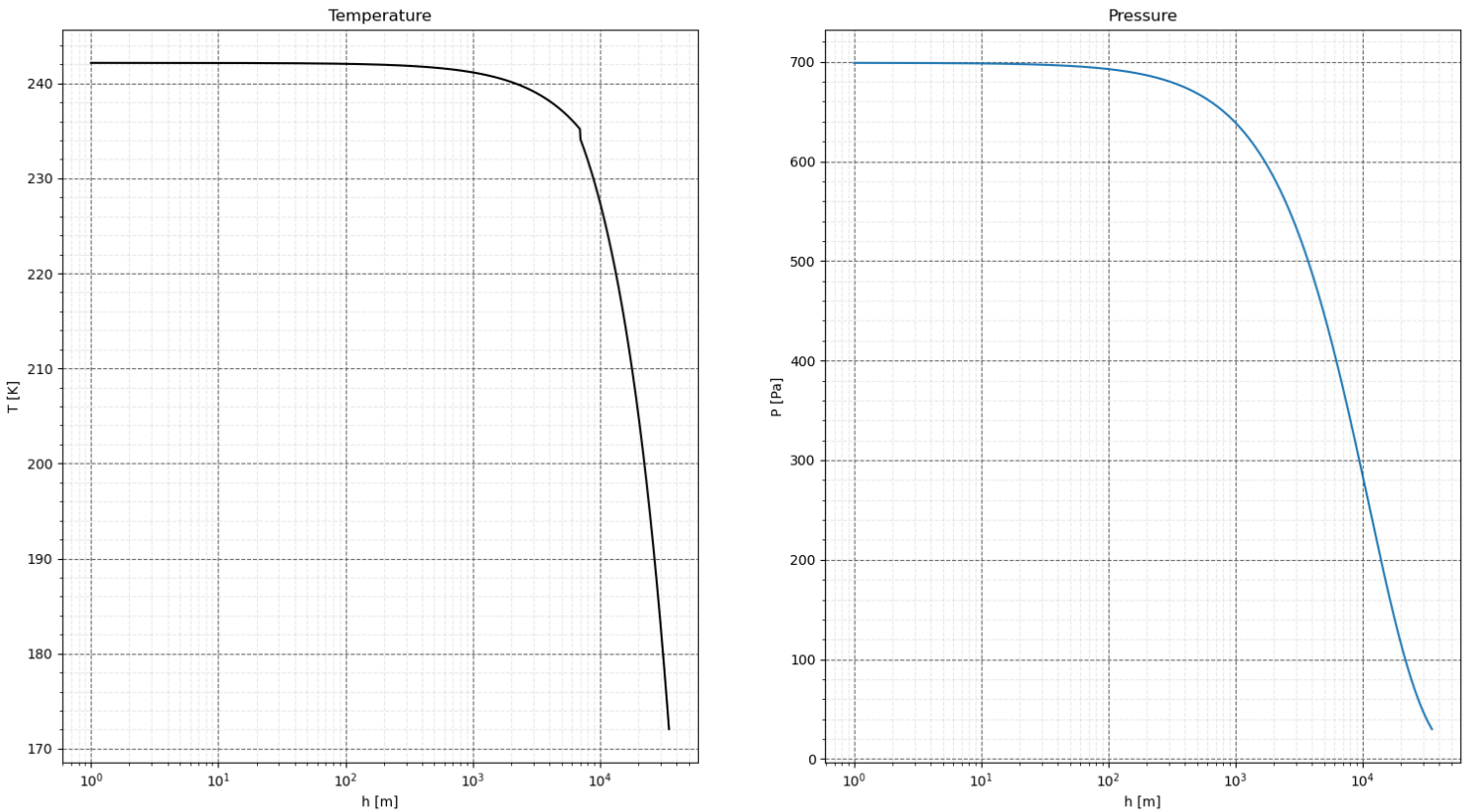
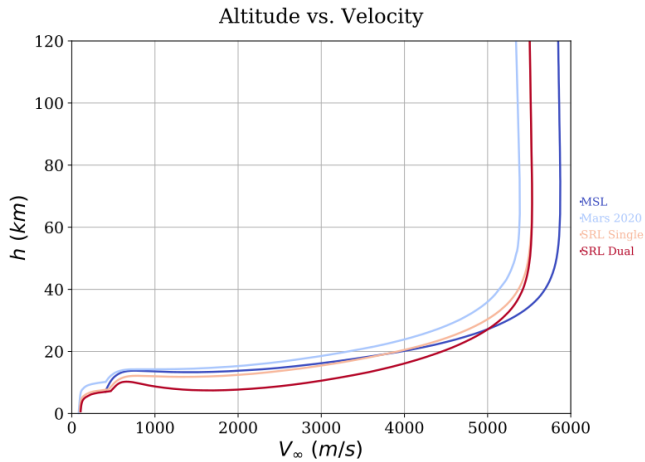


Figure: Atmosphere Model

Selected Cases

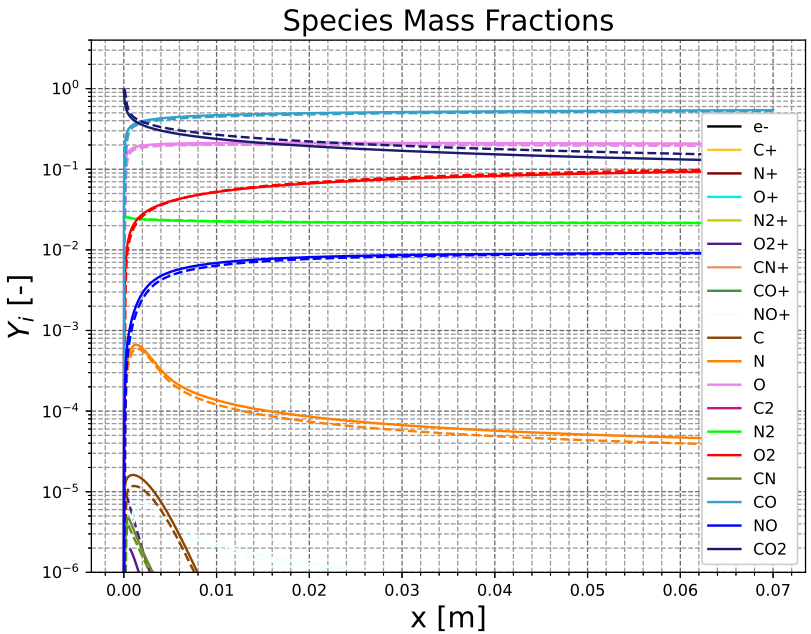
Using planetary entry data from previous missions, the following cases are studied



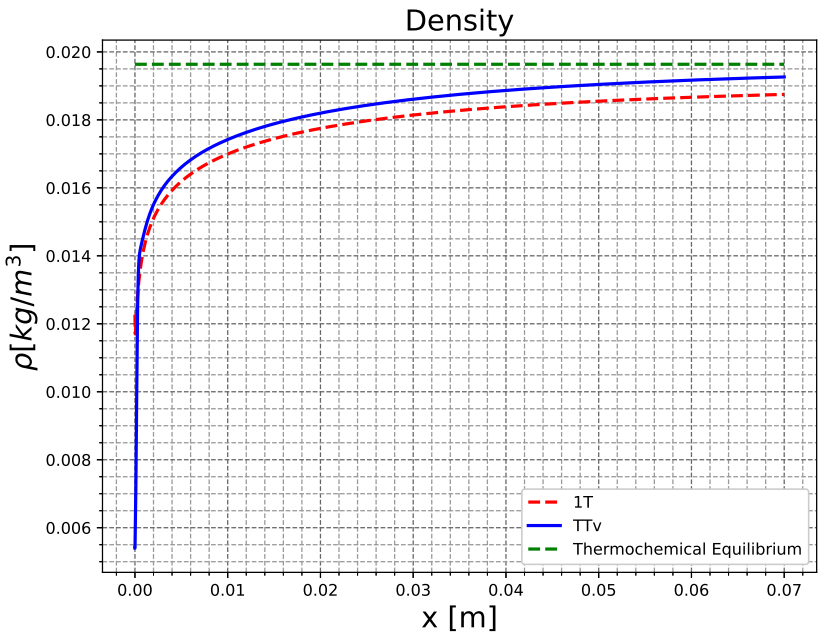
Case 1	
Variable	Value
h	35 [km]
M_∞	23.58 [-]
T_∞	172.05 [K]
P_∞	29.95 [Pa]

Case 2	
Variable	Value
h	1 [km]
M_∞	23.58 [-]
T_∞	241.15 [K]
P_∞	638.83 [Pa]

Case 1, Part 1

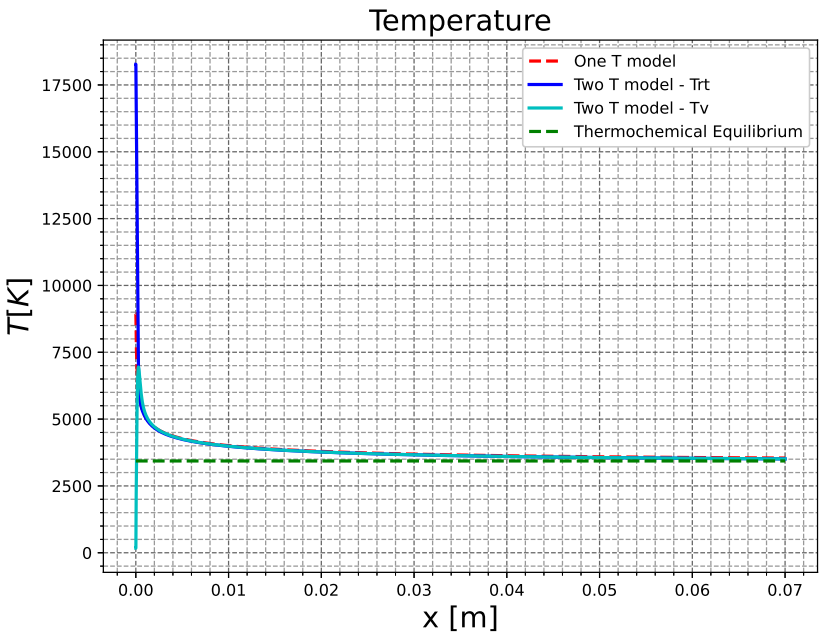


(a) Species

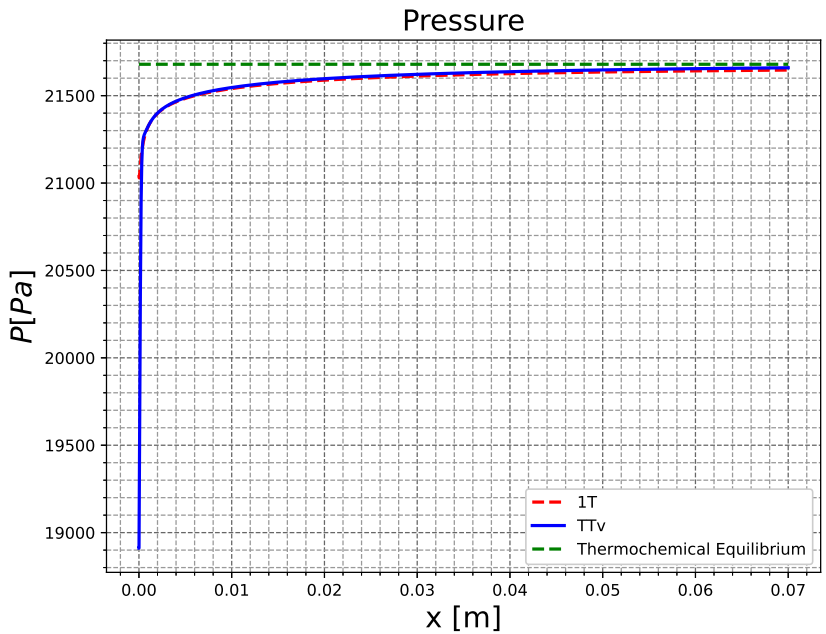


(b) Density

Case 1, Part 2



(a) Temperatures



(b) Pressure

Case 1, Comments

Post Shock	
Variable	Value
U	370 [m/s]
T	8951 [K]
P	21048 [Pa]

Equilibrium	
Variable	Value
U	231 [m/s]
T	3433 [K]
P	21679 [Pa]
ν	$5.71 \cdot 10^3$ [1/s]

1. The flow is very well approximated by thermodynamic equilibrium.
2. The CO2 immediately dissociates into CO and O.
3. Atomic oxygen partially recombines to form molecular oxygen and NO (from the dissociation of molecular nitrogen)
4. CO initially dissociates into C and O, forms CO+, CN. Some NO+ can also be seen. These species later disappear.

Simplified model

Species

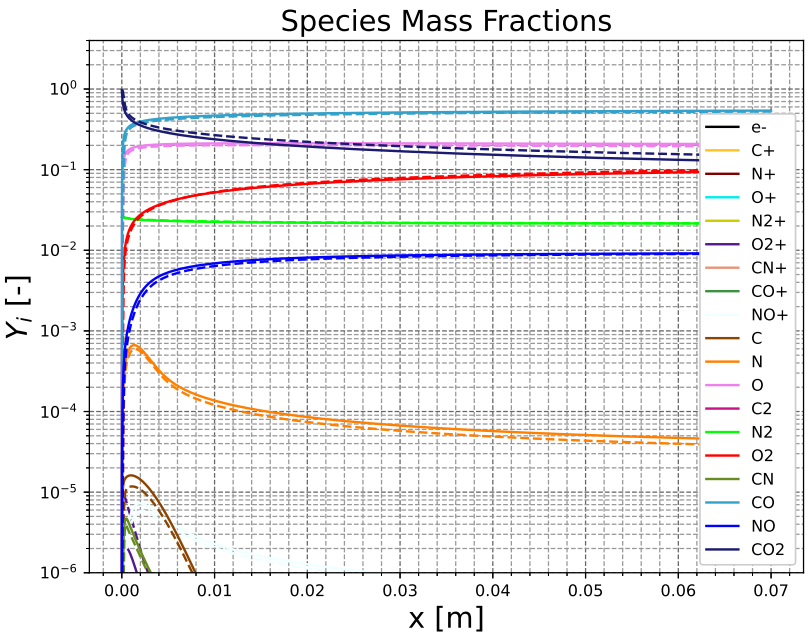
A custom mixture was created with the following species
C,N,O,C2,N2,O2,CN,CO,NO,CO2

19 species	
Variable	Value
U	231 [m/s]
T	3433 [K]
P	21679 [Pa]

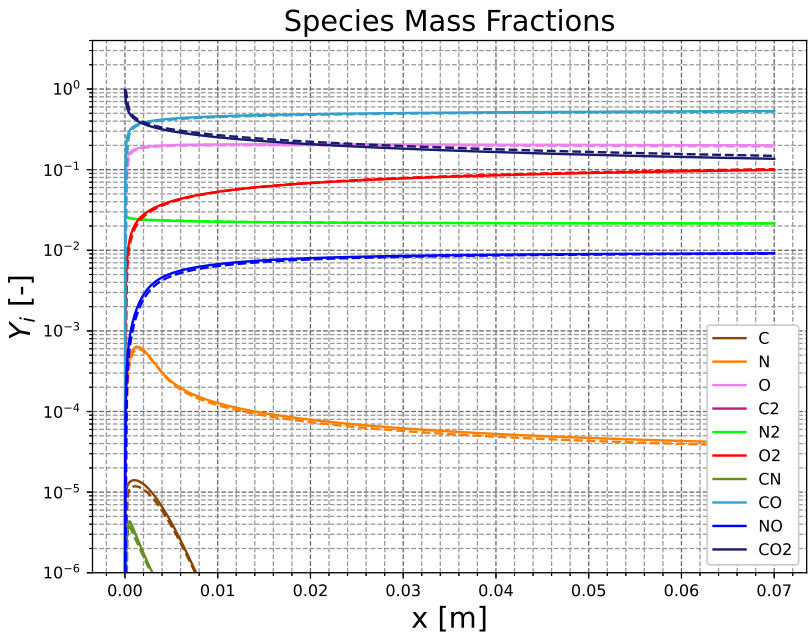
10 species	
Variable	Value
U	231 [m/s]
T	3433 [K]
P	21679 [Pa]

The equilibrium values are the same

Simplified Model



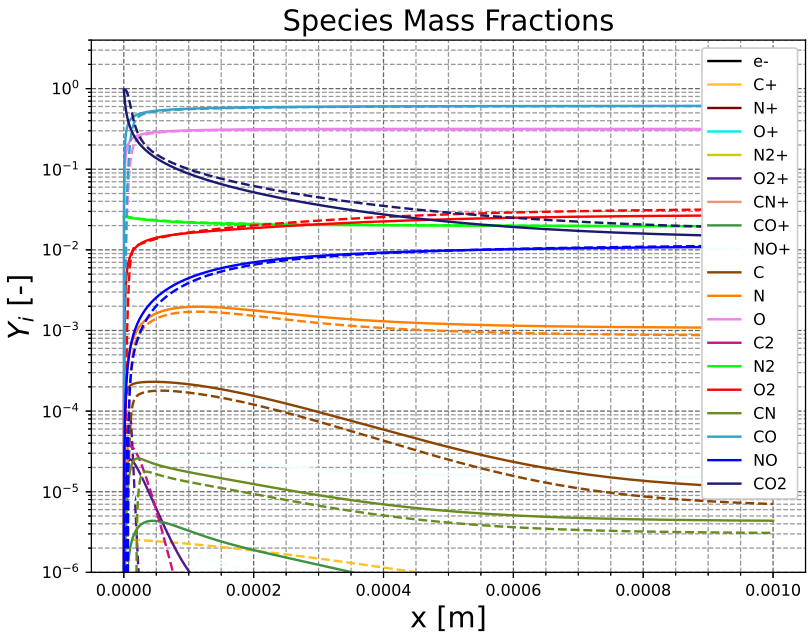
(a) 19 Species Model



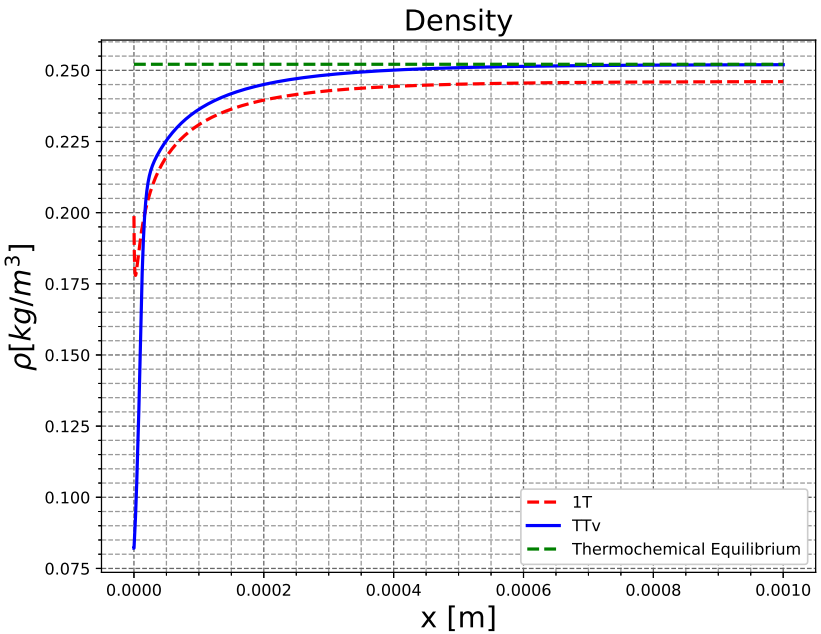
(b) 10 Species Model

The plots are indeed identical, except at the beginning.

Case 2, Part 1

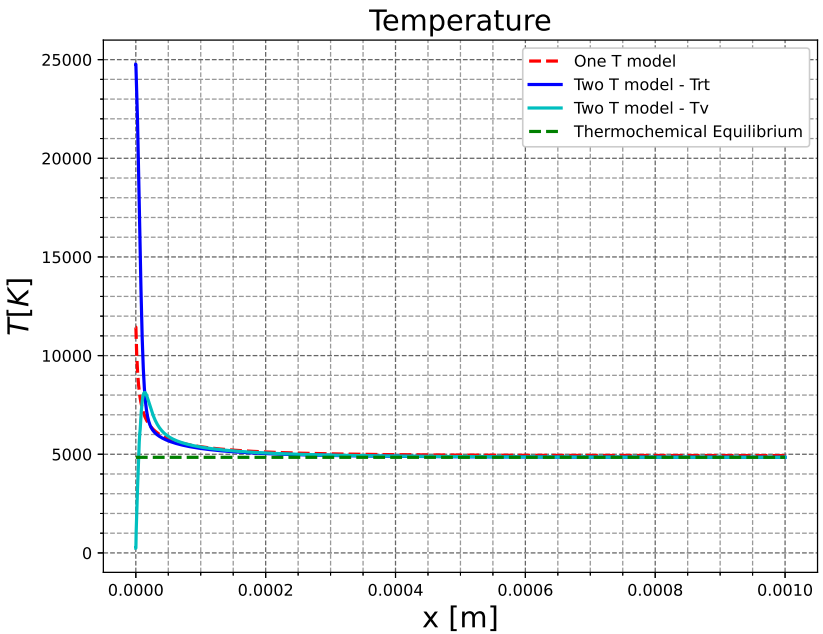


(a) Species

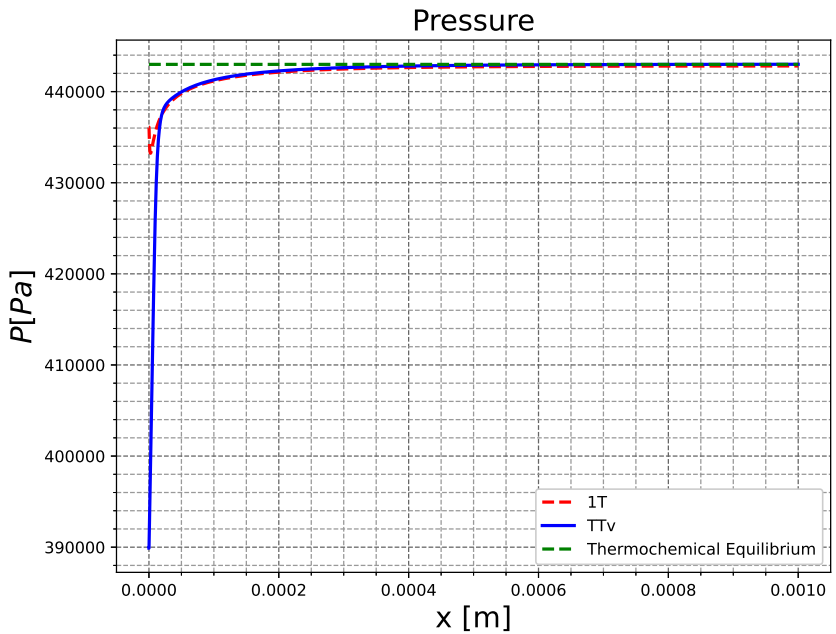


(b) Density

Case 2, Part 2



(a) Temperatures



(b) Pressure

Case 2, comments

Post Shock	
Variable	Value
U	404 [m/s]
T	11443 [K]
P	436105 [Pa]

Equilibrium	
Variable	Value
U	318 [m/s]
T	4845 [K]
P	442988 [Pa]
ν	$3.52 \cdot 10^6$ [1/s]

1. The flow is still in thermodynamic equilibrium the majority of the relaxation region.
2. The 2-Temperature model is still better at predicting equilibrium.
3. The flow is more reactive. Equilibrium is reached faster.
4. CN and NO+ are now present is the mixture.