Computation of Approximate Stagnation Point Heat Flux in Hypersonic Flow at Any Mach Number and Altitude: A Python-Based Numerical Approach

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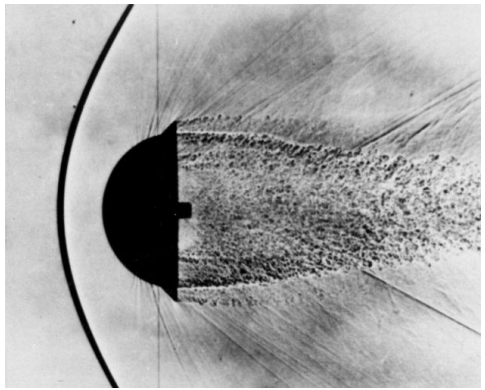
Intro/Background/Purpose

- Hypersonic flow regimes present unique challenges for flight systems: reentry crafts, hypersonic vehicles
  - Extreme temperatures, pressures, heat loads
    - Careful materials selection, thermal & structures tightly coupled, crucial for success of mission
    - Understanding heat rates, total heat load → TPS sizing → mass budgets
  - Variations in geometry cause a large effect on these design parameters
    - Blunt body vs. sharp leading edge
    - Blunt body detached the shock wave, decreases temperature gradients
- For conceptual design and analysis of reentry systems, can model the windward side of the vehicle as sphere with radius Rn
- Blunter body = stronger shock → better energy dissipation



How can we quickly model our blunt body?

- Analytical solutions for hypersonic flow are elusive
- Easily accessible shock relations for supersonic flow do not hold at M>>1
- Air at high temperatures: molecular dissociation and ionization become significant
  - Chemical reactions and equilibrium states must be computed to more accurately model the flow downstream of the hypersonic show wave
- Understanding flow properties downstream of the shock can help predict approximate stagnation point heating
- Approximation methods exist, but require boundary layer edge conditions, to find these, the downstream-shock conditions are required

Purpose

- Approximation methods such as Fay-Riddel Method - derived from boundary layer and stagnation point theories. Greatly simplify the problem, but..
- Many quantities still unknown - properties at the boundary layer edge.
- As a student, high fidelity CFD tools are not readily accessible, nor are they the best tool for the job - conceptual design, preliminary design
- The purpose of this tool is to provide a fast, low compute power hypersonic normal shock wave flow properties calculator that approximates stagnation point heating for a blunt body (sphere) with some nose cone radius R_n

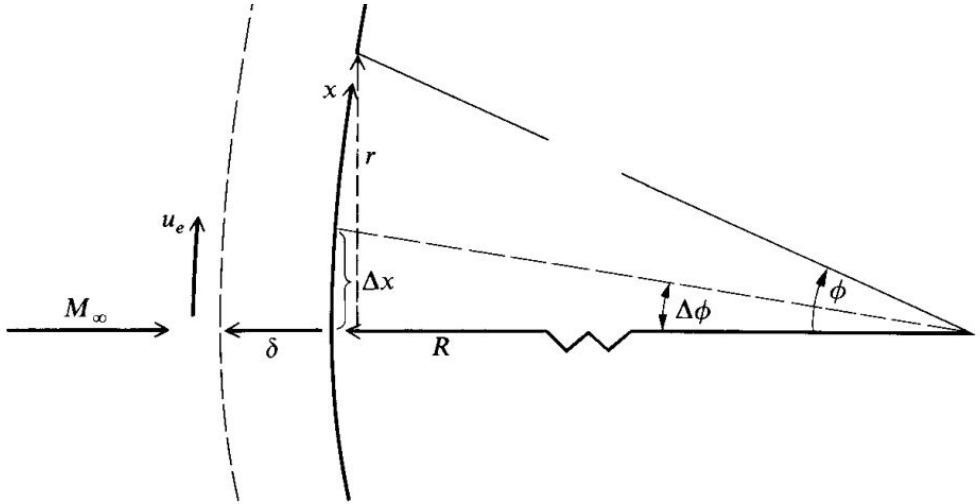
Laminar Boundary Stagnation Point heating

$$q_w = 0.763\, Pr^{-0.6}(\rho_e \mu_e)^{1/2} \sqrt{\frac{du_e}{dx}}\,(h_{aw} - h_w)$$

Van Driest, E. R., "The Problem of Aerodynamic Heating,"

2D Flow

Result very similar to Fay Riddler Method



How to find downstream properties?

$$q_w = 0.763\, Pr^{-0.6}(\rho_e \mu_e)^{1/2} \sqrt{\frac{du_e}{dx}}(h_{aw} - h_w)$$

$$\frac{du_e}{dx} = \frac{1}{R}\sqrt{\frac{2(p_e - p_\infty)}{\rho_e}}$$

$$h_{aw} = h_e + r(h_0 - h_e)$$

Can find boundary layer edge conditions using numerical solver.

Physics, assumptions for solver

- Bow shock approximated as normal shock wave
- Laminar Compressible boundary layer at stagnation point
- Nonisentropic process
- Adiabatic across shock wave, conservation of total temperature
- Implementing chemical equilibrium chemistry allowing for infinite time for gas to reach equilibrium
- Adiabatic wall, wall temperature constant
- Air made up of N_2 and O_2

Governing Equations

Conservation of Mass

$$\rho_1 u_1 = \rho_2 u_2$$

Conservation of Momentum

$$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2$$

Conservation of Energy

$$h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2}$$

Solve for downstream conditions as function of a thermodynamic ratio, in this case the density ratio

$$u_2 = \frac{\rho_1}{\rho_2} u_1$$

$$p_2 = p_1 + \rho_1 u_1^2 \left(1 - \frac{\rho_1}{\rho_2}\right)$$

$$h_2 = h_1 + \frac{u_1^2}{2}\left(1 - \left(\frac{\rho_1}{\rho_2}\right)^2\right)$$

Governing Equations

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Conservation of Momentum

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Conservation of Energy

$$h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2}$$

Using variable *x*, we now have:

$$T(x) = xT_1 + x\frac{u_1^2}{R}(1-x)$$

$$p_2(x) = p_1 + \rho_1 u_1^2 (1-x)$$

$$h_2(x) = h_1 + \frac{1}{2}u_1^2\left(1-x^2\right)$$

How to solve for x?

- Given ***x*** is the ratio of density upstream to downstream of the shock, if we can find a solution for ρ_1/ρ_2 the rest of the thermodynamic values can be computed
- But first: reactive chemistry due to high temperatures!
- Knowing any of the variables on the right, we can uniquely define the chemistry composition
- Let's assume air is made of N_2 and O_2

Variable	Useful Definitions
Partial Pressures (p_i)	$p_i V = \mathcal{N}_i \mathcal{R} T$
Concentrations (C_i)	$C_i = \frac{p_i}{\mathcal{R}T}$
Mole-Mass Ratio (η_i)	$\eta_i = \frac{p_i \nu_i}{\mathcal{R}T}$
Mole Fraction (X_i)	$X_i \equiv \frac{p_i}{p} = \frac{\mathcal{N}_i}{\mathcal{N}}$
Mass Fraction (c_i)	$c_i = \frac{\rho_i}{\rho}$

$$\sum_i p_i = p \qquad R = \sum_i c_i R_i$$

$$\sum_i X_i = 1$$

$$\mathcal{M} = \frac{1}{\sum_i c_i / \mathcal{M}_i} = \sum_i X_i \mathcal{M}_i$$

Reactions occurring in this model

- Thermally perfect gas
- Enthalpy and Energy functions of ***T***
- Enthalpy/internal energy functions of h_i and e_i (each species of gas *i)*

Where vi is the stoichiometric mole number associated with species

$$O_2 \rightleftarrows 2O$$

$$N_2 \rightleftarrows 2N$$

$$NO \rightleftarrows N + O$$

$$NO \rightleftarrows NO + +e^-$$

Gibbs Free Energy

Set Gibbs free energy to zero (equilibrium)

$$\sum_i G_i \mathcal{N}_i = \sum_i \upsilon_i G_i = 0$$

$\boldsymbol{\nu}_i$ is the stoichiometric mole number associated with species

Knowing equilibrium constant $\mathbf{K_P}$ at any temperature we can solve for $\mathbf{p_i}$

$$\prod_i p_i^{\nu_i} = \exp\left(-\sum_i \nu_i \frac{G_i^{p_i=1}}{\mathcal{R}T}\right)$$

Knowing $\mathbf{p_i}$ (or mole fraction, etc) we know the unique chemical composition of the equilibrated gas

$$\prod_i p_i^{\nu_i} = K_p(T)$$

Gathering thermodynamic data

Used data found in: McBride, B. J., Heimmel, S., Ehlers, J. G., and Gordon, S., *Thermodynamic Properties to 6000 K for 210 Substances involving the first 18 elements*, SP-3001, National Aeronautics and Space Administration (NASA), 1963.

- **H(T), S(T)** → can find $K_P(T)$
- Curve fit this data
- Data only provided up to 6000K (discussion on this later)

$$K_p = e^{-\Delta G^{P=1}/\mathscr{R}T}$$

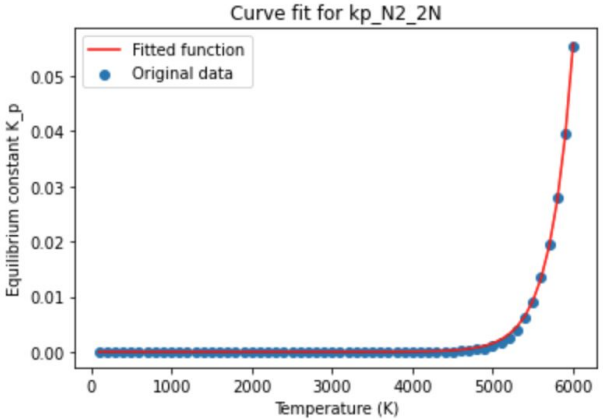
Kp Curve fits

Used python: **scipy.optimize import curve_fit**

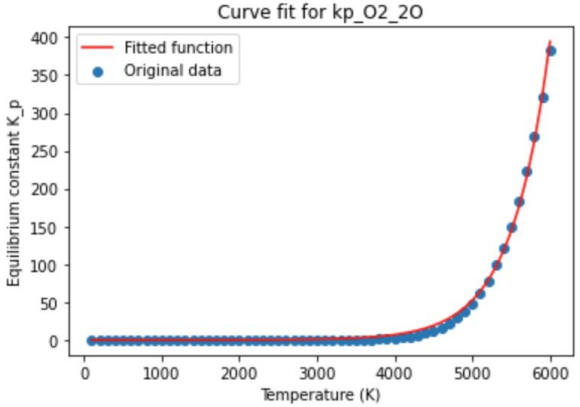
Function: $K_P(T) = A*\exp(B*T) + C$

Fitted $K_P(T)$ for the reaction data available for $N_2 \rightarrow 2N$, $O_2 \rightarrow 2O$, $NO \rightarrow N + O$

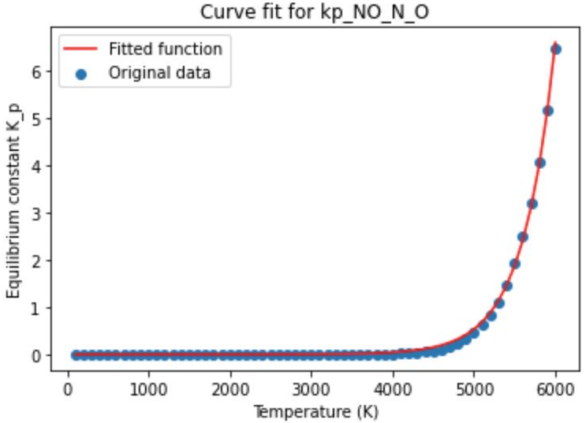
```
A = 3.7223207139967967e-11
B = 21.129359615728184
C = 3.4149407984854826e-44
```




```
A = 0.0026299017557883733
B = 11.917922993490821
C = 5.968074569479879e-18
```




```
A = 2.337861417819774e-06
B = 14.851517292200048
C = 6.669597784777172e-35
```



Knowing Kp for given T gives…

4 equations, 7 unknowns →

$$\frac{X_O^2}{X_{O_2}} = \frac{1}{\rho} K_{p_1}$$

$$\frac{X_N^2}{X_{N_2}} = \frac{1}{\rho} K_{p_2}$$

$$\frac{X_N X_O}{X_{NO}} = \frac{1}{\rho} K_{p_3}$$

$$\frac{X_{NO^+} + X_{e^-}}{X_{NO}} = \frac{1}{\rho} K_{p_4}$$

Need to introduce 3 more equations (conservation of atomic nitrogen, oxygen, charge)

$$2X_{O_2} + X_O + X_{NO} + X_{NO+} = 2X^*_{O_2}$$

$$2X_{N_2} + X_N + X_{NO} + X_{NO+} = 2X^*_{N_2}$$

$$X_{NO+} - X_{e^-} = 0$$

Plug Kp equations into conservation of atomic nitrogen and oxygen equations to produce:

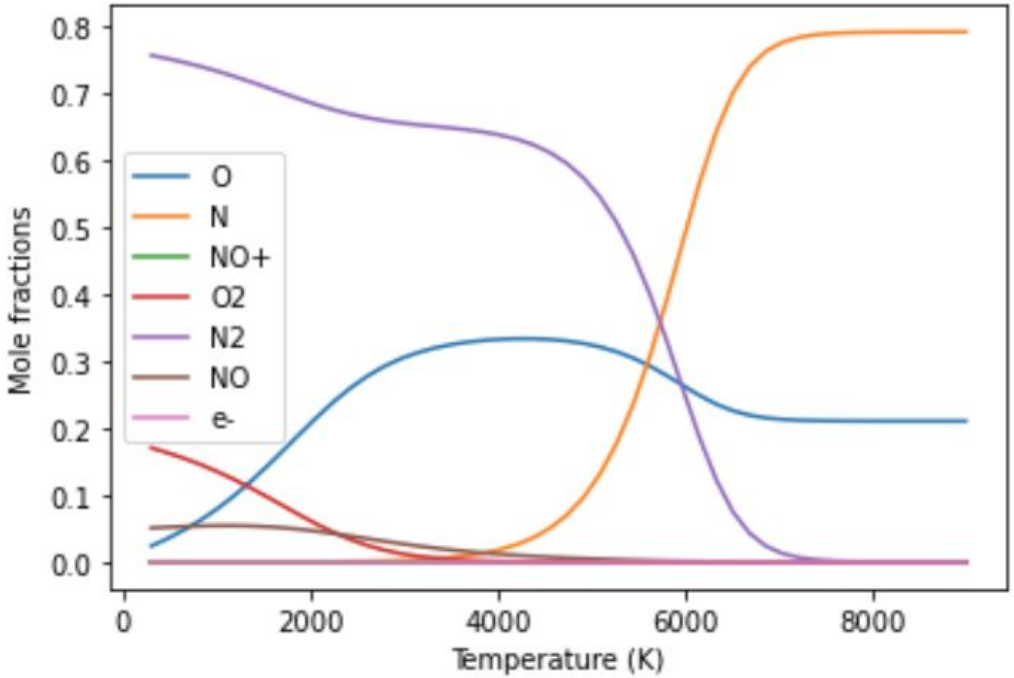
$$\left(\frac{2\rho}{K_{p1}}\right) X_O^2 + \left(1 - \frac{\rho X_N}{K_{p3}}\right) X_O + \left(-2X^*_{O_2} + X_{NO+}\right) = 0$$

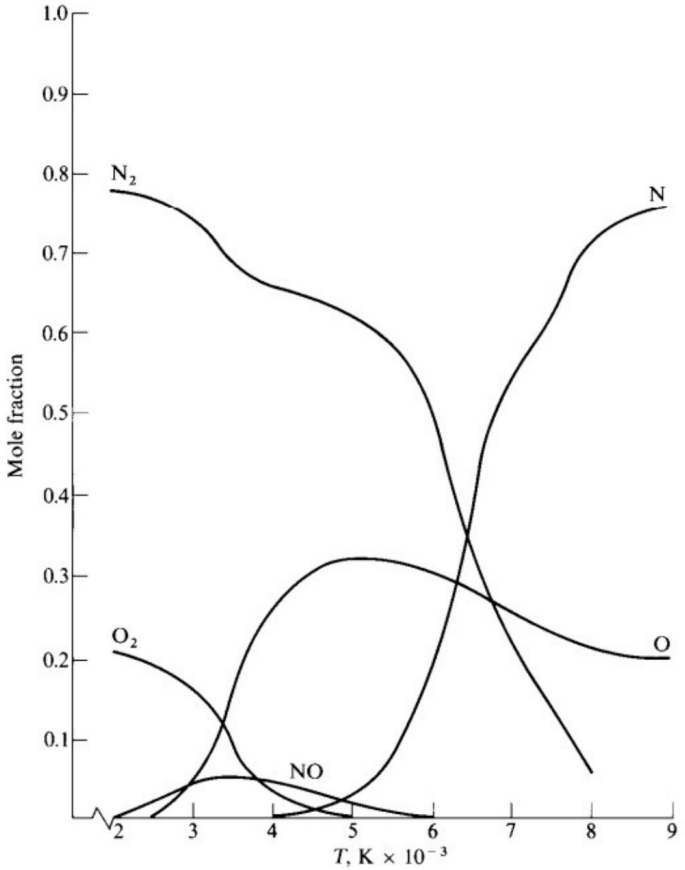
$$\left(\frac{2\rho}{K_{p2}}\right) X_N^2 + \left(1 - \frac{\rho X_N}{K_{p3}}\right) X_O + \left(-2X^*_{N_2} + X_{NO+}\right) = 0$$

Finding positive root with initial values for $X^*_{N2,O2}$ we can get values for X_O and X_N

Results of Chemistry Solver

Tested at 1atm constant pressure. Results good but slightly off, this is most likely due to the curve fits on the thermodynamics data for each reaction, species.





Anderson “Hypersonic and High Temperature Gas Dynamics”

Knowing solution for X_O and X_N gives …

So knowing mole fractions, (or partial pressures, other intensive variables) we know the properties of the gas mixture

Knowing a value for ρ (or in our case ρ_2) can be plugged into the conservation equations that were derived earlier (functions of x where x = ρ_1/ρ_2

$$\eta_i = \frac{X_i}{\sum X_i}$$

$$\mathscr{M}_{\text{mixture}} = \sum (\eta_i \cdot \mathscr{M}_i)$$

$$\rho = \frac{P\mathscr{M}_{\text{mixture}}}{\mathscr{R}T}$$

How to converge a solution on x?

The total enthalpy downstream of the shock is equal to the sensible enthalpy plus the enthalpy of formation for each species plus the $(\frac{1}{2})u^2$ contribution, weighted by each species mole fraction η_i

Need to know sensible enthalpy of each gas species, enthalpy of formation for each gas species

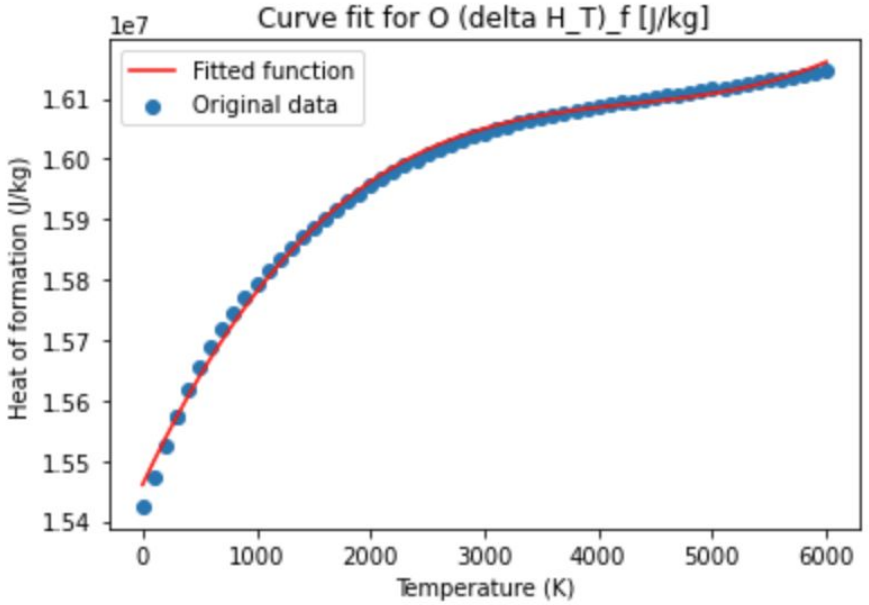
$$\underbrace{h_2 - h_1}_{\text{Change in enthalpy}} = \underbrace{(h_{\text{sens}_2} - h_{\text{sens}_1})}_{\text{Change in sensible enthalpy}} + \underbrace{(e_{0_2} - e_{0_1})}_{\text{Change in zero-point energy}}$$

Change in zero-point energy is the standard heat of formation for that gas species, data fitted as function of Temperature

Heat of Formation Curve fits (data extracted from same thermodynamic properties table from before)

Data for $(\Delta H_f)_i^o$ fit using 3rd degree polynomial

```
Processing y_column: O (delta H_T)_f [J/kg]
[ 6.90561935e-06 -8.88160231e-02  4.01032307e+02  1.54605630e+07]
```



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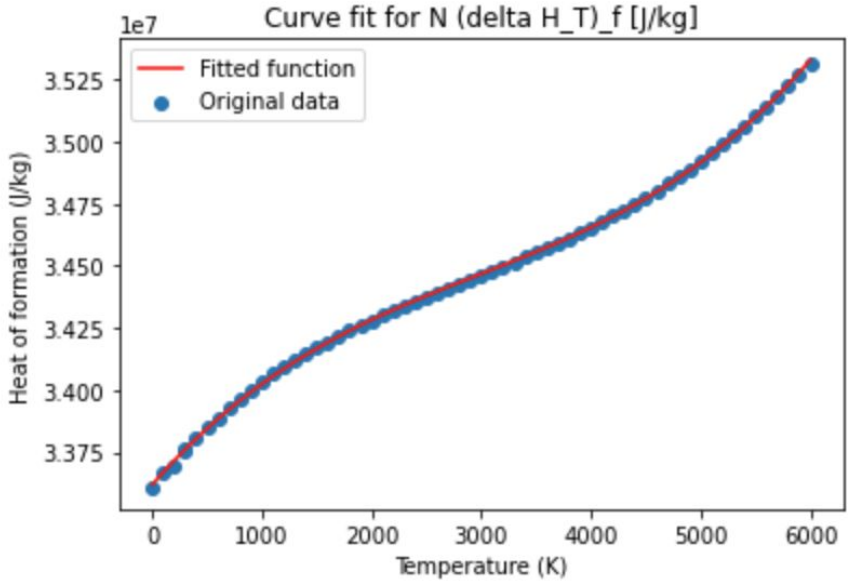
Heat of Formation Curve fits (data extracted from same thermodynamic properties table from before)

Data for $(\Delta H_f)_i^o$ fit using 3rd degree polynomial

```
Processing y_column: N (delta H_T)_f [J/kg]
[ 1.23516218e-05 -1.10465389e-01  5.03010078e+02  3.36201583e+07]
```



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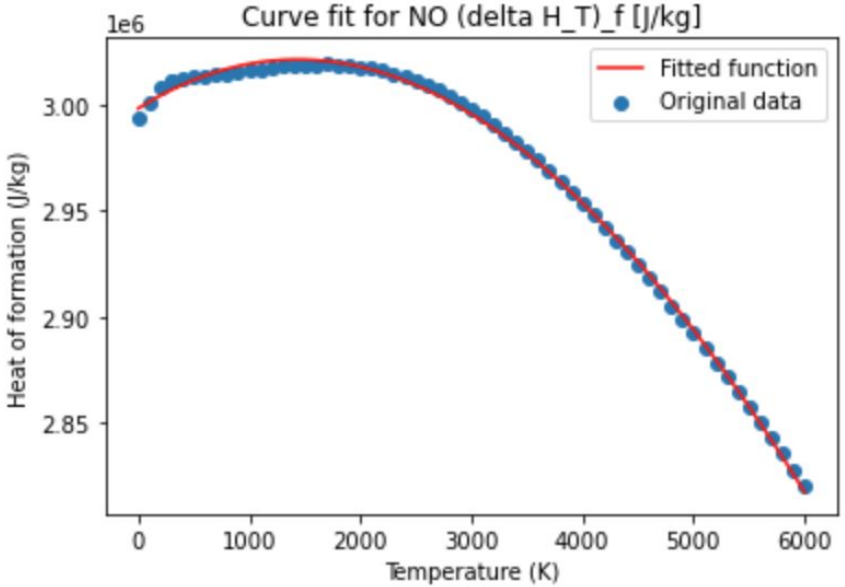
Heat of Formation Curve fits (data extracted from same thermodynamic properties table from before)

Data for $(\Delta H_f)_i^o$ fit using 3rd degree polynomial

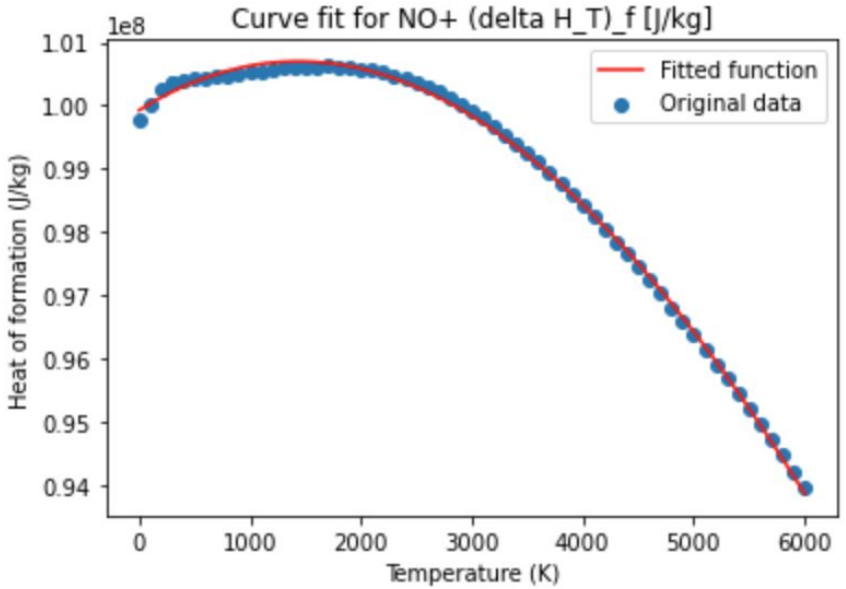
```
Processing y_column: NO (delta H_T)_f [J/kg]
[ 2.44289625e-07 -1.19896083e-02  3.28647520e+01  2.99857388e+06]
```



Heat of Formation Curve fits (data extracted from same thermodynamic properties table from before)

Data for $(\Delta H_f)_i^o$ fit using 3rd degree polynomial

```
Processing y_column: NO+ (delta H_T)_f [J/kg]
[ 8.14084477e-06 -3.99547317e-01  1.09520028e+03  9.99258155e+07]
```



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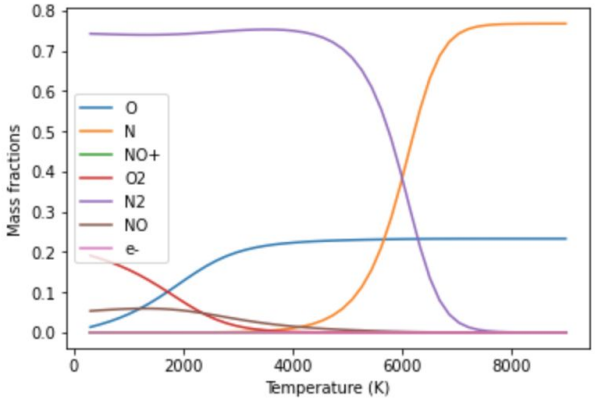
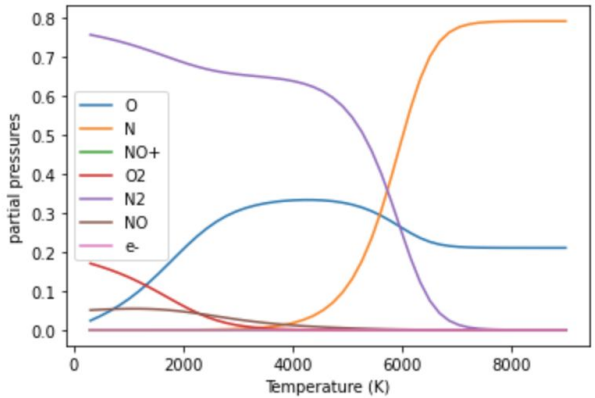
Chemical Composition solver (inputs **T, P)**

- Average 7 iterations per solution
- Example, 300K → 6000K, 50 cases
  Total compute time 1.10 seconds
- Example output of Solve_chemistry(T,P) function






```
1 Solve_chemistry(3000,1)
```

```
0.11768292682926829
CONVERGED
Current T =  3000
Current P =  101325
{'O': 0.3603640152717528, 'N': 0.003064821075105413, 'NO+': 1.5635618046626823e-10, 'O2': 0.013991351215017602, 'N2': 0.7726
409313493235, 'NO': 0.03165331606989169, 'e-': 1.5635618046626823e-10}
iterations to converge =  6
sum of mole/mass ratios =  1.1817144352938036
density of mixture =  0.09917379762257214 kg/m^3
Mixture R constant: R_specific =  340.56374576416084
Molar Mass of Mixture =  0.02441384352683782  kg/mol

(array([3.60364015e-01, 3.06482108e-03, 1.56356180e-10, 1.39913512e-02,
        7.72640931e-01, 3.16533161e-02, 1.56356180e-10]),
 array([3.04950168e-01, 2.59353782e-03, 1.32312999e-10, 1.18398750e-02,
        6.53830493e-01, 2.67859266e-02, 1.32312999e-10]),
 array([1.99841444e-01, 1.48799529e-03, 1.62620730e-10, 1.55183182e-02,
        7.50230708e-01, 3.29215345e-02, 0.00000000e+00]),
 array([3.04950168e-01, 2.59353782e-03, 1.32312999e-10, 1.18398750e-02,
        6.53830493e-01, 2.67859266e-02, 1.32312999e-10]),
 340.56374576416084,
 0.02441384352683782,
 0.09917379762257214)
```

Use Chemistry Solver inside static enthalpy computation

$$h_{\text{mixture}} = \sum_i \eta_i (H - E_0)_i + \sum_i \eta_i \left(\Delta H_f\right)_i^{\circ}$$

Where:

$$(H - E_0)_i = \frac{3}{2}\mathcal{R}T + \mathcal{R}T + \frac{h\nu/kT}{e^{h\nu/kT} - 1}\mathcal{R}T + \mathcal{R}T = \frac{7}{2}\mathcal{R}T + \frac{h\nu/kT}{e^{h\nu/kT} - 1}\mathcal{R}T$$

$$h_t = h_{\text{mixture}} + \frac{1}{2}u^2$$

Use Chemistry Solver inside static enthalpy computation

T = 3000K,
P = 1 atm

```
1 Static_Enthalpy_mixture(3000,1)
```

```
0.11768292682926829
CONVERGED
Current T =  3000 K
Current P =  101325 Pa
{'O': 0.3603640152717528, 'N': 0.003064821075105413, 'NO+': 1.5635618046626823e-10, 'O2': 0.013991351215017602, 'N2': 0.7726
409313493235, 'NO': 0.03165331606989169, 'e-': 1.5635618046626823e-10}
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```

How the solver works

1. **Initialization:**
   a. Compute free stream conditions: enthalpy, density, velocity.

2. **Define Residual Function:**
   a. Calculate difference between computed and thermally perfect enthalpy downstream. (use chemical iterative solver)

3. **Iterative Solution:**
   a. Secant method converges solution for density ratio (x)

4. **Compute Final Properties:**
   a. Determine downstream temperature, density, pressure, and other properties.

5. **Return:**
   a. Density ratio, enthalpy difference (for convergence check), and downstream properties.

Residual Function

$$T(x) = xT_1 + x\frac{u_1^2}{R}(1-x)$$

$$p_2(x) = p_1 + \rho_1 u_1^2 (1-x)$$

$$h_2(x) = h_1 + \frac{1}{2}u_1^2\left(1-x^2\right)$$

Define residual function f(x)

Input: **x (initial guess)**

Return: **residual** (h2 - h2_thermally_perfect) where h2 is computed using conservation of equation and knowing initial h1 and velocity u1, and an initial guess for x. **NEW VALUES FOR T2 and P2 generated → chemistry solver → $h_{mixture}$**

$h_2(x)$ - $h_{2\_mixture}$= residual. Minimize residual using secant method

$$h_{\text{mixture}} = \sum_i \eta_i (H - E_0)_i + \sum_i \eta_i \left(\Delta H_f\right)_i^\circ$$

Secant Method

$$x_2 = x_1 - f(x_1)\frac{x_1 - x_0}{f(x_1) - f(x_0)},$$

$$x_3 = x_2 - f(x_2)\frac{x_2 - x_1}{f(x_2) - f(x_1)},$$

$$\vdots$$

$$x_n = x_{n-1} - f(x_{n-1})\frac{x_{n-1} - x_{n-2}}{f(x_{n-1}) - f(x_{n-2})}.$$

Solver Example

INPUTS:

Parameter	Value
T1	288
Mach_number	15
p1	10132.5
gamma1	1.4

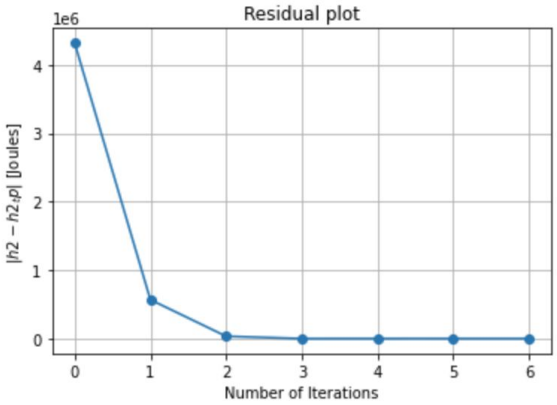
Outputs:

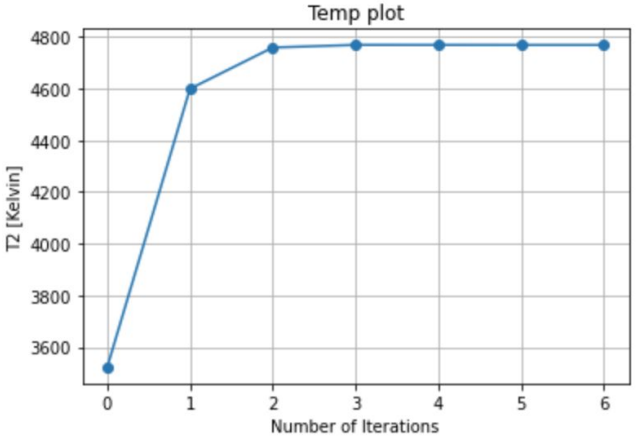
```
sum of mole/mass ratios =  1.2146732943393905
density of mixture =  1.6362746208853745 kg/m^3
Mixture R constant: R_specific =  350.06230446033226
Molar Mass of Mixture =  0.023751400519452858  kg/mol
Density downstream =  1.636274620886198 kg/m^3
____ FLOW SOLVER RESULTS ____
T2 =  5247.621988057359 K
P2 =  3005827.7180780955 Pa
h2 =  16558391.754739717 J/kg
h2tp =  16560081.357987924 J/kg
 _________________
----------
Secant method converged solution:  0.061422
----------
Difference between built in and secant solver =  1.9999999999950613e-06
```

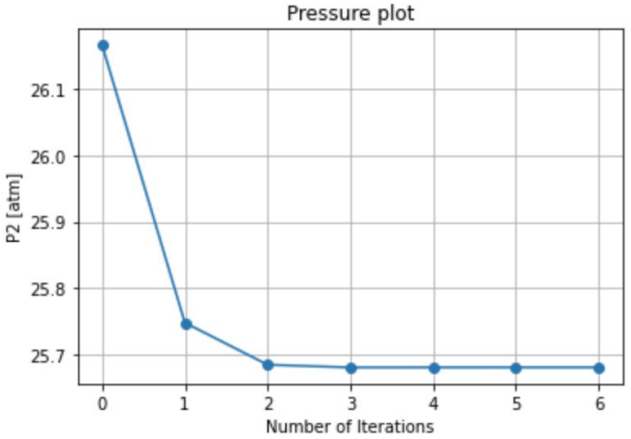
Solver Example

INPUTS:

Parameter	Value
T1	288
Mach_number	15
p1	10132.5
gamma1	1.4





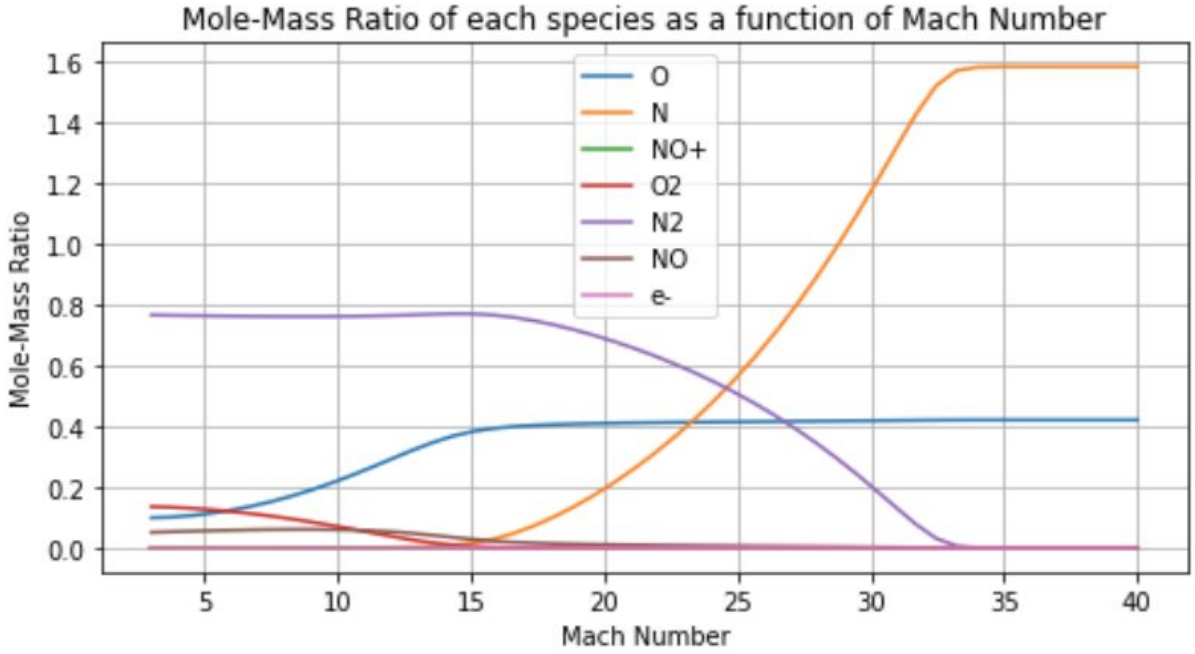


Mole Mass Ratios of gas species vs. Mach

Altitude = 25,000 meters

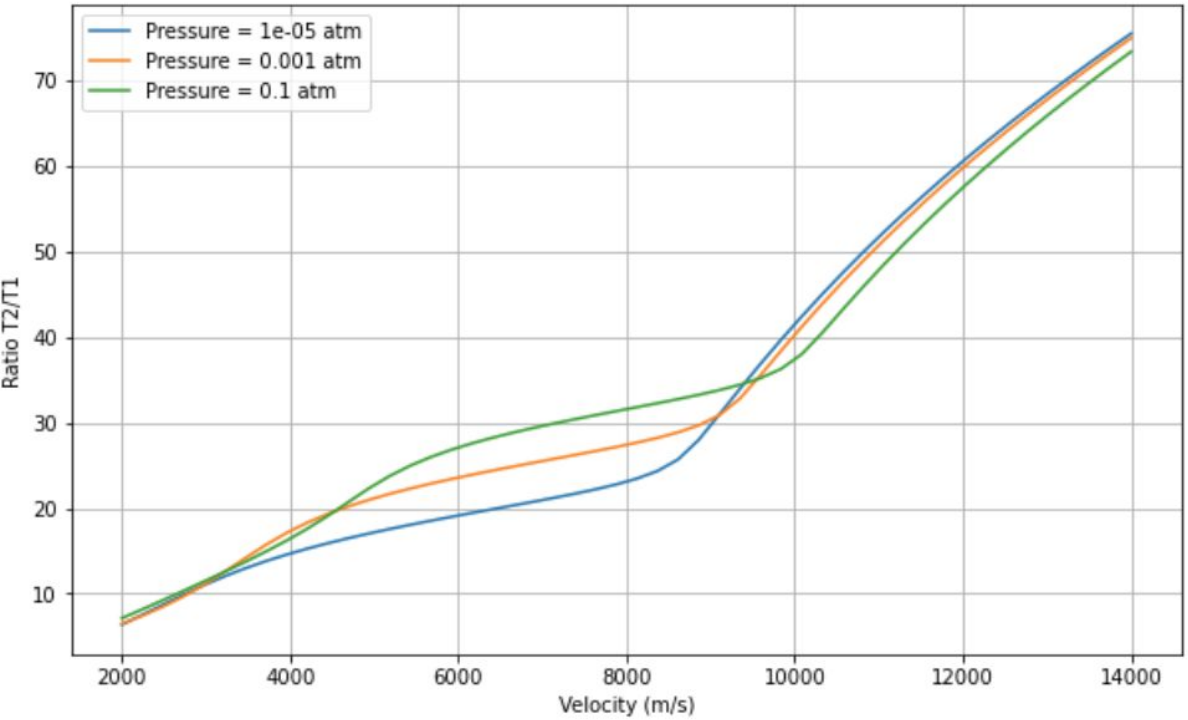
Mach varied from 3 → 40

T1, P1 and ρ_1 held constant, calculated using atm1976 function in code that takes in argument (h = altitude meters) returns T, P, ρ

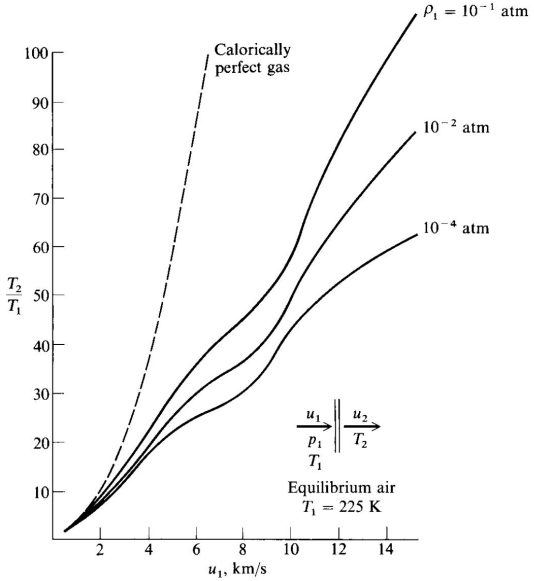


T2/T1 vs V_∞ with varied freestream atmospheric pressure

Comparison to plot in Anderson textbook



608 HYPERSONIC AND HIGH-TEMPERATURE GAS DYNAMICS



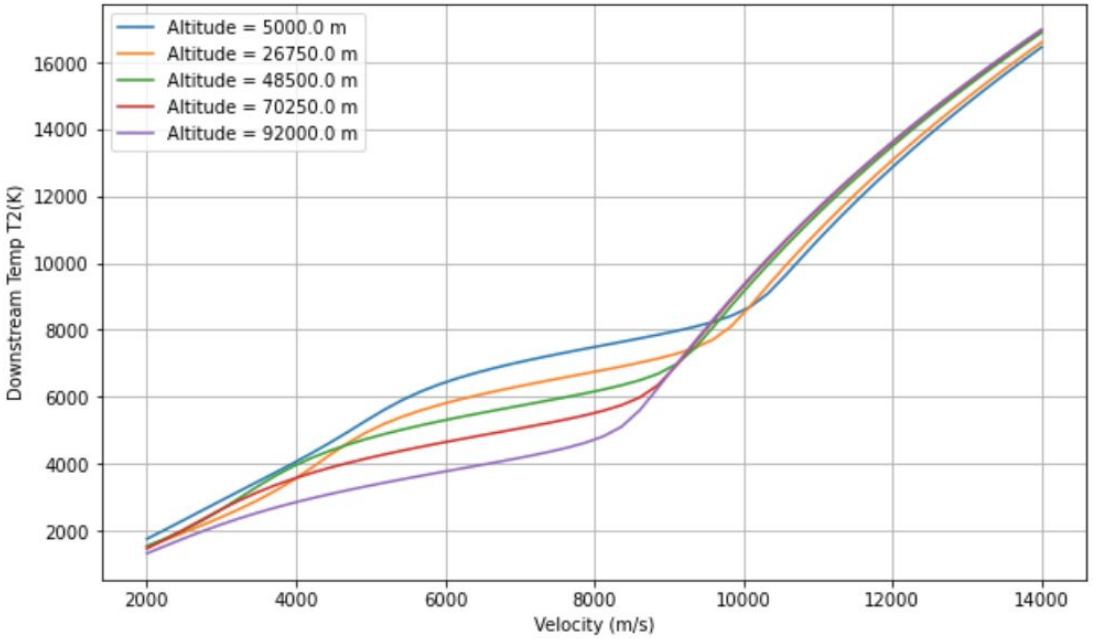
T2 vs free stream velocity at varying atmospheric altitude

Here is the code used as the input for the calculator for example

Mach_numbers = np.linspace(3, 27, 30)

altitudes = np.linspace(5000,92000,5)

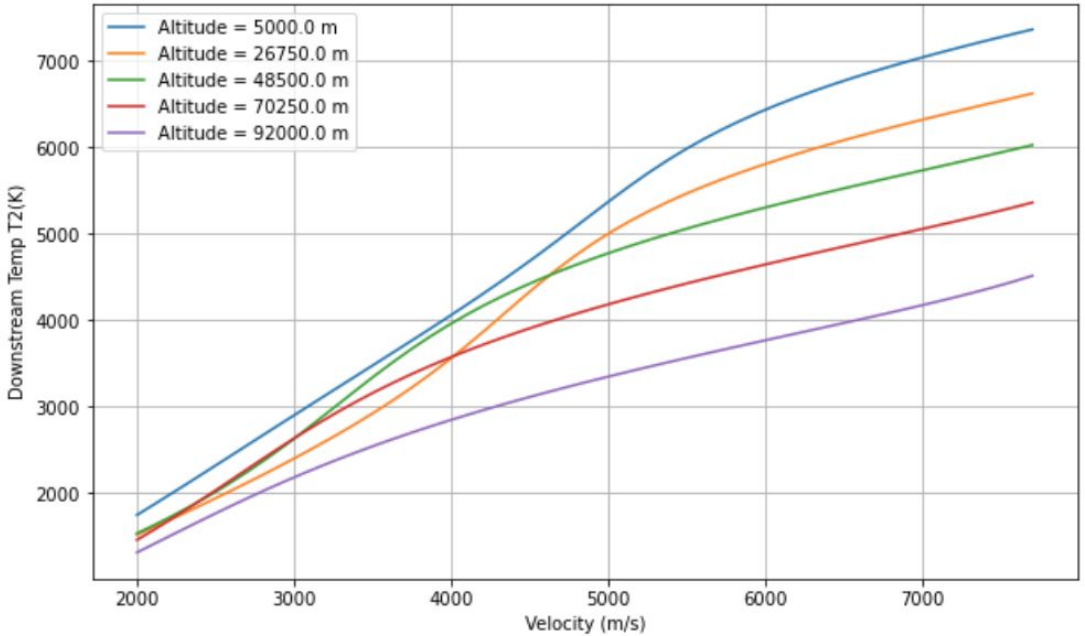
The altitudes feed into atm1976 function to produce freestream conditions

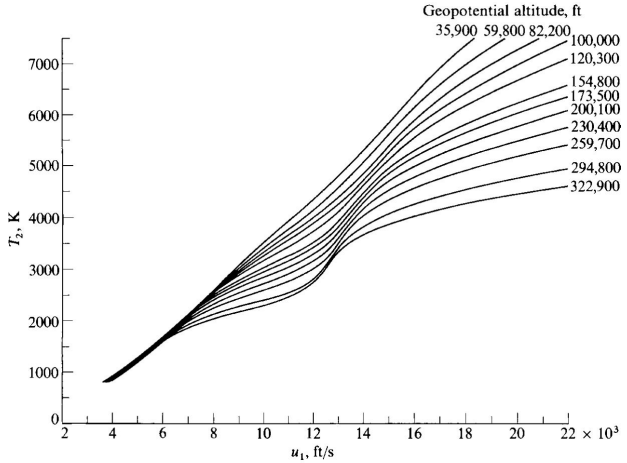


T2 vs free stream velocity at varying atmospheric altitude

Better trend up until 7000-8000 K (due to Kp and delta H curve fits?)

20,000 ft/s = 6096 m/s





Anderson “Hypersonic and High-Temperature and Gas Dynamics”

August 24, 2023

Heat Flux

Fay - Riddler Method/ Van Driest method gives the following solution for sphere with compressible laminar boundary layer behind hypersonic normal shock

$$q_w = 0.763 P_r^{-0.6} (\rho_e \mu_e)^{1/2} \sqrt{\frac{du_e}{dx}} (h_{aw} - h_w)$$

Where we can plug in our numerically computed values where edge conditions are assumed to be equal to downstream (subscript 2) conditions

$$\frac{du_e}{dx} = \frac{1}{R} \sqrt{\frac{2(p_e - p_\infty)}{\rho_e}}$$

$$h_{aw} = h_e + r(h_0 - h_e)$$

In the code, the adiabatic wall temperature can be set by the user.

Tw = constant set by user

R_n = set by user (radius of spherical blunt body in meters)

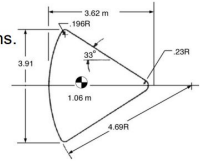
Results, comparisons

MISSION: APOLLO AS-501 (APOLLO-4)
PLANET: EARTH
LAUNCH: NOV 9, 1967
ENTRY: NOV 9, 1967

MISSION DESCRIPTION: Test of Saturn V launch vehicle and overall reentry operations.

INSTRUMENTATION: 17 pressure sensors all worked, and 23 calorimeters worked initially. Radiometer functioned well.

NOTES: TPS thickness: Ablator = 4.32 cm, braised stainless-steel substructure (PH 15-7 MO) = 5.08 cm. Insulation: (TG-15,000) = 2.03 cm, aluminum honeycomb (2014-T6 and 5052-H39) = 3.81 cm Manufacturer: AVCO Corp.



Trajectory		Geometry		Aero/thermal		TPS		Parachutes	
Entry angle	Inertial -6.93 Relative-7.19° Entry altitude 121.92 km	**Shape**	Capsule: 33° cone	**Velocity at peak heat**	10.04 km/s	**Forebody material designation**	Avco 5026-39 HC	**Type**	(1) 2 conical ribbon drogue parachutes, (2) 3 ringshot pilot parachutes, (3) 3 ringsail main parachutes
Entry velocity: inertial & relative	Inertial: 11.14 km/s Relative: 10.73 km/s	**Nose radius**	4.66 m, 3 m effective	**Peak convective heating**	219 W/cm²	**Forebody thickness & mass**	TPS thickness: Ablator = 4.32 cm, braised stainless-steel substructure (PH 15-7 MO) = 5.08 cm	**Deployment method**	(1) mortar (2) drogue parachute (3) pilot parachute
Trim L/D (specify trim α)	0.37 < L/D < 0.44 24° < α <28°	**Base area**	12.08 m²	**Peak radiative heating**	317 W/cm²	**Ablating Ejected**	Ablated: yes Ejected: no	**Reference diameter / area**	(1) 4.9 m dia. (2) 2.2 m dia. (3) 25.5 m dia.
Control method	Roll modulation	**Vehicle mass**	5424.5 kg	**Integrated total heatload**	24122 J/cm²	**TPS integration method**	Honeycomb bonded to substructure; cells filled with ablative compound	**Deployment mach**	~0.7
Ballistic co-eff.	~340 kg/m²	**Payload mass**	N/A	**PH stag. pressure**	0.542 atm	**Aftbody material designation**		**Deployment dynamic pressure**	
Peak deceleration	8.79 g	**TPS mass fraction, inc.insul.**	13.7%	**Peak stag. heating rate**	527 W/cm² peak	**Aftbody thickness & mass**		**Parachute materials**	

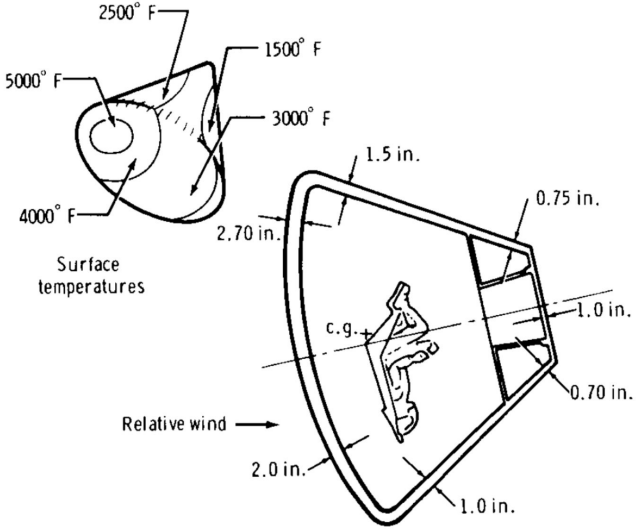


Figure 2.- Command module ablator thickness.

Results, Comparison

Compare to Apollo test data

Rn = 4.69, velocity = 10.4 km/s, Tw = 5000K

Peak stagnation (test data) = 527 W/cm^2

Calculator = 622 W/cm^2

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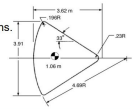

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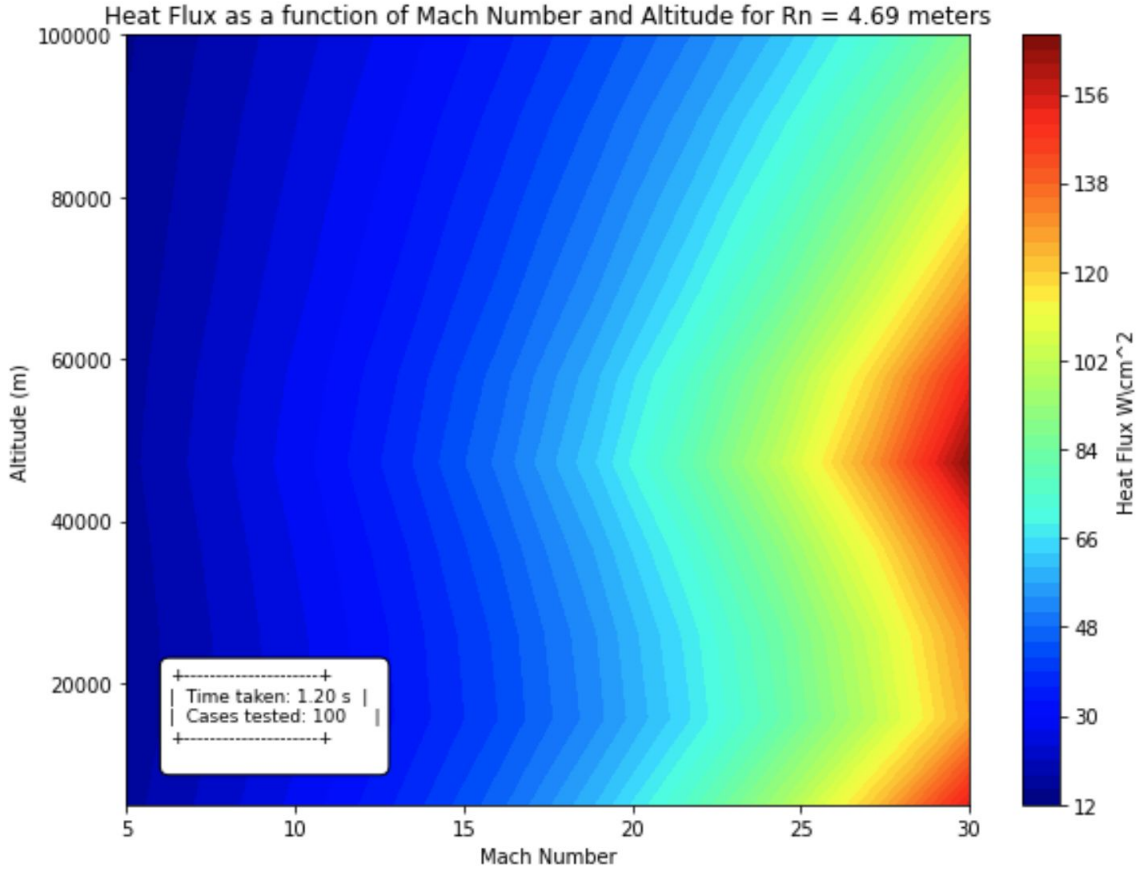
```
1  Heat_Flux_Solver_v3(70000,10400,4.69,5000)
 ____________________
-495.6553449332714
9293.500000301012
Density =  6.205854342383742 kg/m^3
16552468.804516856 Pa
163.36016584768672 atm
576.0577817483268
57413206.62320827
      converged: True
           flag: 'converged'
 function_calls: 32
     iterations: 31
           root: 0.02528428165547628
velocity edge 262.9565292169533
Dynamic Viscosity =  0.00013855777596535204
2496.250387576082
Velocity =  10400
HEAT RATE =  621.534199667807  W/cm^2

6215341.99667807
```

Results. Heat flux as function of altitude and Mach

Note, 100 test cases took 1.20seconds to complete.



SJSU SAN JOSÉ STATE UNIVERSITY

Contributions

- Provide students in engineering with an easy to access, easy to use tool to approximate hypersonic shock layer flow conditions and the stagnation point heating on a spherical blunt body nose cone
- Having preliminary values for temperature, pressure, density, heat rates can help determine preliminary TPS sizing, vehicle sizing, mass constraints, etc
- Allows to rapidly perform systems trade studies
- Open source with contribution welcome!

Future work

- Implement better data and thus curve fits for chemistry reactions
- Clean up bugs
- Improve user experience, usability
- Convert functions into classes and create callable python library
- Add shear stress calculations
- Improve calculations by computing gamma(T) downstream of shock
- Push revised version to github for public access
  https://github.com/antonkulinich/Reentry-Peak-Heating-Python-Anton-Kulinich-TFWS

Acknowledgments

Dr. Yawo Ezunkpe - Hypersonics Professor

Jesse Franklin and Javaneh Keikha - hypersonics class mates