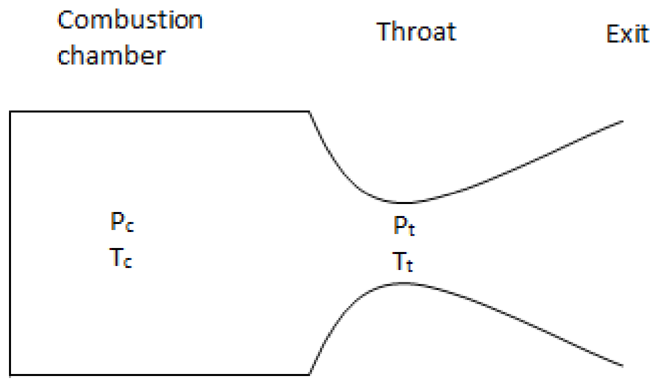
Performance of a Monomethylhydrazine-Dinotrogen Tetroxide Rocket

Liquid Monomethylhydrazine (CH_6N_2) and Dinitrogen Tetroxide (N_2O_4) are burned in the combustion chamber of a rocket engine. The oxidizer to fuel ratio is 2.5 (i.e. in the ratio of 1 mole of CH_6N_2 to 1.2518 moles of N_2O_4)



This application will calculate

- the adiabatic flame temperature and composition of the combustion products (i.e. in the combustion chamber)
- the pressures and temperatures in the throat and exit
- and the theoretical rocket performance, including the ideal specific impulse, characteristic velocity, and sonic velocity.

Monomethylhydrazine and Dinitrogen Tetroxide are commonly used in spacecraft rocket engines as a fuel and oxidizer. The thrusters used by SpaceX's Dragon spacecraft, for example, use this combination.

Assumptions:
- The combustion chamber is large compared to the throat, hence an infinite area ratio
- The flow composition is "frozen" at the combustion chamber, i.e. the composition does not change through the nozzle expansion (i.e. reaction rate is slow compared to flowrate)
- The combustion products only contain CO, HNO, H_2O, NO_2, O, CO_2, HO_2, H_2O_2, N_2, OH, H, H_2, NO, N_2O and O_2. No other species are considered.

Ideal gas constant

$$R := 8.3144$$

Chamber pressure

$$P_c := 50.0\ \mathbf{bar}$$

Atmospheric pressure

$$P_a := 101325\ \mathbf{Pa}$$

Standard pressure

$$P_s := 1\ \mathbf{bar}$$

Molecular weights

$$\text{Property} := \text{ThermophysicalData:-Property}$$

$$mw_{C6HN2L} := \text{Property}(\text{"MolarMass"}, \text{"CH6N2(L)"}, \text{useunits}) = 46.072\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{N2O5L} := \text{Property}(\text{"MolarMass"}, \text{"N2O4(L)"}, \text{useunits}) = 92.011\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{CO} := \text{Property}(\text{"MolarMass"}, \text{"CO"}, \text{useunits}) = 28.010\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{HNO} := \text{Property}(\text{"MolarMass"}, \text{"HNO"}, \text{useunits}) = 31.014\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{H2O} := \text{Property}(\text{"MolarMass"}, \text{"H2O"}, \text{useunits}) = 18.015\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{NO2} := \text{Property}(\text{"MolarMass"}, \text{"NO2"}, \text{useunits}) = 46.006\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{O} := \text{Property}(\text{"MolarMass"}, \text{"O"}, \text{useunits}) = 15.999\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{CO2} := \text{Property}(\text{"MolarMass"}, \text{"CO2"}, \text{useunits}) = 44.010\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{HO2} := \text{Property}(\text{"MolarMass"}, \text{"HO2"}, \text{useunits}) = 33.007\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{H2O2} := \text{Property}(\text{"MolarMass"}, \text{"H2O2"}, \text{useunits}) = 34.015\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{N2} := -\text{Property}(\text{"MolarMass"}, \text{"N2"}, \text{useunits}) = -28.013\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{OH} := \text{Property}(\text{"MolarMass"}, \text{"OH"}, \text{useunits}) = 17.007\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{H} := \text{Property}(\text{"MolarMass"}, \text{"H"}, \text{useunits}) = 1.008\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{H2} := \text{Property}(\text{"MolarMass"}, \text{"H2"}, \text{useunits}) = 2.016\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$$mw_{NO} := \text{Property}(\text{"MolarMass"}, \text{"NO"}, \text{useunits}) = 30.006\ \frac{\mathbf{g}}{\mathbf{mol}}$$

$mw_{N2O} := Property("MolarMass", "N2O", useunits) = 44.013 \frac{g}{mol}$

$mw_{O2} := Property("MolarMass", "O2", useunits) = 31.999 \frac{g}{mol}$

Specific heat capacity at constant pressure

$Cp_{CO} := Property("Cpmolar", "CO", "temperature" = T)$

$Cp_{HNO} := Property("Cpmolar", "HNO", "temperature" = T)$

$Cp_{H2O} := Property("Cpmolar", "H2O", "temperature" = T)$

$Cp_{NO2} := Property("Cpmolar", "NO2", "temperature" = T)$

$Cp_{O} := Property("Cpmolar", "O", "temperature" = T)$

$Cp_{CO2} := Property("Cpmolar", "CO2", "temperature" = T)$

$Cp_{HO2} := Property("Cpmolar", "HO2", "temperature" = T)$

$Cp_{H2O2} := Property("Cpmolar", "H2O2", "temperature" = T)$

$Cp_{N2} := Property("Cpmolar", "N2", "temperature" = T)$

$Cp_{OH} := Property("Cpmolar", "OH", "temperature" = T)$

$Cp_{H} := Property("Cpmolar", "H", "temperature" = T)$

$Cp_{H2} := Property("Cpmolar", "H2", "temperature" = T)$

$Cp_{NO} := Property("Cpmolar", "NO", "temperature" = T)$

$Cp_{N2O} := Property("Cpmolar", "N2O", "temperature" = T)$

$Cp_{O2} := Property("Cpmolar", "O2", "temperature" = T)$

Enthalpies

$h_{CO} := Property("Hmolar", "CO", "temperature" = T)$

$h_{HNO} := Property("Hmolar", "HNO", "temperature" = T)$

$h_{H2O} := \text{Property}(\text{"Hmolar", "H2O", "temperature"} = T)$

$h_{NO2} := \text{Property}(\text{"Hmolar", "NO2", "temperature"} = T)$

$h_{O} := \text{Property}(\text{"Hmolar", "O", "temperature"} = T)$

$h_{CO2} := \text{Property}(\text{"Hmolar", "CO2", "temperature"} = T)$

$h_{HO2} := \text{Property}(\text{"Hmolar", "HO2", "temperature"} = T)$

$h_{H2O2} := \text{Property}(\text{"Hmolar", "H2O2", "temperature"} = T)$

$h_{N2} := \text{Property}(\text{"Hmolar", "N2", "temperature"} = T)$

$h_{OH} := \text{Property}(\text{"Hmolar", "OH", "temperature"} = T)$

$h_{H} := \text{Property}(\text{"Hmolar", "H", "temperature"} = T)$

$h_{H2} := \text{Property}(\text{"Hmolar", "H2", "temperature"} = T)$

$h_{NO} := \text{Property}(\text{"Hmolar", "NO", "temperature"} = T)$

$h_{N2O} := \text{Property}(\text{"Hmolar", "N2O", "temperature"} = T)$

$h_{O2} := \text{Property}(\text{"Hmolar", "O2", "temperature"} = T)$

$h_{C} := \text{Property}(\text{"Hmolar", "C(gr)", "temperature"} = T)$

Entropies

$s_{CO} := \text{Property}(\text{"Smolar", "CO", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{HNO} := \text{Property}(\text{"Smolar", "HNO", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{H2O} := \text{Property}(\text{"Smolar", "H2O", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{NO2} := \text{Property}(\text{"Smolar", "NO2", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{O} := \text{Property}(\text{"Smolar", "O", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{CO2} := \text{Property}(\text{"Smolar", "CO2", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{HO2} := \text{Property}(\text{"Smolar", "HO2", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{H2O2} := \text{Property}(\text{"Smolar", "H2O2", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{N2} := \text{Property}(\text{"Smolar", "N2", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{OH} := \text{Property}(\text{"Smolar", "OH", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{H} := \text{Property}(\text{"Smolar", "H", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{H2} := \text{Property}(\text{"Smolar", "H2", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{NO} := \text{Property}(\text{"Smolar", "NO", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{N2O} := \text{Property}(\text{"Smolar", "N2O", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{O2} := \text{Property}(\text{"Smolar", "O2", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

$s_{C} := \text{Property}(\text{"Smolar", "C(gr)", "temperature"} = T) - R \cdot \ln(P_c / P_s)$

Enthalpy of formation

$h_{f\_CH6N2L} := \text{Property}(\text{"HeatOfFormation", "CH6N2(L)"}) = 5.420 \times 10^{4}$

$h_{f\_N2O4L} := \text{Property}(\text{"HeatOfFormation","N2O4(L)"}) = -1.755 \times 10^{4}$

$h_{f\_CO} := \text{Property}(\text{"HeatOfFormation", "CO"}) = -1.105 \times 10^{5}$

$h_{f\_HNO} := \text{Property}(\text{"HeatOfFormation", "HNO"}) = 1.020 \times 10^{5}$

$h_{f\_H2O} := \text{Property}(\text{"HeatOfFormation", "H2O"}) = -2.418 \times 10^{5}$

$h_{f\_NO2} := \text{Property}(\text{"HeatOfFormation", "NO2"}) = 3.419 \times 10^{4}$

$h_{f\_O} := \text{Property}(\text{"HeatOfFormation", "O"}) = 2.492 \times 10^{5}$

$h_{f\_CO2} := \text{Property}(\text{"HeatOfFormation", "CO2"}) = -3.935 \times 10^{5}$

$h_{f\_HO2} := \text{Property}(\text{"HeatOfFormation", "HO2"}) = 1.202 \times 10^{4}$

$h_{f\_H2O2} := \text{Property}(\text{"HeatOfFormation", "H2O2"}) = -1.359 \times 10^{5}$

$h_{f\_N2} := \text{Property}(\text{"HeatOfFormation", "N2"}) = 0.$

$h_{f\_OH} := \text{Property}(\text{"HeatOfFormation", "OH"}) = 3.728 \times 10^{4}$

$h_{f\_H} := \text{Property}(\text{"HeatOfFormation"}, \text{"H"}) = 2.180 \times 10^5$

$h_{f\_H2} := \text{Property}(\text{"HeatOfFormation"}, \text{"H2"}) = 0.$

$h_{f\_NO} := \text{Property}(\text{"HeatOfFormation"}, \text{"NO"}) = 9.127 \times 10^4$

$h_{f\_N2O} := \text{Property}(\text{"HeatOfFormation"}, \text{"N2O"}) = 8.160 \times 10^4$

$h_{f\_O2} := \text{Property}(\text{"HeatOfFormation"}, \text{"O2"}) = 0.$

Reference enthalpies

$h_{r\_CO} := \text{eval}(h_{CO}, T = 298.15) = -1.105 \times 10^5$

$h_{r\_HNO} := \text{eval}(h_{HNO}, T = 298.15) = 1.020 \times 10^5$

$h_{r\_H2O} := \text{eval}(h_{H2O}, T = 298.15) = -2.418 \times 10^5$

$h_{r\_NO2} := \text{eval}(h_{NO2}, T = 298.15) = 3.419 \times 10^4$

$h_{r\_O} := \text{eval}(h_{O}, T = 298.15) = 2.492 \times 10^5$

$h_{r\_CO2} := \text{eval}(h_{CO2}, T = 298.15) = -3.935 \times 10^5$

$h_{r\_HO2} := \text{eval}(h_{HO2}, T = 298.15) = 1.202 \times 10^4$

$h_{r\_H2O2} := \text{eval}(h_{H2O2}, T = 298.15) = -1.359 \times 10^5$

$h_{r\_N2} := \text{eval}(h_{N2}, T = 298.15) = 9.916 \times 10^{-6}$

$h_{r\_OH} := \text{eval}(h_{OH}, T = 298.15) = 3.728 \times 10^4$

$h_{r\_H} := \text{eval}(h_{H}, T = 298.15) = 2.180 \times 10^5$

$h_{r\_H2} := \text{eval}(h_{H2}, T = 298.15) = -4.958 \times 10^{-6}$

$h_{r\_NO} := \text{eval}(h_{NO}, T = 298.15) = 9.127 \times 10^4$

$h_{r\_N2O} := \text{eval}(h_{N2O}, T = 298.15) = 8.160 \times 10^4$

$h_{r\_O2} := \text{eval}(h_{O2}, T = 298.15) = 0.$

Gibbs energy of formation

$$g_{CO} := h_{CO} - (h_C + 0.5 \cdot h_{O2}) - T \cdot (s_{CO} - (s_C + 0.5 \cdot s_{O2}))$$

$$g_{HNO} := h_{HNO} - (0.5 \cdot h_{H2} + 0.5 \cdot h_{O2} + 0.5 \cdot h_{N2}) - T \cdot (s_{HNO} - (0.5 \cdot s_{H2} + 0.5 \cdot s_{O2} + 0.5 \cdot s_{N2}))$$

$$g_{H2O} := h_{H2O} - (h_{H2} + 0.5 \cdot h_{O2}) - T \cdot (s_{H2O} - (s_{H2} + 0.5 \cdot s_{O2}))$$

$$g_{NO2} := h_{NO2} - (0.5 \cdot h_{N2} + h_{O2}) - T \cdot (s_{NO2} - (0.5 \cdot s_{N2} + s_{O2}))$$

$$g_O := h_O - 0.5 \cdot h_{O2} - T \cdot (s_O - 0.5 \cdot s_{O2})$$

$$g_{CO2} := h_{CO2} - (h_C + h_{O2}) - T \cdot (s_{CO2} - (s_C + s_{O2}))$$

$$g_{HO2} := h_{HO2} - (0.5 \cdot h_{H2} + h_{O2}) - T \cdot (s_{HO2} - (0.5 \cdot s_{H2} + s_{O2}))$$

$$g_{H2O2} := h_{H2O2} - (h_{H2} + h_{O2}) - T \cdot (s_{H2O2} - (s_{H2} + s_{O2}))$$

$$g_{N2} := 0$$

$$g_{OH} := h_{OH} - (0.5 \cdot h_{H2} + 0.5 \cdot h_{O2}) - T \cdot (s_{OH} - (0.5 \cdot s_{H2} + 0.5 \cdot s_{O2}))$$

$$g_H := h_H - 0.5 \cdot h_{H2} - T \cdot (s_H - 0.5 \cdot s_{H2})$$

$$g_{H2} := 0$$

$$g_{NO} := h_{NO} - (0.5 \cdot h_{N2} + 0.5 \cdot h_{O2}) - T \cdot (s_{NO} - (0.5 \cdot s_{N2} + 0.5 \cdot s_{O2}))$$

$$g_{N2O} := h_{N2O} - (h_{N2} + 0.5 \cdot h_{O2}) - T \cdot (s_{N2O} - (s_{N2} + 0.5 \cdot s_{O2}))$$

$$g_{O2} := 0$$

Ratio of nozzle exit and combustion chamber throat area

$$epsilon := 1$$

Ratio of exit area to throat area

$$AeAt := 1.58$$

Mach number at throat (=1 for choked flow)

$$M_t := 1$$

Calculate the equilibrium composition

Constraints

$$con_1 := n_{CO} + n_{CO2} = 1$$

$$con_2 := n_{HNO} + 2 \cdot n_{H2O} + n_{HO2} + 2 \cdot n_{H2O2} + n_{OH} + n_H + 2 \cdot n_{H2} = 6$$

$$con_3 := n_{CO} + n_{HNO} + n_{H2O} + 2 \cdot n_{NO2} + n_O + 2 \cdot n_{CO2} + 2 \cdot n_{HO2} + 2 \cdot n_{H2O2} + n_{OH} + n_{NO} + n_{N2O} + 2 \cdot n_{O2} = 4 \cdot 1.2518$$

$$con_4 := n_{HNO} + n_{NO2} + 2 \cdot n_{N2} + n_{NO} + 2 \cdot n_{N2O} = 2 + 2 \cdot 1.2518$$

Total moles of combustion products

$$n_{total} := n_{CO} + n_{HNO} + n_{H2O} + n_{NO2} + n_O + n_{CO2} + n_{HO2} + n_{H2O2} + n_{N2} + n_{OH} + n_H + n_{H2} + n_{NO} + n_{N2O} + n_{O2}$$

For a given temperature, minimizing the Gibbs Free Energy of the combustion products will give the equilibrium composition

$$\begin{aligned} g_{total} := {} & n_{CO} \cdot \left(g_{CO} + R \cdot T \cdot \ln\left(\frac{n_{CO}}{n_{total}} \right) \right) + n_{HNO} \cdot \left(g_{HNO} + R \cdot T \cdot \ln\left(\frac{n_{HNO}}{n_{total}} \right) \right) \\ & + n_{H2O} \cdot \left(g_{H2O} + R \cdot T \cdot \ln\left(\frac{n_{H2O}}{n_{total}} \right) \right) + n_{NO2} \cdot \left(g_{NO2} + R \cdot T \cdot \ln\left(\frac{n_{NO2}}{n_{total}} \right) \right) \\ & + n_O \cdot \left(g_O + R \cdot T \cdot \ln\left(\frac{n_O}{n_{total}} \right) \right) + n_{CO2} \cdot \left(g_{CO2} + R \cdot T \cdot \ln\left(\frac{n_{CO2}}{n_{total}} \right) \right) \\ & + n_{HO2} \cdot \left(g_{HO2} + R \cdot T \cdot \ln\left(\frac{n_{HO2}}{n_{total}} \right) \right) + n_{H2O2} \cdot \left(g_{H2O2} + R \cdot T \cdot \ln\left(\frac{n_{H2O2}}{n_{total}} \right) \right) \\ & + n_{N2} \cdot \left(g_{N2} + R \cdot T \cdot \ln\left(\frac{n_{N2}}{n_{total}} \right) \right) + n_{OH} \cdot \left(g_{OH} + R \cdot T \cdot \ln\left(\frac{n_{OH}}{n_{total}} \right) \right) \\ & + n_H \cdot \left(g_H + R \cdot T \cdot \ln\left(\frac{n_H}{n_{total}} \right) \right) + n_{H2} \cdot \left(g_{H2} + R \cdot T \cdot \ln\left(\frac{n_{H2}}{n_{total}} \right) \right) \\ & + n_{NO} \cdot \left(g_{NO} + R \cdot T \cdot \ln\left(\frac{n_{NO}}{n_{total}} \right) \right) + n_{N2O} \cdot \left(g_{N2O} + R \cdot T \cdot \ln\left(\frac{n_{N2O}}{n_{total}} \right) \right) \\ & + n_{O2} \cdot \left(g_{O2} + R \cdot T \cdot \ln\left(\frac{n_{O2}}{n_{total}} \right) \right) \end{aligned}$$

Hence the values of n1, n2, n3, n4, n5, n6, n7 and n8 are given by the numeric solution of these equations, where L1 and L2 are the Lagrange multipliers.

$$eqComposition_1 := L_1 \cdot \frac{\partial}{\partial n_{CO}} lhs(con_1) + L_2 \cdot \frac{\partial}{\partial n_{CO}} lhs(con_2) + L_3 \cdot \frac{\partial}{\partial n_{CO}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{CO}} lhs(con_4) = \frac{d}{dn_{CO}} g_{total}$$

$$eqComposition_2 := L_1 \cdot \frac{d}{dn_{HNO}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{HNO}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{HNO}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{HNO}} lhs(con_4) = \frac{d}{dn_{HNO}} g_{total}$$

$$eqComposition_3 := L_1 \cdot \frac{d}{dn_{H2O}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{H2O}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{H2O}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{H2O}} lhs(con_4) = \frac{d}{dn_{H2O}} g_{total}$$

$$eqComposition_4 := L_1 \cdot \frac{d}{dn_{NO2}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{NO2}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{NO2}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{NO2}} lhs(con_4) = \frac{d}{dn_{NO2}} g_{total}$$

$$eqComposition_5 := L_1 \cdot \frac{d}{dn_{O}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{O}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{O}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{O}} lhs(con_4) = \frac{d}{dn_{O}} g_{total}$$

$$eqComposition_6 := L_1 \cdot \frac{d}{dn_{CO2}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{CO2}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{CO2}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{CO2}} lhs(con_4) = \frac{d}{dn_{CO2}} g_{total}$$

$$eqComposition_7 := L_1 \cdot \frac{d}{dn_{HO2}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{HO2}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{HO2}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{HO2}} lhs(con_4) = \frac{d}{dn_{HO2}} g_{total}$$

$$eqComposition_8 := L_1 \cdot \frac{d}{dn_{H2O2}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{H2O2}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{H2O2}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{H2O2}} lhs(con_4) = \frac{d}{dn_{H2O2}} g_{total}$$

$$eqComposition_9 := L_1 \cdot \frac{d}{dn_{N2}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{N2}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{N2}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{N2}} lhs(con_4) = \frac{d}{dn_{N2}} g_{total}$$

$$eqComposition_{10} := L_1 \cdot \frac{d}{dn_{OH}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{OH}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{OH}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{OH}} lhs(con_4) = \frac{d}{dn_{OH}} g_{total}$$

$$eqComposition_{11} := L_1 \cdot \frac{d}{dn_{H}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{H}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{H}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{H}} lhs(con_4) = \frac{d}{dn_{H}} g_{total}$$

$$eqComposition_{12} := L_1 \cdot \frac{d}{dn_{H2}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{H2}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{H2}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{H2}} lhs(con_4) = \frac{d}{dn_{H2}} g_{total}$$

$$eqComposition_{13} := L_1 \cdot \frac{d}{dn_{NO}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{NO}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{NO}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{NO}} lhs(con_4) = \frac{d}{dn_{NO}} g_{total}$$

$$eqComposition_{14} := L_1 \cdot \frac{d}{dn_{N2O}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{N2O}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{N2O}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{N2O}} lhs(con_4) = \frac{d}{dn_{N2O}} g_{total}$$

$$eqComposition_{15} := L_1 \cdot \frac{d}{dn_{O2}} lhs(con_1) + L_2 \cdot \frac{d}{dn_{O2}} lhs(con_2) + L_3 \cdot \frac{d}{dn_{O2}} lhs(con_3) + L_4 \cdot \frac{d}{dn_{O2}} lhs(con_4) = \frac{d}{dn_{O2}} g_{total}$$

The flame temperature is given by equating the heat of the reactants to the heat of the products

$$H_{reactants} := 1 \cdot h_{f\_CH6N2L} + 1.2518 \cdot h_{f\_N2O4L} = 3.223 \times 10^4$$

$$\begin{aligned} H_{products} := {} & n_{CO} \cdot (h_{f\_CO} + (h_{CO} - h_{r\_CO})) + n_{HNO} \cdot (h_{f\_HNO} + (h_{HNO} - h_{r\_HNO})) \\ & + n_{H2O} \cdot (h_{f\_H2O} + (h_{H2O} - h_{r\_H2O})) + n_{NO2} \cdot (h_{f\_NO2} + (h_{NO2} - h_{r\_NO2})) \\ & + n_{O} \cdot (h_{f\_O} + (h_{O} - h_{r\_O})) + n_{CO2} \cdot (h_{f\_CO2} + (h_{CO2} - h_{r\_CO2})) \\ & + n_{HO2} \cdot (h_{f\_HO2} + (h_{HO2} - h_{r\_HO2})) + n_{H2O2} \cdot (h_{f\_H2O2} + (h_{H2O2} - h_{r\_H2O2})) \\ & + n_{N2} \cdot (h_{f\_N2} + (h_{N2} - h_{r\_N2})) + n_{OH} \cdot (h_{f\_OH} + (h_{OH} - h_{r\_OH})) \\ & + n_{H} \cdot (h_{f\_H} + (h_{H} - h_{r\_H})) + n_{H2} \cdot (h_{f\_H2} + (h_{H2} - h_{r\_H2})) \\ & + n_{NO} \cdot (h_{f\_NO} + (h_{NO} - h_{r\_NO})) + n_{N2O} \cdot (h_{f\_N2O} + (h_{N2O} - h_{r\_N2O})) \\ & + n_{O2} \cdot (h_{f\_O2} + (h_{O2} - h_{r\_O2})) \end{aligned}$$

$$flameTemp := H_{reactants} = H_{products}$$

Numerical solution of equilibrium composition and flame temperature

$$\begin{aligned} sys := \{ & eqComposition_1, eqComposition_2, eqComposition_3 \\ & , eqComposition_4, eqComposition_4, eqComposition_5, eqComposition_6 \\ & , eqComposition_7, eqComposition_8, eqComposition_9, eqComposition_{10} \\ & , eqComposition_{11}, eqComposition_{12}, eqComposition_{13}, eqComposition_{14} \\ & , eqComposition_{15}, con_1, con_2, con_3, con_4, flameTemp \} \end{aligned}$$

$$\begin{aligned} estimates := \{ & L_1 = -1000, L_2 = -1000, L_3 = -1000, L_4 = -1000, T = 3000 \\ & , n_{CO} = 0.1, n_{HNO} = 0.1, n_{H2O} = 0.1, n_{NO2} = 0.1, n_{O} = 0.1, n_{CO2} = 0.1, n_{HO2} = 0.1 \\ & , n_{H2O2} = 0.1, n_{N2} = 0.1, n_{OH} = 0.1, n_{H} = 0.1, n_{H2} = 0.1, n_{NO} = 0.1, n_{N2O} = 0.1 \\ & , n_{O2} = 0.1 \} \end{aligned}$$

$$res := fsolve(sys, estimates)$$

Hence the temperature in the rocket combustion chamber is

$$T_c := eval(T, res)\ \mathbf{K} = 3.348 \times 10^3\ \mathbf{K}$$

Equilibrium composition of the combustion products (mole fraction)

$$mol_{CO} := eval(n_{CO}, res) = 0.453$$

$$mol_{HNO} := eval(n_{HNO}, res) = 8.183 \times 10^{-5}$$

$$mol_{H2O} := eval(n_{H2O}, res) = 2.529$$

$$mol_{NO2} := eval(n_{NO2}, res) = 1.472 \times 10^{-4}$$

$$mol_{O} := eval(n_{O}, res) = 0.056$$

$$mol_{CO2} := eval(n_{CO2}, res) = 0.547$$

$$mol_{HO2} := eval(n_{HO2}, res) = 6.306 \times 10^{-4}$$

$$mol_{H2O2} := eval(n_{H2O2}, res) = 8.772 \times 10^{-5}$$

$$mol_{N2} := eval(n_{N2}, res) = 2.194$$

$$mol_{OH} := eval(n_{OH}, res) = 0.341$$

$$mol_{H} := eval(n_{H}, res) = 0.078$$

$$mol_{H2} := eval(n_{H2}, res) = 0.261$$

$$mol_{NO} := eval(n_{NO}, res) = 0.116$$

$$mol_{N2O} := eval(n_{N2O}, res) = 3.050 \times 10^{-5}$$

$$mol_{O2} := eval(n_{O2}, res) = 0.209$$

Total number of moles

$$mol_{total} := mol_{CO} + mol_{HNO} + mol_{H2O} + mol_{NO2} + mol_{O} + mol_{CO2} + mol_{HO2} + mol_{H2O2} + mol_{N2} + mol_{OH} + mol_{H} + mol_{H2} + mol_{NO} + mol_{N2O} + mol_{O2}$$

$$mol_{total} = 6.784$$

Mole fractions in the combustion products

$$molFrac_{CO} := \frac{mol_{CO}}{mol_{total}} = 0.067$$

$$molFrac_{HNO} := \frac{mol_{HNO}}{mol_{total}} = 1.206 \times 10^{-5}$$

$$molFrac_{H2O} := \frac{mol_{H2O}}{mol_{total}} = 0.373$$

$$molFrac_{NO2} := \frac{mol_{NO2}}{mol_{total}} = 2.169 \times 10^{-5}$$

$$molFrac_{O} := \frac{mol_{O}}{mol_{total}} = 0.008$$

$$molFrac_{CO2} := \frac{mol_{CO2}}{mol_{total}} = 0.081$$

$$molFrac_{HO2} := \frac{mol_{HO2}}{mol_{total}} = 9.296 \times 10^{-5}$$

$$molFrac_{H2O2} := \frac{mol_{H2O2}}{mol_{total}} = 1.293 \times 10^{-5}$$

$$molFrac_{N2} := \frac{mol_{N2}}{mol_{total}} = 0.323$$

$$molFrac_{OH} := \frac{mol_{OH}}{mol_{total}} = 0.050$$

$$molFrac_{H} := \frac{mol_{H}}{mol_{total}} = 0.011$$

$$molFrac_{H2} := \frac{mol_{H2}}{mol_{total}} = 0.038$$

$$molFrac_{NO} := \frac{mol_{NO}}{mol_{total}} = 0.017$$

$$molFrac_{N2O} := \frac{mol_{N2O}}{mol_{total}} = 4.496 \times 10^{-6}$$

$$molFrac_{O2} := \frac{mol_{O2}}{mol_{total}} = 0.031$$

Ideal gas constant

$$R := 8.3144\ J \cdot mol^{-1} \cdot K^{-1}$$

Gravity

$$grav := 9.81\ m \cdot s^{-2}$$

Molecular weight of the combustion products

$$Mw_{mix} := molFrac_{CO} \cdot mw_{CO} + molFrac_{HNO} \cdot mw_{HNO} + molFrac_{H2O} \cdot mw_{H2O} + molFrac_{NO2} \cdot mw_{NO2} + molFrac_{O} \cdot mw_{O} + molFrac_{CO2} \cdot mw_{CO2} + molFrac_{HO2} \cdot mw_{HO2} + molFrac_{H2O2} \cdot mw_{H2O2} + molFrac_{N2} \cdot mw_{N2} + molFrac_{OH} \cdot mw_{OH} + molFrac_{H} \cdot mw_{H} + molFrac_{H2} \cdot mw_{H2} + molFrac_{NO} \cdot mw_{NO} + molFrac_{N2O} \cdot mw_{N2O} + molFrac_{O2} \cdot mw_{O2}$$

$$Mw_{mix} = 5.653\ \frac{g}{mol}$$

Specific heat capacity at constant pressure at constant pressure

$$Cp_c := eval(molFrac_{CO} \cdot Cp_{CO} + molFrac_{HNO} \cdot Cp_{HNO} + molFrac_{H2O} \cdot Cp_{H2O} + molFrac_{NO2} \cdot Cp_{NO2} + molFrac_{O} \cdot Cp_{O} + molFrac_{CO2} \cdot Cp_{CO2} + molFrac_{HO2} \cdot Cp_{HO2} + molFrac_{H2O2} \cdot Cp_{H2O2} + molFrac_{N2} \cdot Cp_{N2} + molFrac_{OH} \cdot Cp_{OH} + molFrac_{H} \cdot Cp_{H} + molFrac_{H2} \cdot Cp_{H2} + molFrac_{NO} \cdot Cp_{NO} + molFrac_{N2O} \cdot Cp_{N2O} + molFrac_{O2} \cdot Cp_{O2}, T = T_c)$$

$$Cp_c = 46.817\ \frac{m^2 \cdot kg}{s^2 \cdot mol \cdot K}$$

Specific heat capacity (at constant volume) in the combustion chamber

$$Cv_c := Cp_c - R = 38.502\ \frac{J}{mol \cdot K}$$

Isentropic expansion coefficient in the chamber

$$k_c := \frac{Cp_c}{Cv_c} = 1.216$$

Mach number at exit

$$M_e := \text{fsolve}\left(AeAt = \frac{\left(\frac{k_c+1}{2}\right)^{-\frac{k_c+1}{2\cdot\left(k_c-1\right)}} \cdot \left(1 + \frac{k_c - 1}{2}\cdot M_e^2\right)^{\frac{k_c+1}{2\cdot\left(k_c-1\right)}}}{M_e}, M_e = 1 \right)$$

$$M_e = 0.410$$

Throat temperature

$$T_t := T_c \cdot \left(1 + \frac{k_c - 1}{2}\cdot M_t^2\right)^{-1} = 3.022 \times 10^3\ \mathbf{K}$$

Exit temperature

$$T_e := T_c \cdot \left(1 + \frac{k_c - 1}{2}\cdot M_e^2\right)^{-1} = 3.288 \times 10^3\ \mathbf{K}$$

Specific heat capacity (at constant pressure) at throat

$$\begin{aligned} Cp_t := \text{eval}\big(& molFrac_{CO}\cdot Cp_{CO} + molFrac_{HNO}\cdot Cp_{HNO} + molFrac_{H2O}\cdot Cp_{H2O} \\ &+ molFrac_{NO2}\cdot Cp_{NO2} + molFrac_{O}\cdot Cp_{O} + molFrac_{CO2}\cdot Cp_{CO2} \\ &+ molFrac_{HO2}\cdot Cp_{HO2} + molFrac_{H2O2}\cdot Cp_{H2O2} + molFrac_{N2}\cdot Cp_{N2} \\ &+ molFrac_{OH}\cdot Cp_{OH} + molFrac_{H}\cdot Cp_{H} + molFrac_{H2}\cdot Cp_{H2} + molFrac_{NO}\cdot Cp_{NO} \\ &+ molFrac_{N2O}\cdot Cp_{N2O} + molFrac_{O2}\cdot Cp_{O2}, T = T_t\big) \end{aligned}$$

$$Cp_t = 46.273\ \frac{\mathbf{J}}{\mathbf{mol\cdot K}}$$

Isentropic expansion coefficient at throat

$$k_t := \frac{Cp_t}{Cp_t - R} = 1.219$$

Throat pressure

$$P_t := P_c \cdot \left(1 + \frac{k_c - 1}{2} \cdot M_t^2\right)^{\frac{k_c}{1 - k_c}} = 28.070\ \mathbf{bar}$$

Exit pressure

$$P_e := P_c \cdot \left(1 + \frac{k_t - 1}{2} \cdot M_e^2\right)^{\frac{k_t}{1 - k_t}} = 45.168\ \mathbf{bar}$$

Chamber gas density

$$\rho_c := \frac{P_c \cdot Mw_{mix}}{R \cdot T_c} = 1.015\ \frac{\mathbf{kg}}{\mathbf{m^3}}$$

Throat gas density

$$\rho_t := \frac{P_t \cdot Mw_{mix}}{R \cdot T_t} = 0.632\ \frac{\mathbf{kg}}{\mathbf{m^3}}$$

Sonic velocity in chamber

$$sonicVelocity_c := \sqrt{\frac{k_c \cdot P_c}{\rho_c}} = 2.447 \times 10^3\ \frac{\mathbf{m}}{\mathbf{s}}$$

Sonic velocity in throat

$$sonicVelocity_t := \sqrt{\frac{k_t \cdot P_t}{\rho_t}} = 2.328 \times 10^3\ \frac{\mathbf{m}}{\mathbf{s}}$$

Throat velocity for an isentropic nozzle

$$V_t := \sqrt{\frac{2 \cdot T_c \cdot R}{Mw_{mix}} \cdot \frac{k_c}{k_c - 1} \cdot \left(1 - \left(\frac{P_t}{P_c}\right)^{\frac{k_c - 1}{k_c}}\right)} = 2.325 \times 10^3 \ \frac{m}{s}$$

Ideal specific impulse

$$Isp_{ideal} := \frac{V_t}{grav} = 236.984 \ s$$

Ideal specific impulse as defined by NASA CEA

$$Isp_{ideal\_NASA} := V_t = 2.325 \times 10^3 \ \frac{m}{s}$$

Ideal specific impulse in a vacuum

$$Isp_{vac} := \frac{1}{grav} \cdot \left(V_t + \frac{P_t}{\rho_t \cdot V_t}\right) = 431.880 \ s$$

Characteristic velocity (Cstar)

$$Cstar := \sqrt{\frac{R \cdot T_c}{k_c \cdot Mw_{mix}} \cdot \left(\frac{k_c + 1}{2}\right)^{\frac{k_c + 1}{k_c - 1}}} = 3.406 \times 10^3 \ \frac{m}{s}$$