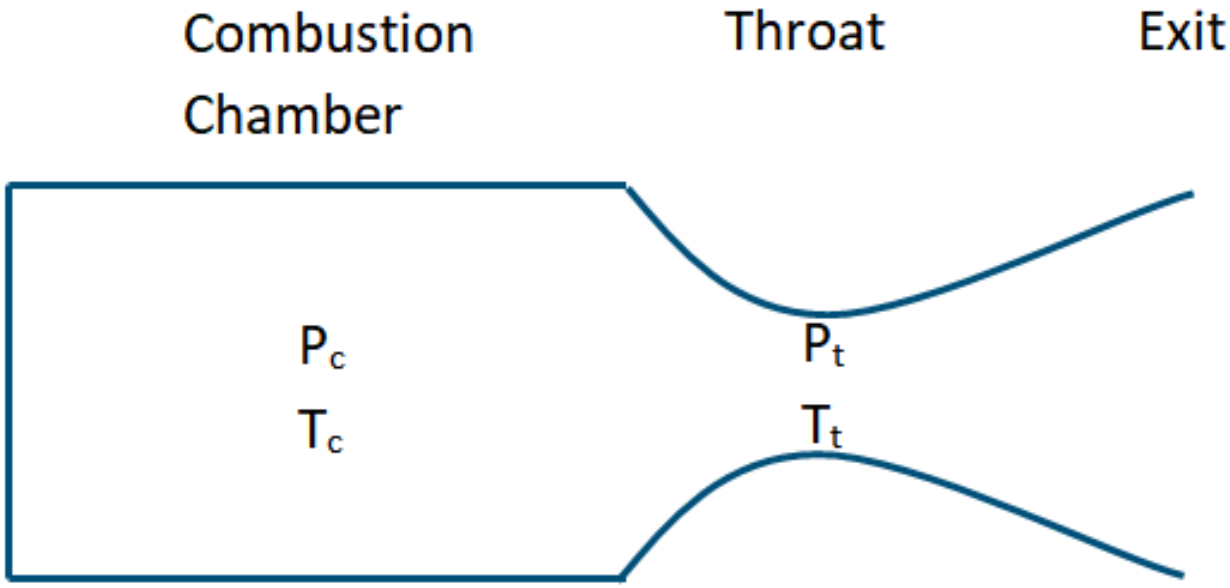
Theoretical Performance of a LOX-LH2 Rocket

Introduction

Liquid hydrogen (at 20.27 K) and liquid oxygen (at 90.17 K) are burned in the combustion chamber (with an infinite area ratio) of a rocket.



The combustion products contain H_2, O_2, H, O, OH, HO_2 and H_2O_2

Chemical	In Feed	In Products
H_2	1	n1
O_2	0.34974	n2
H_2O		n3

O		n4
H		n5
OH		n6
HO_2		n7
H_2O_2		n8

This application will calculate

- the adiabatic flame temperature and composition of the combustion products
- the pressures and temperatures in the throat and exit
- and the theoretical rocket performance, including the ideal specific impulse, characteristic velocity, sonic velocity and more

Assumptions

- The combustion chamber is large compared to the throat, hence the assumption of an infinite area ratio
- The flow composition does not change through the nozzle expansion (i.e. reaction rate is slow compared to flowrate). This is also known as "frozen" flow

Physical Properties

```
> restart:
> with(ThermophysicalData:-Chemicals):
```

Enthalpies

```
> h_O2   := Property("Hmolar", "O2",   "temperature" = T):
  h_H2   := Property("Hmolar", "H2",   "temperature" = T):
  h_H2O  := Property("Hmolar", "H2O",  "temperature" = T):
  h_OH   := Property("Hmolar", "OH",   "temperature" = T):
  h_H    := Property("Hmolar", "H",    "temperature" = T):
  h_O    := Property("Hmolar", "O",    "temperature" = T):
  h_HO2  := Property("Hmolar", "HO2",  "temperature" = T):
  h_H2O2 := Property("Hmolar", "H2O2", "temperature" = T):
```

Entropies

```
> s_O2   := Property("Smolar", "O2",   "temperature" = T)  - R *
  ln(P_c/P_s):
  s_H2   := Property("Smolar", "H2",   "temperature" = T)  - R *
  ln(P_c/P_s):
  s_H2O  := Property("Smolar", "H2O",  "temperature" = T)  - R *
  ln(P_c/P_s):
  s_OH   := Property("Smolar", "OH",   "temperature" = T)  - R *
  ln(P_c/P_s):
  s_H    := Property("Smolar", "H",    "temperature" = T)  - R *
```

```
ln(P_c/P_s):
s_O    := Property("Smolar", "O",    "temperature" = T)  - R *
ln(P_c/P_s):
s_HO2  := Property("Smolar", "HO2",  "temperature" = T)  - R *
ln(P_c/P_s):
s_H2O2 := Property("Smolar", "H2O2", "temperature" = T)  - R *
ln(P_c/P_s):
```

Enthalpy of formation

```
> h_f_O2L  := Property("HeatOfFormation", "O2(L)");
  h_f_H2L  := Property("HeatOfFormation", "H2(L)");
  h_f_O2   := Property("HeatOfFormation", "O2");
  h_f_H2   := Property("HeatOfFormation", "H2");
  h_f_H2O  := Property("HeatOfFormation", "H2O");
  h_f_OH   := Property("HeatOfFormation", "OH");
  h_f_H    := Property("HeatOfFormation", "H");
  h_f_O    := Property("HeatOfFormation", "O");
  h_f_HO2  := Property("HeatOfFormation", "HO2");
  h_f_H2O2 := Property("HeatOfFormation", "H2O2");
```

$$h\_f\_O2L := -12979.000$$

$$h\_f\_H2L := -9012.000$$

$$h\_f\_O2 := 0.$$

$$h\_f\_H2 := 0.$$

$$h\_f\_H2O := -241826.000$$

$$h\_f\_OH := 37278.206$$

$$h\_f\_H := 217998.828$$

$$h\_f\_O := 249175.003$$

$$h\_f\_HO2 := 12020.000$$

$$h\_f\_H2O2 := -135880.000 \quad \textbf{(2.1)}$$

Reference enthalpies

```
> h_r_O2   := eval(h_O2,   T = 298.15);
  h_r_H2   := eval(h_H2,   T = 298.15);
  h_r_H2O  := eval(h_H2O,  T = 298.15);
  h_r_OH   := eval(h_OH,   T = 298.15);
  h_r_H    := eval(h_H,    T = 298.15);
  h_r_O    := eval(h_O,    T = 298.15);
  h_r_HO2  := eval(h_HO2,  T = 298.15);
  h_r_H2O2 := eval(h_H2O2, T = 298.15)
```

$$h\_r\_O2 := 0.$$

$$h\_r\_H2 := -4.95794231\,10^{-6}$$

$$h\_r\_H2O := -241826.0005$$

$$h\_r\_OH := 37278.20600$$

$$h\_r\_H := 217998.8279$$

$$h\_r\_O := 249175.0027$$

$$h\_r\_HO2 := 12019.99997$$

$$h\_r\_H2O2 := -135880.0000 \quad \textbf{(2.2)}$$

Gibbs Free Energy of Formation of the combustion products

```
> Gibbs_H2 := proc(temp)
     return 0
  end proc:

> Gibbs_O2 := proc(temp)
     return 0
  end proc:

> Gibbs_H2O := proc(temp)
     local DeltaH, DeltaS, DeltaG:
     DeltaH := eval(h_H2O - (h_H2 + 0.5*h_O2), T = temp):
     DeltaS := eval(s_H2O - (s_H2 + 0.5*s_O2), T = temp):
     DeltaG := DeltaH - DeltaS*temp:
  end proc:

> Gibbs_O := proc(temp)
     local DeltaH, DeltaS, DeltaG:
     DeltaH := eval(h_O - 0.5*h_O2, T = temp):
     DeltaS := eval(s_O - 0.5*s_O2, T = temp):
     DeltaG := DeltaH - DeltaS*temp:
     return DeltaG:
  end proc:

> Gibbs_H := proc(temp)
     local DeltaH, DeltaS, DeltaG:
     DeltaH := eval(h_H - 0.5*h_H2, T = temp):
     DeltaS := eval(s_H - 0.5*s_H2, T = temp):
     DeltaG := DeltaH - DeltaS*temp:
     return DeltaG:
  end proc:

> Gibbs_OH := proc(temp)
     local DeltaH, DeltaS, DeltaG:
     DeltaH := eval(h_OH - (0.5*h_H2 + 0.5*h_O2), T = temp):
     DeltaS := eval(s_OH - (0.5*s_H2 + 0.5*s_O2), T = temp):
     DeltaG := DeltaH - DeltaS*temp:
     return DeltaG:
  end proc:

> Gibbs_HO2 := proc(temp)
     local DeltaH, DeltaS, DeltaG:
     DeltaH := eval(h_HO2 - (0.5*h_H2 + h_O2), T = temp):
     DeltaS := eval(s_HO2 - (0.5*s_H2 + s_O2), T = temp):
     DeltaG := DeltaH - DeltaS*temp:
     return DeltaG:
  end proc:

  Gibbs_H2O2 := proc(temp)
     local DeltaH, DeltaS, DeltaG:
     DeltaH := eval(h_H2O2 - (h_H2 + h_O2), T = temp):
     DeltaS := eval(s_H2O2 - (s_H2 + s_O2), T = temp):
     DeltaG := DeltaH - DeltaS*temp:
     return DeltaG:
  end proc:
```

Ideal gas constant

```
> R := 8.3144:
```

Chamber Pressure

```
> P_c := 53.3172 * Unit(bar):
```

Atmospheric Pressure

```
> P_a := 1.01325 * Unit(bar):
```

Standard pressure

```
> P_s := 1.0 * Unit(bar):
```

Ratio of nozzle exit and combustion chamber throat area

```
> epsilon := 1.0:
```

Ratio of exit area to throat area

```
> AeAt := 1.58:
```

Moles of H_2 and O_2 fed into combustion chamber (only the ratio is important)

```
> N_H2L := 1:
  N_O2L := 0.34974:
```

Mach number at throat (= 1 for choked flow)

```
> M_t := 1:
```

Equilibrium Composition

Equating the moles of chemicals in the reactants and products gives

N_H2L H_2 + N_O2L O_2 → n1 H_2 + n2 O_2 + n3 H_2O + n4 H + n5 O + n6 OH + n7 HO_2 + n8 H_2O_2

Balance on H atoms

2 n1 + 2 n3 + n4 + n6 + n7 + 2 n8 = 2 * N_H2L

Balance on O atoms

2 n2 + n3 + n5 + n6 + 2 n7 + 2 n8 = 2 * N_O2L

Hence the constraints are

```
> con1 := 2 * n1 + 2 * n3 + n4 + n6 + n7 + 2 * n8 = 2 * N_H2L:
> con2 := 2 * n2 + n3 + n5 + n6 + 2 * n7 + 2 * n8 = 2 * N_O2L:
```

Total moles of products

```
> nt := n1 + n2 + n3 + n4 + n5 + n6 + n7 + n8:
```

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

```
> gibbs :=   n1 * (Gibbs_H2(T)   + R * T * ln(n1/nt))
           + n2 * (Gibbs_O2(T)   + R * T * ln(n2/nt))
           + n3 * (Gibbs_H2O(T)  + R * T * ln(n3/nt))
           + n4 * (Gibbs_H(T)    + R * T * ln(n4/nt))
           + n5 * (Gibbs_O(T)    + R * T * ln(n5/nt))
           + n6 * (Gibbs_OH(T)   + R * T * ln(n6/nt))
           + n7 * (Gibbs_HO2(T)  + R * T * ln(n7/nt))
           + n8 * (Gibbs_H2O2(T) + R * T * ln(n8/nt)):
```

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 := L1 * diff(lhs(con1), n1) + L2 * diff(lhs(con2),
  n1) = diff(gibbs, n1),
                   L1 * diff(lhs(con1), n2) + L2 * diff(lhs(con2),
  n2) = diff(gibbs, n2),
                   L1 * diff(lhs(con1), n3) + L2 * diff(lhs(con2),
  n3) = diff(gibbs, n3),
                   L1 * diff(lhs(con1), n4) + L2 * diff(lhs(con2),
  n4) = diff(gibbs, n4),
                   L1 * diff(lhs(con1), n5) + L2 * diff(lhs(con2),
  n5) = diff(gibbs, n5),
                   L1 * diff(lhs(con1), n6) + L2 * diff(lhs(con2),
  n6) = diff(gibbs, n6),
                   L1 * diff(lhs(con1), n7) + L2 * diff(lhs(con2),
  n7) = diff(gibbs, n7),
                   L1 * diff(lhs(con1), n8) + L2 * diff(lhs(con2),
  n8) = diff(gibbs, n8):
```

Heat Balance

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

```
> H_reactants := N_H2L * h_f_H2L + N_O2L * h_f_O2L;
```

$$-13.55 \times 10^{3} \tag{4.1}$$

```
> H_products := + n1 * (h_f_H2   + (h_H2   - h_r_H2))
                + n2 * (h_f_O2   + (h_O2   - h_r_O2))
                + n3 * (h_f_H2O  + (h_H2O  - h_r_H2O))
                + n4 * (h_f_H    + (h_H    - h_r_H))
                + n5 * (h_f_O    + (h_O    - h_r_O))
                + n6 * (h_f_OH   + (h_OH   - h_r_OH))
                + n7 * (h_f_HO2  + (h_HO2  - h_r_HO2))
                + n8 * (h_f_H2O2 + (h_H2O2 - h_r_H2O2)):
> flameTemp := H_reactants = H_products:
```

Numerical Solution of Equilibrium Composition and Flame Temperature

```
> res:=fsolve({eqComposition, flameTemp, con1, con2}, {L1 =
  -1000, L2=-1000, T = 3000, n1 = 0.1, n2 = 0.1, n2 = 0.1, n3 =
```

```
  0.1, n4 = 0.1, n5 = 0.1, n6 = 0.1, n7 = 0.1, n8 = 0.1})
```

$$res := \{L1 = -17182.81432,\ L2 = -89531.03079,\ T = 3383.844425,\ n1 = 0.3061915322,\ n2 = 0.001788202357,\ n3 = 0.6590840027,\ n4 = 0.03479245713,\ n5 = 0.002147607467,\ n6 = 0.03462930001,\ n7 = 0.00001551202423,\ n8 = 5.83055171810^{-6}\} \quad (5.1)$$

Hence the temperature in the rocket combustion chamber is

```
> T_c := eval(T,res) * Unit(K)
```

$$T\_c := 3383.844425\ \mathrm{K} \quad (5.2)$$

The equilibrium composition of the combustion products are (in moles)

```
> mol_H2   := eval(n1 ,res);
  mol_O2   := eval(n2 ,res);
  mol_H2O  := eval(n3 ,res);
  mol_H    := eval(n4 ,res);
  mol_O    := eval(n5 ,res);
  mol_OH   := eval(n6 ,res);
  mol_HO2  := eval(n7 ,res);
  mol_H2O2 := eval(n8 ,res);
```

$$306.19 \times 10^{-3}$$
$$1.79 \times 10^{-3}$$
$$659.08 \times 10^{-3}$$
$$34.79 \times 10^{-3}$$
$$2.15 \times 10^{-3}$$
$$34.63 \times 10^{-3}$$
$$15.51 \times 10^{-6}$$
$$5.83 \times 10^{-6} \quad (5.3)$$

```
> mol_total := mol_H2 + mol_H2O + mol_O2 + mol_H + mol_O + mol_OH
  + mol_HO2 + mol_H2O2
```

$$mol\_total := 1.038654444 \quad (5.4)$$

Mole fractions in the combustion products

```
> molFrac_H2   := mol_H2/mol_total;
  molFrac_O2   := mol_O2/mol_total;
  molFrac_H2O  := mol_H2O/mol_total;
  molFrac_H    := mol_H/mol_total;
  molFrac_O    := mol_O/mol_total;
  molFrac_OH   := mol_OH/mol_total;
  molFrac_HO2  := mol_HO2/mol_total;
  molFrac_H2O2 := mol_H2O2/mol_total;
```

$$molFrac\_H2 := 0.2947963435$$
$$molFrac\_O2 := 0.001721652824$$
$$molFrac\_H2O := 0.6345556085$$
$$molFrac\_H := 0.03349762506$$
$$molFrac\_O := 0.002067682355$$
$$molFrac\_OH := 0.03334053997$$

$$molFrac\_HO2 := 0.00001493473053$$
$$molFrac\_H2O2 := 5.61356257810^{-6} \quad \textbf{(5.5)}$$

Ideal Performance of an Infinite Area Ratio Rocket

```
> with(Units[Simple]):
```

Ideal gas constant

```
> R := 8.3144 * Unit(J/mol/K):
```

Gravity

```
> grav := 9.81*Unit(m/s^2):
```

Molecular weight of the combustion products

```
> Mw_mix :=   molFrac_H2   * Property("MolarMass", "H2",
  useunits)
            + molFrac_H2O  * Property("MolarMass", "H2O",
  useunits)
            + molFrac_O2   * Property("MolarMass", "O2",
  useunits)
            + molFrac_H    * Property("MolarMass", "H",
  useunits)
            + molFrac_O    * Property("MolarMass", "O",
  useunits)
            + molFrac_OH   * Property("MolarMass", "OH",
  useunits)
            + molFrac_HO2  * Property("MolarMass", "HO2",
  useunits)
            + molFrac_H2O2 * Property("MolarMass", "H2O2",
  useunits)
```

$$12.72 \frac{g}{mol} \quad \textbf{(6.1)}$$

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

```
> Cp_c_mol :=   molFrac_H2   * Property("Cpmolar", "H2",
  "temperature" = T_c)
              + molFrac_H2O  * Property("Cpmolar", "H2O",
  "temperature" = T_c)
              + molFrac_O2   * Property("Cpmolar", "O2",
  "temperature" = T_c)
              + molFrac_O    * Property("Cpmolar", "O",
  "temperature" = T_c)
              + molFrac_H    * Property("Cpmolar", "H",
  "temperature" = T_c)
              + molFrac_OH   * Property("Cpmolar", "OH",
  "temperature" = T_c)
              + molFrac_HO2  * Property("Cpmolar", "HO2",
  "temperature" = T_c)
              + molFrac_H2O2 * Property("Cpmolar", "H2O2",
  "temperature" = T_c)
```

(6.2)

$$50.02 \ \frac{J}{mol\,K} \tag{6.2}$$

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

```
> Cv_c_mol := Cp_c_mol - R
```

$$41.70 \ \frac{J}{mol\,K} \tag{6.3}$$

Isentropic expansion coefficient in the chamber

```
> Gamma_c := Cp_c_mol / Cv_c_mol
```

$$1.199 \tag{6.4}$$

Mach number at exit

```
> M_e := fsolve(AeAt = ((Gamma_c + 1)/2) ^ (-(Gamma_c + 1)/(2 *
  (Gamma_c - 1))) * (1 + 0.5 * (Gamma_c - 1) * M_e^2)^((Gamma_c +
  1)/(2 * (Gamma_c - 1)))/M_e, M_e = 1)
```

$$.41 \tag{6.5}$$

Throat temperature

```
> T_t := T_c * (1 + (Gamma_c - 1)/2 * M_t^2)^(-1)
```

$$3077.11\ K \tag{6.6}$$

Exit temperature

```
> T_e := T_c * (1 + (Gamma_c - 1)/2 * M_e^2)^(-1)
```

$$3327.85\ K \tag{6.7}$$

Specific heat capacity (at constant pressure) at throat

```
> Cp_t_mol :=   molFrac_H2   * Property("Cpmolar", "H2",
  "temperature" = T_t)
              + molFrac_H2O  * Property("Cpmolar", "H2O",
  "temperature" = T_t)
              + molFrac_O2   * Property("Cpmolar", "O2",
  "temperature" = T_t)
              + molFrac_H    * Property("Cpmolar", "H",
  "temperature" = T_t)
              + molFrac_O    * Property("Cpmolar", "O",
  "temperature" = T_t)
              + molFrac_OH   * Property("Cpmolar", "OH",
  "temperature" = T_t)
              + molFrac_HO2  * Property("Cpmolar", "HO2",
  "temperature" = T_t)
              + molFrac_H2O2 * Property("Cpmolar", "H2O2",
  "temperature" = T_t)
```

$$49.25 \ \frac{J}{mol\,K} \tag{6.8}$$

Isentropic expansion coefficient at throat

```
> Gamma_t := Cp_t_mol / (Cp_t_mol - R )
```

$$1.203 \tag{6.9}$$

Throat pressure

```
> P_t := P_c * (1 + (Gamma_c - 1)/2 * M_t^2)^(Gamma_c / (1 -
```

```
Gamma_c))
```

$$30.10\ \text{bar} \tag{6.10}$$

Exit pressure

```
> P_e := P_c * (1 + (Gamma_t - 1)/2 * M_e^2)^(Gamma_t / (1 -
  Gamma_t))
```

$$48.21\ \text{bar} \tag{6.11}$$

Chamber gas density

```
> rho_c := P_c * Mw_mix/(R * T_c)
```

$$2.41\ \frac{\text{kg}}{\text{m}^3} \tag{6.12}$$

Throat gas density

```
> rho_t :=  P_t * Mw_mix/(R * T_t )
```

$$1.50\ \frac{\text{kg}}{\text{m}^3} \tag{6.13}$$

Sonic velocity in chamber and throat

```
> sonicVelocity_c := sqrt((Gamma_c * P_c/rho_c))
```

$$1629.02\ \frac{\text{m}}{\text{s}} \tag{6.14}$$

```
> sonicVelocity_t := sqrt((Gamma_t * P_t/rho_t))
```

$$1555.86\ \frac{\text{m}}{\text{s}} \tag{6.15}$$

Throat velocity for an isentropic nozzle

$$> V\_t := \sqrt{\frac{2 \cdot T\_cR}{Mw\_mix} \cdot \frac{Gamma\_c}{Gamma\_c - 1} \left(1 - \left(\frac{P\_t}{P\_c}\right)^{\frac{Gamma\_c - 1}{Gamma\_c}}\right)}$$

$$1553.44\ \frac{\text{m}}{\text{s}} \tag{6.16}$$

Ideal specific impulse

```
> Isp_ideal := V_t / grav
```

$$158.35\ \text{s} \tag{6.17}$$

Ideal specific impulse as defied by NASA CEA

```
> Isp_ideal_NASA := V_t
```

$$1553.44\ \frac{\text{m}}{\text{s}} \tag{6.18}$$

Ideal specific impulse in a vacuum.

```
> Isp_vac := V_t + P_t / (rho_t * V_t)
```

$$2848.65\ \frac{\text{m}}{\text{s}} \tag{6.19}$$

Characteristic velocity (C-Star)

```
> Cstar := sqrt(1 / Gamma_c * ((Gamma_c + 1)/2) ^ ((Gamma_c + 1)/
  (Gamma_c - 1)) * R / Mw_mix * T_c)
```

$$2294.05\ \frac{m}{s} \tag{6.20}$$