

$$\gamma := 1.47 \quad M_m := 28.01 \frac{\text{gram}}{\text{mol}} \quad R_s := \frac{R_m}{M_m} = 296.8394 \cdot \frac{1}{\text{K}} \frac{\text{J}}{\text{kg}} \quad R_s = 296.8394 \frac{\text{Gy}}{\text{K}}$$

$$A_3 := 100000 \text{ micron}^2 = 0.1 \text{ mm}^2 \quad A_4 := 100 \cdot \pi \text{ micron}^2 \quad A_5 := 400 \cdot \pi \text{ micron}^2 = 1.2566 \cdot 10^{-9} \text{ m}^2$$

$$T_\theta := 300 \text{ K} \quad p_\theta := 1.5 \text{ bar} \quad A_2 := A_4 \quad A_1 := A_5$$

$$L_{c.1} := 40 \text{ micron} \quad L_{c.2} := 20 \text{ micron} \quad L_{c.3} := 40 \text{ micron} \quad L_{c.4} := 20 \text{ micron} \quad L_{c.5} := 40 \text{ micron}$$

Function Definitions:

Variable Definitions:

Isentropic Massflow:

$$\text{massflow}(\gamma, M, A, T_t, p_t) := A \cdot p_t \cdot \sqrt{\frac{\gamma}{R_s \cdot T_t}} \cdot M \cdot \left(1 + \frac{\gamma-1}{2} \cdot M^2\right)^{-\frac{\gamma+1}{2 \cdot (\gamma-1)}} \quad \text{molecules\_per\_sec}(\text{mdot}, M_m) := \text{mdot} \cdot \frac{N_A}{M_m}$$

Dynamic Viscosity using sutherlands formular:

$$\mu_{ref} := 1.716 \cdot 10^{-5} \frac{\text{N s}}{\text{m}^2} \quad T_{ref} := 276 \text{ K} \quad S_\mu := 111 \text{ K} \quad p_{crit.ratio} := \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} = 0.5168$$

$$\text{sutherland}(T) := \mu_{ref} \cdot \left(\frac{T}{T_{ref}}\right)^{\frac{3}{2}} \cdot \frac{T_{ref} + S_\mu}{T + S_\mu} \quad T_{crit.ratio} := \frac{2}{\gamma+1} = 0.8097$$

Knudsen number:

$$\text{knudsen}(p, T, L_c) := \frac{\text{sutherland}(T) \cdot R_s}{p \cdot L_c} \cdot \sqrt{\frac{\pi \cdot M_m \cdot T}{2 \cdot \text{K} \cdot N_A}}$$

Reynolds number:

$$\text{reynolds}(p, T, L_c, Ma, \gamma) := \frac{Ma}{\text{knudsen}(p, T, L_c)} \cdot \sqrt{\frac{\gamma \cdot \pi}{2}}$$

Isentropic Relations:

$$\text{temp\_to\_total}(\gamma, M) := \left(1 + \frac{\gamma-1}{2} \cdot M^2\right)^{-1} \quad \text{pressure\_to\_total}(\gamma, M) := \left(1 + \frac{\gamma-1}{2} \cdot M^2\right)^{-\frac{\gamma}{\gamma-1}} \quad \text{density\_to\_total}(\gamma, M) := \left(1 + \frac{\gamma-1}{2} \cdot M^2\right)^{-\frac{1}{\gamma-1}}$$

Machnumber solvers:

$$\text{solve\_machnumber\_sub}(A_{ratio}, \gamma) := \text{solve}\left(\frac{1}{M} \cdot \left(\left(\frac{2}{\gamma+1}\right) \cdot \left(1 + \frac{\gamma-1}{2} \cdot M^2\right)\right)^{\frac{\gamma+1}{2 \cdot (\gamma-1)}} - A_{ratio} = 0, M, 0, 1\right)$$

$$\text{solve\_machnumber\_super}(A_{ratio}, \gamma) := \text{solve}\left(\frac{1}{M} \cdot \left(\left(\frac{2}{\gamma+1}\right) \cdot \left(1 + \frac{\gamma-1}{2} \cdot M^2\right)\right)^{\frac{\gamma+1}{2 \cdot (\gamma-1)}} - A_{ratio} = 0, M, 1, 12\right)$$

$$\left(\text{terminal\_velocity}(R, T_\theta, \gamma) := \sqrt{2 \cdot R \cdot \frac{\gamma}{\gamma-1} \cdot T_\theta}\right)$$

### Chapter 3.3: one-dimensional isentropic case

Position 3 (middle of Reactor):

$$M_{3.1} := \text{solve\_machnumber\_sub}(318, \gamma) = \blacksquare \quad \text{From external Solver:} \quad M_{3.2} := \text{solve\_machnumber\_super}(318, \gamma) = 10.543$$

$$M_{3.1} := 0.0018$$

$$m_{3.1} := \text{massflow}(\gamma, M_{3.1}, A_3, T_\theta, p_\theta) = 1.097 \cdot 10^{-7} \frac{\text{kg}}{\text{s}} \quad m_{3.2} := \text{massflow}(\gamma, M_{3.2}, A_3, T_\theta, p_\theta) = 1.1006 \cdot 10^{-7} \frac{\text{kg}}{\text{s}}$$

$$p_{3.1.to.total} := \text{pressure\_to\_total}(\gamma, M_{3.1}) = 1 \quad p_{3.2.to.total} := \text{pressure\_to\_total}(\gamma, M_{3.2}) = 3.2891 \cdot 10^{-5}$$

$$T_{3.1.to.total} := \text{temp\_to\_total}(\gamma, M_{3.1}) = 1 \quad T_{3.2.to.total} := \text{temp\_to\_total}(\gamma, M_{3.2}) = 0.0369$$

Position 2 & 4 (nozzle throats):

$$m_{2.4} := \text{massflow} \left( \gamma, 1, A_4, T_\theta, p_\theta \right) = 1.0995 \cdot 10^{-7} \frac{\text{kg}}{\text{s}}$$

$$m_{1D\_isen} := \text{molecules\_per\_sec} \left( m_{2.4}, M_m \right) = 2.364 \cdot 10^{18} \frac{1}{\text{s}}$$

$$p_{2.4.to.total} := \text{pressure\_to\_total} \left( \gamma, 1 \right) = 0.5168$$

$$\rho_{2.4.to.total} := \text{density\_to\_total} \left( \gamma, 1 \right) = 0.6382$$

$$T_{2.4.to.total} := \text{temp\_to\_total} \left( \gamma, 1 \right) = 0.8097$$

Position 5 (outlet nozzle exit plane):

$$M_{5.1} := \text{solve\_machnumber\_sub} \left( 4, \gamma \right) = 0.1455$$

$$M_{5.2} := \text{solve\_machnumber\_super} \left( 4, \gamma \right) = 3.063$$

$$m_{5.1} := \text{massflow} \left( \gamma, M_{5.1}, A_5, T_\theta, p_\theta \right) = 1.0995 \cdot 10^{-7} \frac{\text{kg}}{\text{s}}$$

$$m_{5.2} := \text{massflow} \left( \gamma, M_{5.2}, A_5, T_\theta, p_\theta \right) = 1.0995 \cdot 10^{-7} \frac{\text{kg}}{\text{s}}$$

$$p_{5.1.to.total} := \text{pressure\_to\_total} \left( \gamma, M_{5.1} \right) = 0.9846$$

$$p_{5.2.to.total} := \text{pressure\_to\_total} \left( \gamma, M_{5.2} \right) = 0.0262$$

$$\rho_{5.1.to.total} := \text{density\_to\_total} \left( \gamma, M_{5.1} \right) = 0.9895$$

$$\rho_{5.2.to.total} := \text{density\_to\_total} \left( \gamma, M_{5.2} \right) = 0.0839$$

$$T_{5.1.to.total} := \text{temp\_to\_total} \left( \gamma, M_{5.1} \right) = 0.9951$$

$$T_{5.2.to.total} := \text{temp\_to\_total} \left( \gamma, M_{5.2} \right) = 0.312$$

## Chapter 3.3: one-dimensional isentropic knudsen and reynolds numbers

knudsen numbers:

$$Kn_1 := \text{knudsen} \left( p_\theta, T_\theta, L_{c.1} \right) = 0.0011$$

$$Kn_{2.4} := \text{knudsen} \left( p_\theta \cdot p_{2.4.to.total}, T_\theta \cdot T_{2.4.to.total}, L_{c.2} \right) = 0.0034$$

$$Kn_{3.1} := \text{knudsen} \left( p_\theta \cdot p_{3.1.to.total}, T_\theta \cdot T_{3.1.to.total}, L_{c.3} \right) = 0.0011$$

$$Kn_{3.2} := \text{knudsen} \left( p_\theta \cdot p_{3.2.to.total}, T_\theta \cdot T_{3.2.to.total}, L_{c.3} \right) = 0.1589$$

$$Kn_{5.1} := \text{knudsen} \left( p_\theta \cdot p_{5.1.to.total}, T_\theta \cdot T_{5.1.to.total}, L_{c.5} \right) = 0.0012$$

$$Kn_{5.2} := \text{knudsen} \left( p_\theta \cdot p_{5.2.to.total}, T_\theta \cdot T_{5.2.to.total}, L_{c.5} \right) = 0.0085$$

reynolds numbers:

$$Re_1 := \text{reynolds} \left( p_\theta, T_\theta, L_{c.1}, \theta, \gamma \right) = 0$$

$$Re_{2.4} := \text{reynolds} \left( p_\theta \cdot p_{2.4.to.total}, T_\theta \cdot T_{2.4.to.total}, L_{c.2}, 1 \right)$$

$$Re_{3.1} := \text{reynolds} \left( p_\theta \cdot p_{3.1.to.total}, T_\theta \cdot T_{3.1.to.total}, L_{c.3}, M_{3.1}, \gamma \right) = 2.3964$$

$$Re_{3.2} := \text{reynolds} \left( p_\theta \cdot p_{3.2.to.total}, T_\theta \cdot T_{3.2.to.total}, L_{c.3}, M \right)$$

$$Re_{5.1} := \text{reynolds} \left( p_\theta \cdot p_{5.1.to.total}, T_\theta \cdot T_{5.1.to.total}, L_{c.5}, M_{5.1}, \gamma \right) = 191.8725$$

$$Re_{5.2} := \text{reynolds} \left( p_\theta \cdot p_{5.2.to.total}, T_\theta \cdot T_{5.2.to.total}, L_{c.5}, M \right)$$

## Chapter 3.5: Disconncted Reservoirs (Isentropic):

$$M_{D.iso} := \left( 1 + \frac{\gamma - 1}{2} \right)^{-\frac{\gamma + 1}{2 \cdot (\gamma - 1)}} = 0.5743$$

$$p_{ratio} := \text{pressure\_to\_total} \left( \gamma, M_{D.iso} \right) = 0.7918$$

$$T_{ratio} := \text{temp\_to\_total} \left( \gamma, M_{D.iso} \right) = 0.9281$$

$$\rho_{ratio} := \text{density\_to\_total} \left( \gamma, M_{D.iso} \right) = 0.7209$$

$$m_{D.iso} := \text{massflow} \left( \gamma, M_{D.iso}, A_2, T_\theta, p_\theta \right) = 9.037 \cdot 10^{-8} \frac{\text{kg}}{\text{s}}$$

$$q_{m.D.isen} := \text{molecules\_per\_sec} \left( m_{D.iso}, M_m \right) = 1.9429 \cdot 10^{18} \frac{1}{\text{s}}$$

## Chapter 3.5: Disconncted Reservoirs (Isothermal):

$$f := \left( -\frac{1}{\gamma-1} + \sqrt{\frac{1}{(\gamma-1)^2} + \frac{2}{\gamma-1} \cdot \left( \frac{2}{\gamma+1} \right)^{\frac{\gamma+1}{\gamma-1}}} \right) \quad M_{D.term} := \sqrt{f} = 0.5546$$

$$f = 0.3076$$

$$p_{ratio} := pressure\_to\_total \left( \gamma , M_{D.term} \right) = 0.8039 \quad T_{ratio} := temp\_to\_total \left( \gamma , M_{D.term} \right) = 0.9326$$

$$\rho_{ratio} := density\_to\_total \left( \gamma , M_{D.term} \right) = 0.862$$

$$m_{D.term} := massflow \left( \gamma , M_{D.term} , A_2 , T_{\theta} , p_{\theta} \right) = 8.8392 \cdot 10^{-8} \frac{kg}{s}$$

$$q_{m.D.iso} := molecules\_per\_sec \left( m_{D.term} , M_m \right) = 1.9004 \cdot 10^{18} \text{ Hz}$$

Chapter 3.5: Formulation with leak (isentropic connection):

$$m_{L.isen} \left( A , \gamma , T_r , p_r \right) := A \cdot p_r \cdot \sqrt{\frac{\gamma}{R_s \cdot T_r}} \cdot \left( 1 - \left( 1 + \frac{\gamma-1}{2} \right)^{-\frac{\gamma+1}{2 \cdot (\gamma-1)}} \right)$$

$$p_r := p_{crit.ratio} \cdot p_{\theta} = 0.7752 \text{ bar} \quad T_r := T_{crit.ratio} \cdot T_{\theta} = 242.915 \text{ K}$$

$$m_{L.isen} := m_{L.isen} \left( A_4 , \gamma , T_r , p_r \right) = 4.6808 \cdot 10^{-8} \frac{kg}{s}$$

$$q_{m.L.isen} := molecules\_per\_sec \left( m_{L.isen} , M_m \right) = 1.0064 \cdot 10^{18} \text{ Hz}$$

Chapter 3.5: Formulation with leak (isothermal connection):

$$m_{L.iso} \left( A , \gamma , T , p_r \right) := A \cdot p_r \cdot \sqrt{\frac{\gamma}{R_s \cdot T}} \cdot \left( 1 + \frac{\gamma-1}{2} \right)^{-\frac{\gamma+1}{2 \cdot (\gamma-1)}} \cdot \left( \left( 1 + \frac{\gamma-1}{2} \right)^{\frac{\gamma}{\gamma-1}} - 1 \right)$$

$$m_{L.isot} := m_{L.iso} \left( A_4 , \gamma , T_{\theta} , p_r \right) = 5.3133 \cdot 10^{-8} \frac{kg}{s}$$

$$q_{m.L.iso} := molecules\_per\_sec \left( m_{L.isot} , M_m \right) = 1.1424 \cdot 10^{18} \text{ Hz}$$

Chapter 3.6: Maximum turning angle

$$\theta_{max} := \frac{\pi}{2} \cdot \left( \sqrt{\frac{\gamma+1}{\gamma-1}} - 1 \right) - \sqrt{\frac{\gamma+1}{\gamma-1}} \cdot \operatorname{atan} \left( \sqrt{\frac{\gamma-1}{\gamma+1} \cdot \left( M_{5.2}^2 - 1 \right)} \right) + \operatorname{atan} \left( \sqrt{M_{5.2}^2 - 1} \right) = 68.912 \text{ deg}$$

Terminal velocity:

$$v_{infty} := terminal\_velocity \left( R_s , T_{\theta} , \gamma \right) = 746.3562 \frac{m}{s}$$

$$T_{max} := 600 \text{ K}$$

$$v_{infty} := terminal\_velocity \left( R_s , T_{max} , \gamma \right) = 1055.5071 \frac{m}{s}$$