

Variable Definitions:

$$\begin{aligned} \gamma &:= 1.47 & M_m &:= 28.01 \frac{\text{gram}}{\text{mol}} & R_s &:= \frac{R_m}{M_m} = 296.8394 \cdot \frac{1}{\text{K}} \frac{\text{J}}{\text{kg}} \\ A_3 &:= 100000 \text{ micron}^2 = 0.1 \text{ mm}^2 & A_4 &:= 100 \cdot \pi \text{ micron}^2 & A_5 &:= 400 \cdot \pi \text{ micron}^2 \\ T_t &:= 500 \text{ K} & p_t &:= 1.5 \text{ bar} & A_2 &:= A_4 & A_1 &:= A_5 \\ L_{c.1} &:= 40 \text{ micron} & L_{c.2} &:= 40 \text{ micron} & L_{c.3} &:= 40 \text{ micron} & L_{c.4} &:= 20 \text{ micron} & L_{c.5} &:= 40 \text{ micron} \end{aligned}$$

Function Definitions:

Isentropic Massflow:

$$\text{massflow}(\gamma, M, A, T_t, p_t) := A \cdot p_t \cdot \sqrt{\frac{\gamma}{R_s \cdot T_t}} \cdot M \cdot \left(1 + \frac{\gamma-1}{2} \cdot M^2\right)^{-\frac{\gamma+1}{2 \cdot (\gamma-1)}}$$

Dynamic Viscosity using sutherlands formular:

$$\begin{aligned} \mu_{ref} &:= 1.716 \cdot 10^{-5} \frac{\text{N s}}{\text{m}} & T_{ref} &:= 276 \text{ K} & S_\mu &:= 111 \text{ K} & p_{crit.ratio} &:= \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} = 0.5168 \\ \text{sutherland}(T) &:= \mu_{ref} \cdot \left(\frac{T}{T_{ref}}\right)^{\frac{3}{2}} \cdot \frac{T_{ref} + S_\mu}{T + S_\mu} & T_{crit.ratio} &:= \frac{2}{\gamma+1} = 0.8097 \end{aligned}$$

Knudsen number:

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

Reynolds number:

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

Isentropic Relations:

$$\begin{aligned} \text{temp_to_total}(\gamma, M) &:= \left(1 + \frac{\gamma-1}{2} \cdot M^2\right)^{-1} & \text{pressure_to_total}(\gamma, M) &:= \left(1 + \frac{\gamma-1}{2} \cdot M^2\right)^{-\frac{\gamma}{\gamma-1}} \\ \text{density_to_total}(\gamma, M) &:= \left(1 + \frac{\gamma-1}{2} \cdot M^2\right)^{-\frac{1}{\gamma-1}} \end{aligned}$$

Machnumber solvers:

$$\begin{aligned} \text{solve_machnumber_sub}(A_{ratio}, \gamma) &:= \text{solve} \left(\frac{1}{M} \cdot \left(\left(\frac{2}{\gamma+1} \right) \cdot \left(1 + \frac{\gamma-1}{2} \cdot M^2 \right) \right)^{\frac{\gamma+1}{2 \cdot (\gamma-1)}} - A_{ratio} = 0, M, 0, 1 \right) \\ \text{solve_machnumber_super}(A_{ratio}, \gamma) &:= \text{solve} \left(\frac{1}{M} \cdot \left(\left(\frac{2}{\gamma+1} \right) \cdot \left(1 + \frac{\gamma-1}{2} \cdot M^2 \right) \right)^{\frac{\gamma+1}{2 \cdot (\gamma-1)}} - A_{ratio} = 0, M, 1, 12 \right) \end{aligned}$$

Chapter 3.3: one-dimensional isentropic case

Position 3 (middle of Reactor):

$$\begin{aligned} M_{3.1} &:= \text{solve_machnumber_sub}(318, \gamma) = \blacksquare & \text{From external Solver:} & & M_{3.2} &:= \text{solve_machnumber_super}(318, \gamma) = 10.543 \\ & & M_{3.1} &:= 0.0018 \end{aligned}$$

$$\begin{aligned} m_{3.1} &:= \text{massflow}(\gamma, M_{3.1}, A_3, T_t, p_t) = 8.4972 \cdot 10^{-8} \frac{\text{kg}}{\text{s}} & m_{3.2} &:= \text{massflow}(\gamma, M_{3.2}, A_3, T_t, p_t) = 8.5253 \cdot 10^{-8} \frac{\text{kg}}{\text{s}} \end{aligned}$$

$$p_{3.1.to.total} := pressure_to_total \left(\gamma, M_{3.1} \right) = 1$$

$$T_{3.1.to.total} := temp_to_total \left(\gamma, M_{3.1} \right) = 1$$

$$p_{3.2.to.total} := pressure_to_total \left(\gamma, M_{3.2} \right) = 3.2891 \cdot 10^{-5}$$

$$T_{3.2.to.total} := temp_to_total \left(\gamma, M_{3.2} \right) = 0.0369$$

Position 2 & 4 (nozzle throats):

$$m_{2.4} := massflow \left(\gamma, 1, A_4, T_t, p_t \right) = 8.517 \cdot 10^{-8} \frac{\text{kg}}{\text{s}}$$

$$p_{2.4.to.total} := pressure_to_total \left(\gamma, 1 \right) = 0.5168$$

$$\rho_{2.4.to.total} := density_to_total \left(\gamma, 1 \right) = 0.6382$$

$$T_{2.4.to.total} := temp_to_total \left(\gamma, 1 \right) = 0.8097$$

Position 5 (outlet nozzle exit plane):

$$M_{5.1} := solve_machnumber_sub \left(4, \gamma \right) = 0.1455$$

$$m_{5.1} := massflow \left(\gamma, M_{5.1}, A_5, T_t, p_t \right) = 8.5169 \cdot 10^{-8} \frac{\text{kg}}{\text{s}}$$

$$p_{5.1.to.total} := pressure_to_total \left(\gamma, M_{5.1} \right) = 0.9846$$

$$\rho_{5.1.to.total} := density_to_total \left(\gamma, M_{5.1} \right) = 0.9895$$

$$T_{5.1.to.total} := temp_to_total \left(\gamma, M_{5.1} \right) = 0.9951$$

$$M_{5.2} := solve_machnumber_super \left(4, \gamma \right) = 3.063$$

$$m_{5.2} := massflow \left(\gamma, M_{5.2}, A_5, T_t, p_t \right) = 8.517 \cdot 10^{-8} \frac{\text{kg}}{\text{s}}$$

$$p_{5.2.to.total} := pressure_to_total \left(\gamma, M_{5.2} \right) = 0.0262$$

$$\rho_{5.2.to.total} := density_to_total \left(\gamma, M_{5.2} \right) = 0.0839$$

$$T_{5.2.to.total} := temp_to_total \left(\gamma, M_{5.2} \right) = 0.312$$

Chapter 3.3: one-dimensional isentropic knudsen and reynolds numbers

knudsen numbers:

$$Kn_1 := knudsen \left(p_t, T_t, L_{c.1} \right) = 0.0021 \quad Kn_{2.4} := knudsen \left(p_t \cdot p_{2.4.to.total}, T_t \cdot T_{2.4.to.total}, L_{c.2} \right) = 0.0032$$

$$Kn_{3.1} := knudsen \left(p_t \cdot p_{3.1.to.total}, T_t \cdot T_{3.1.to.total}, L_{c.3} \right) = 0.0021 \quad Kn_{3.2} := knudsen \left(p_t \cdot p_{3.2.to.total}, T_t \cdot T_{3.2.to.total}, L_{c.3} \right) = 0.4161$$

$$Kn_{5.1} := knudsen \left(p_t \cdot p_{5.1.to.total}, T_t \cdot T_{5.1.to.total}, L_{c.5} \right) = 0.0022 \quad Kn_{5.2} := knudsen \left(p_t \cdot p_{5.2.to.total}, T_t \cdot T_{5.2.to.total}, L_{c.5} \right) = 0.0181$$

reynolds numbers:

$$Re_1 := reynolds \left(p_t, T_t, L_{c.1}, 0.001, \gamma \right) = 1.4035 \quad Re_{2.4} := reynolds \left(p_t, T_t, L_{c.2}, 1, \gamma \right) = 0.0014$$

$$Re_{3.1} := reynolds \left(p_t, T_t, L_{c.3}, M_{3.1}, \gamma \right) = 0.7797 \quad Re_{3.2} := reynolds \left(p_t, T_t, L_{c.3}, M_{3.2}, \gamma \right) = 0.0001$$

$$Re_{5.1} := reynolds \left(p_t, T_t, L_{c.5}, M_{5.1}, \gamma \right) = 0.0096 \quad Re_{5.2} := reynolds \left(p_t, T_t, L_{c.5}, M_{5.2}, \gamma \right) = 0.0005$$

Chapter 3.5: Disconneted Reservoirs (Isentropic):

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

$$p_{ratio} := pressure_to_total \left(\gamma, M_{D.iso} \right) = 0.7918 \quad T_{ratio} := temp_to_total \left(\gamma, M_{D.iso} \right) = 0.9281$$

$$\rho_{ratio} := density_to_total \left(\gamma, M_{D.iso} \right) = 0.8531$$

$$m_{D.term} := massflow \left(\gamma, M_{D.iso}, A_2, T_t, p_t \right) = 7 \cdot 10^{-8} \frac{\text{kg}}{\text{s}}$$

Chapter 3.5: Disconncted Reservoirs (Isothermal):

$$f := \left(-\frac{1}{\gamma-1} + \sqrt{\frac{1}{(\gamma-1)^2} + \frac{2}{\gamma-1} \cdot \left(\frac{2}{\gamma+1} \right)^{\frac{\gamma+1}{\gamma-1}}} \right) = 0.3076 \quad M_{D.term} := \sqrt{f} = 0.5546$$

$$p_{ratio} := pressure_to_total(\gamma, M_{D.term}) = 0.8039 \quad T_{ratio} := temp_to_total(\gamma, M_{D.term}) = 0.9326$$

$$\rho_{ratio} := density_to_total(\gamma, M_{D.term}) = 0.862$$

$$m_{D.term} := massflow(\gamma, M_{D.term}, A_2, T_t, \rho_t) = 6.8468 \cdot 10^{-8} \frac{\text{kg}}{\text{s}}$$

Chapter 3.5: Formulation with leak (isentropic connection):

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

$$p_r := p_{crit.ratio} \cdot p_t = 0.7752 \text{ bar} \quad T_r := T_{crit.ratio} \cdot T_t = 404.8583 \text{ K}$$

$$m_{L.isen}(A_4, \gamma, T_r, p_r) = 3.6258 \cdot 10^{-8} \frac{\text{kg}}{\text{s}}$$

Chapter 3.5: Formulation with leak (isothermal connection):

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

$$m_{L.iso}(A_4, \gamma, T_r, p_r) = 4.5737 \cdot 10^{-8} \frac{\text{kg}}{\text{s}}$$

Chapter 3.2: expected knudsen number

Test:

$$\alpha := 0.06 \frac{\text{Pa}}{\frac{\text{K}}{2}}$$

$$Kn := knudsen(1 \text{ bar}, 300 \text{ K}, 20 \text{ micron}) = 0.0034$$

$$p := \alpha \cdot \frac{T_t}{0.1} = 0.0671 \text{ bar}$$

$$p := 1 \text{ bar} \quad a := \frac{p \cdot Kn}{\frac{T_t}{2}} = 0.0021 \frac{\text{Pa}}{\frac{\text{K}}{2}}$$

Chapter 3.6: Maximum turning angle

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