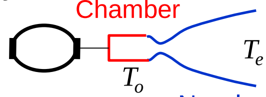
Thermochemistry Overview

- For chemical rockets, we have already examined some aspects of propellant storage and **ideal** nozzle flow
  - e.g., non-reacting gas



- But what can happen to propellant going through nozzle?
  - e.g., NH_3, N_2, H_2 products of hydrazine resistojet
    - at T_o=2500 K, p_o=50 psi we might expect mostly N_2, H_2 and H in the products
    - ideal calculation of T_e (for p_e/p_o~10^{-3})

$$T_e = T_o\left(10^{-3}\right)^{\gamma/(\gamma-1)}$$
$$T_e = 500-700K$$

  - will composition change at these lower temperatures (less H, H_2; more NH_3)?
    - will change MW, c_p and T_e

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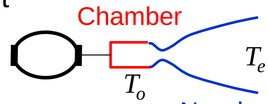


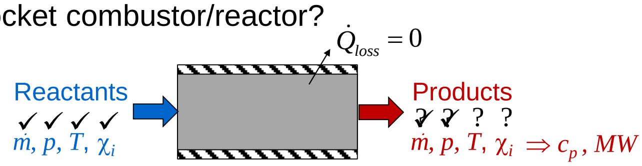
- Also, how do we determine conditions exiting combustion/reaction chamber ?
  - most accurate calculation requires understanding flow field and finite rate chemistry (reaction rates)
  - but is there approach that can provide a good estimate of T_o and composition (MW, c_p, …) ?

Equilibrium Thermochemistry

- Answer is yes – **Chemical Equilibrium**
- For most rocket combustors
  - the exit T_o and composition (major products) can be reasonably approximated assuming chemical equilibrium
- For nozzles
  - the chemical equilibrium assumption provides an **upper bound** on the nozzle exit velocity and thus the rocket performance
  - **frozen flow** (no composition change, very slow reactions) provides a **lower bound**

Our Problem: Combustor Example

- What is general form of chemical equilibrium problem for rocket combustor/reactor?



  - steady – e.g., apply mass conservation ($\dot{m}_{out} = \dot{m}_{in}$)
  - often near constant pressure internally ($p_{out} = p_{in}$)
  - often also assume adiabatic
- So generally we need to do find
  - product composition (mole χ or mass Y fractions)
  - (adiabatic) product (flame) temperature (e.g, T_o)