AUTOMOTIVE CO2 MITIGATION USING AN ONBOARD BOSCH REACTOR: ANALYSIS

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OBJECTIVE

- Determine the technical and economic requirements of an automotive CO_2 reduction system
  - Determine preferred carbon product and method of expulsion from vehicle
  - Determine cost contributors
- Conduct a techno-economic and lifecycle analysis of implementing an automotive Bosch reactor
  - Determine the optimal operating conditions
  - Determine the optimal design

AUTOMOTIVE CO_2 REDUCTION

- Preferred carbon product
  - Non-corrosive
  - Cheap to dispose
  - Non-gaseous
- Cost Goals
  - Minimize the amount of hydrogen required to store onboard
  - Determine feasibility of regenerative and non-regenerative catalysts
  - Need to mitigate carbon "coking" on catalyst surface

BOSCH REACTION

- Composed of 4 different reactions

Reaction	Formula	ΔH
Reverse Water Gas Shift	$CO_2 + H_2 \rightarrow CO + H_2O$	41 kJ/mol
Hydrogenation	$CO + H_2 \rightarrow C(s) + H_2O$	-131 kJ/mol
Boudouard	$2CO \rightarrow C(s) + CO_2$	-172 kJ/mol
Sabatier	$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$	-165.4 kJ/mol

REACTION RATES (EQUILIBRIUM CONSTANTS)

- Developed by solving each species' transport equation simultaneously with its energy balance
- Temperature dependent equilibrium constants developed by comparing fugacity ratios to differences in Gibb's free energies at actual and reference conditions (chemical activity)

$$K_i = \exp\left[\frac{\lambda_1}{T^2} + \frac{\lambda_2}{T} + \lambda_3\right]$$

Description	Reaction	Equation	λ_1	λ_2	λ_3
1. CO_2 Methanation	$CO_2 + 4H_2 \rightleftharpoons CH_4 + 2H_2O$	Eq. 1	-730,726.0	24,125.3	-26.9616
2. CO Methanation	$CO + 3H_2 \rightleftharpoons CH_4 + H_2O$	Eq. 2	-538,798.1	28,062.7	-30.7759
3. Reverse WGS	$CO_2 + H_2 \rightleftharpoons CO + H_2O$	Eq. 4	-191,928.1	-3,937.4	3.8143
4. Hydrogenation	$CO + H_2 \rightleftharpoons C(s) + H_2O$	Eq. 5	-121,003.4	16,573.0	-17.3858
5. Boudouard	$2CO \rightleftharpoons C(s) + CO_2$	Eq. 6	70,924.7	20,510.4	-21.2000

REACTION RATES (GAS PHASE EQUILIBRIA)

- Methanation
- RWGS
- Hydrogenation
- Boudouard

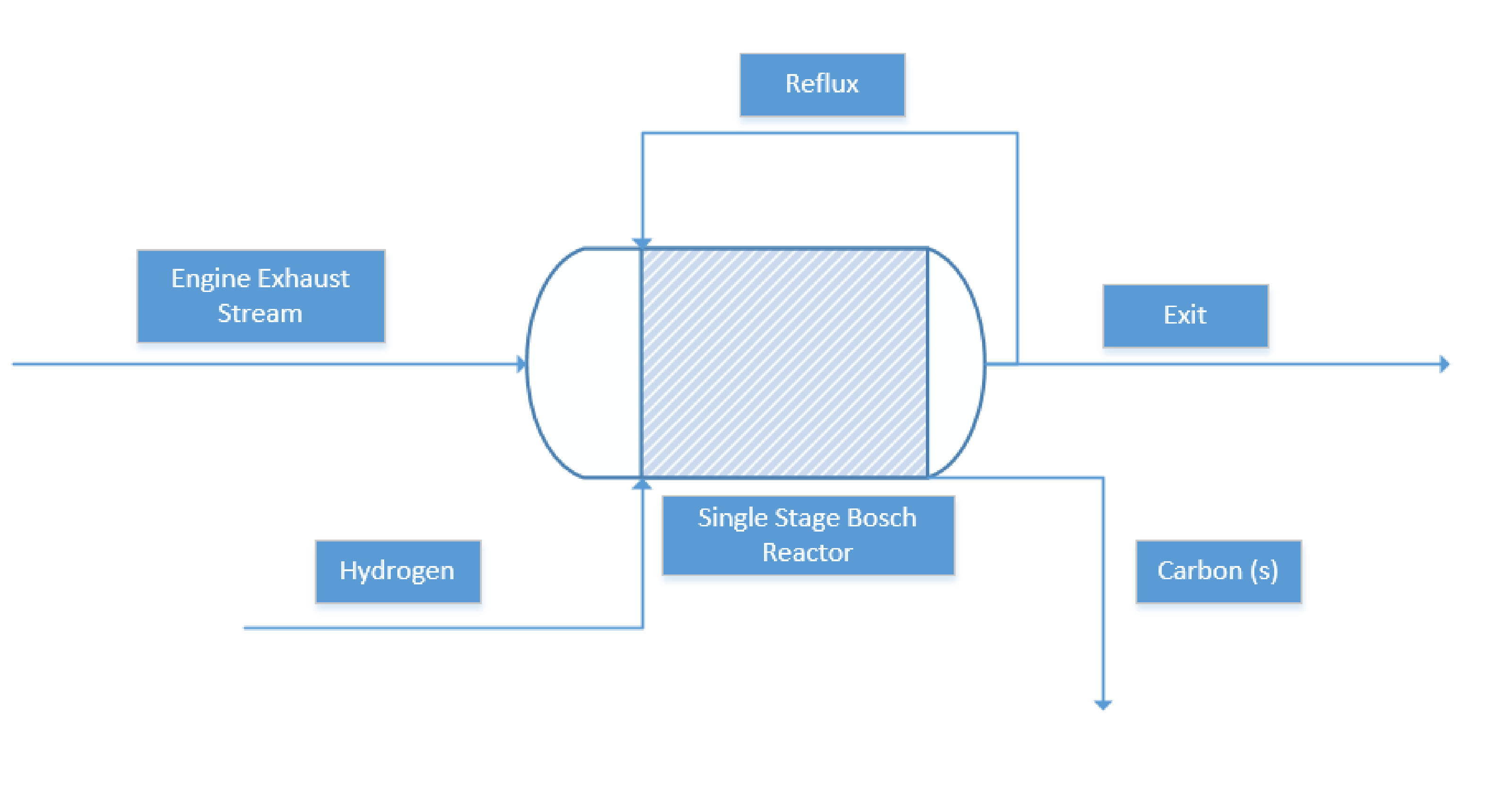
$$r_1 = \frac{k_1 K_{CO_2,1} K_{H_2,1}^4 z_{CO_2} z_{H_2}^4 P^5}{\left(1 + K_{CO_2,1} P z_{CO_2} + K_{H_2,1} P z_{H_2}\right)^5} (1 - \eta)$$

$$r_3 = k_3 \rho P \left(z_{CO_2} z_{H_2} K_3 - z_{CO} z_{H_2O}\right)$$

$$r_4 = k_4 \rho \left(z_{CO} z_{H_2} K_4 P - z_{H_2O}\right)$$

$$r_5 = \frac{\rho_{\text{cat}} \epsilon_o k_B^+ K_{CO,5} \left(P z_{CO} - \frac{1}{K_B^*} \frac{z_{CO_2}}{z_{CO}}\right)}{\left(1 + K_{CO,5} P z_{CO} + \frac{1}{K_{O,CO_2} K_{CO,5}} \frac{z_{CO_2}}{z_{CO}}\right)^2}$$

PROPOSED REACTOR DESIGN

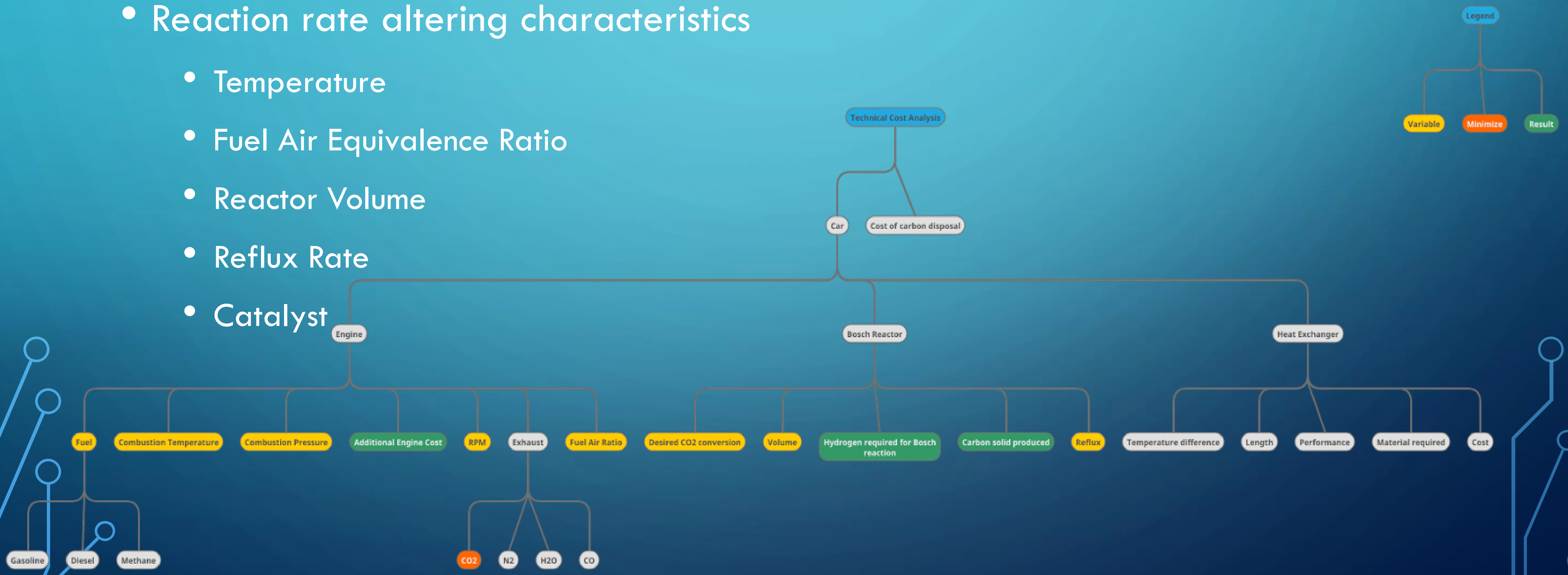


CATALYST COKING

- Assume nickel catalyst is completely regenerative
  - Needs mechanical or magnetic agitation
- For ~105kg CO_2 in 1 tank of fuel
  - 1.38 kg steel wool required (packing density = $0.2 g/cm^3$)
    - Volume steel wool required to avoid coking disadvantage = $0.0069 m^3$

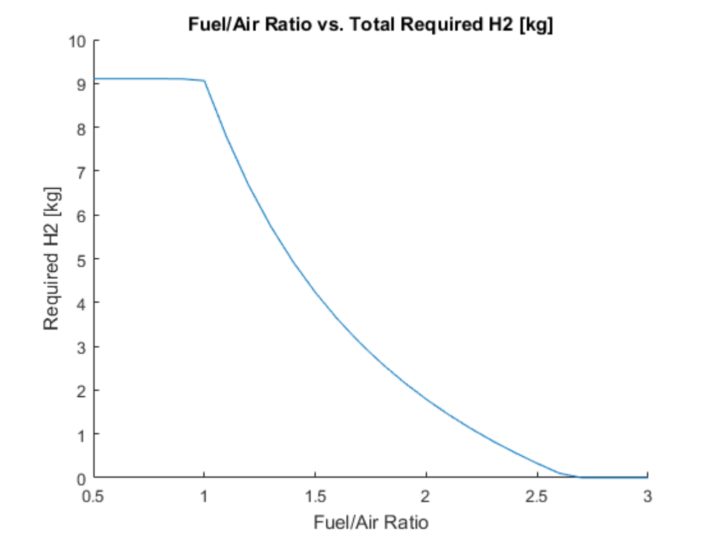
PROCESS CONSIDERATIONS

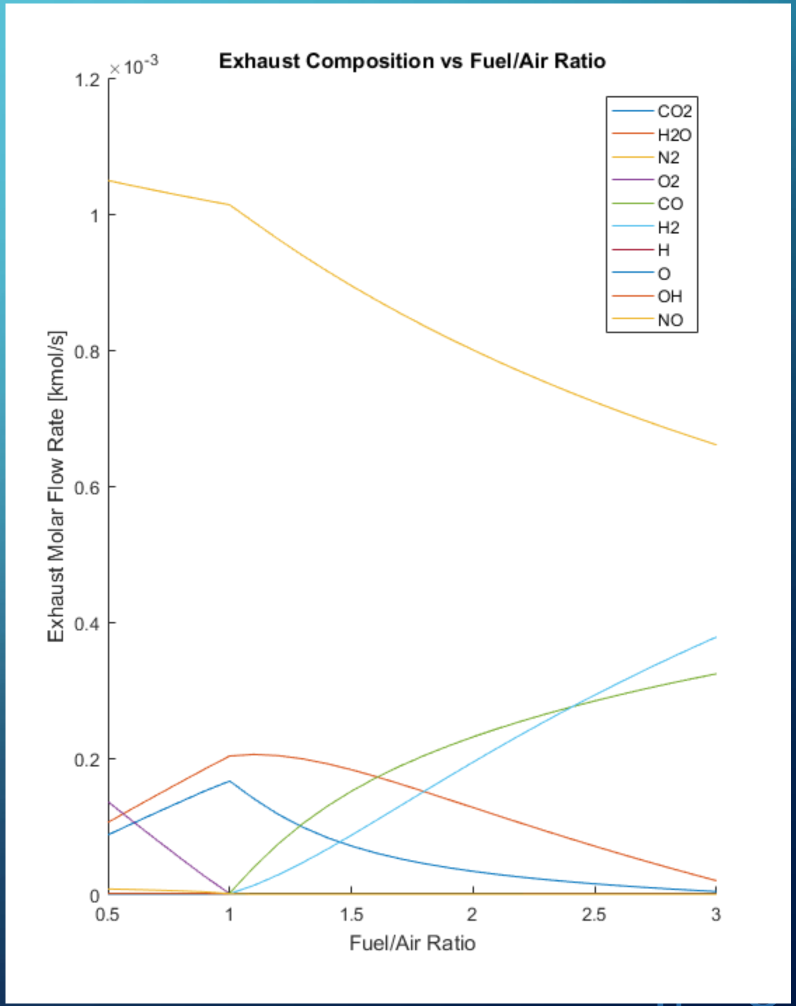
- Reaction rate altering characteristics
  - Temperature
  - Fuel Air Equivalence Ratio
  - Reactor Volume
  - Reflux Rate
  - Catalyst



ENGINE EXHAUST STREAM

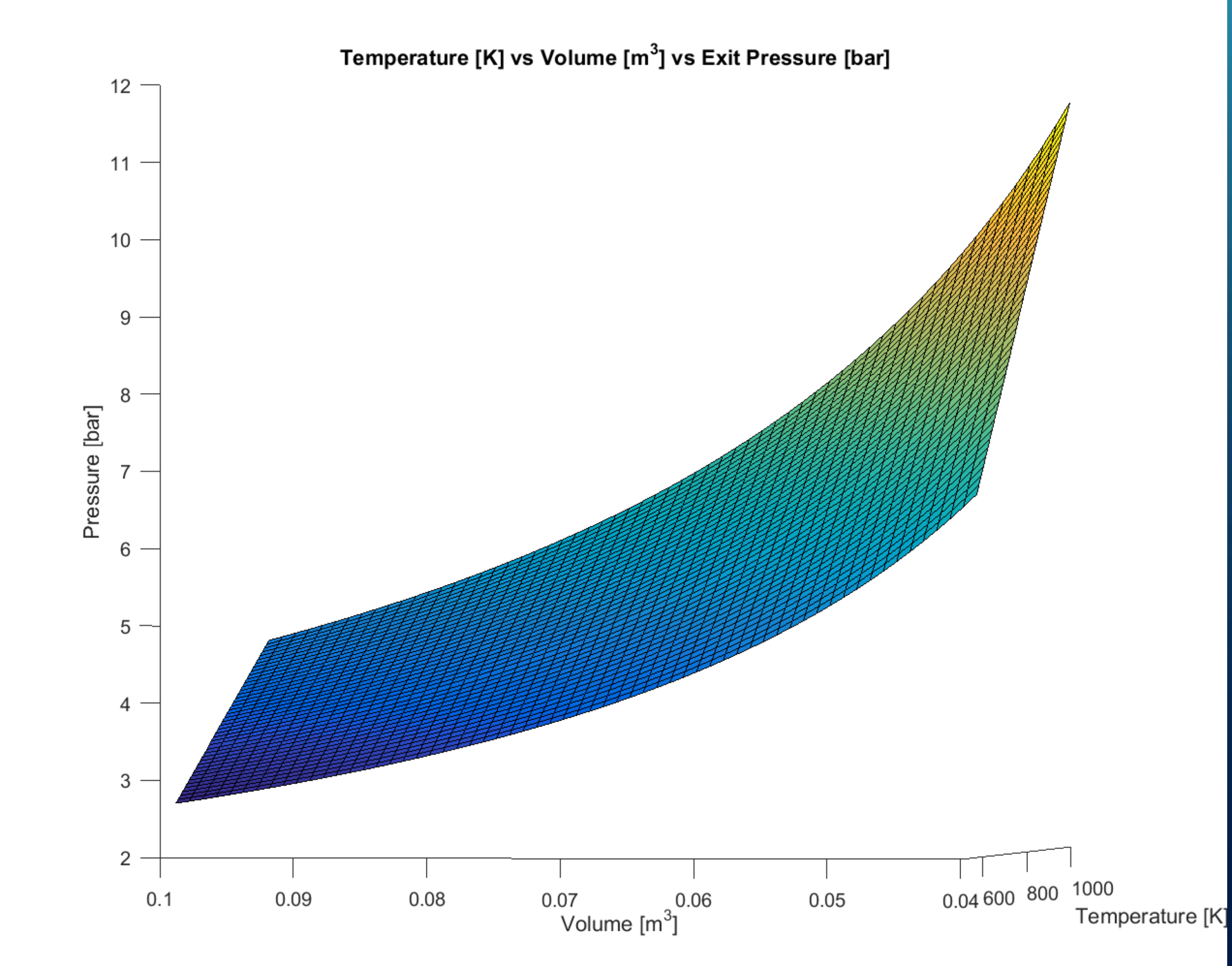
- Higher Fuel/Air Equivalence Ratio → More H_2 produced in combustion
  - Less H_2 required in onboard tanks
  - Higher concentration of CO
  - Decreases fuel economy





EFFECT OF REACTOR VOLUME

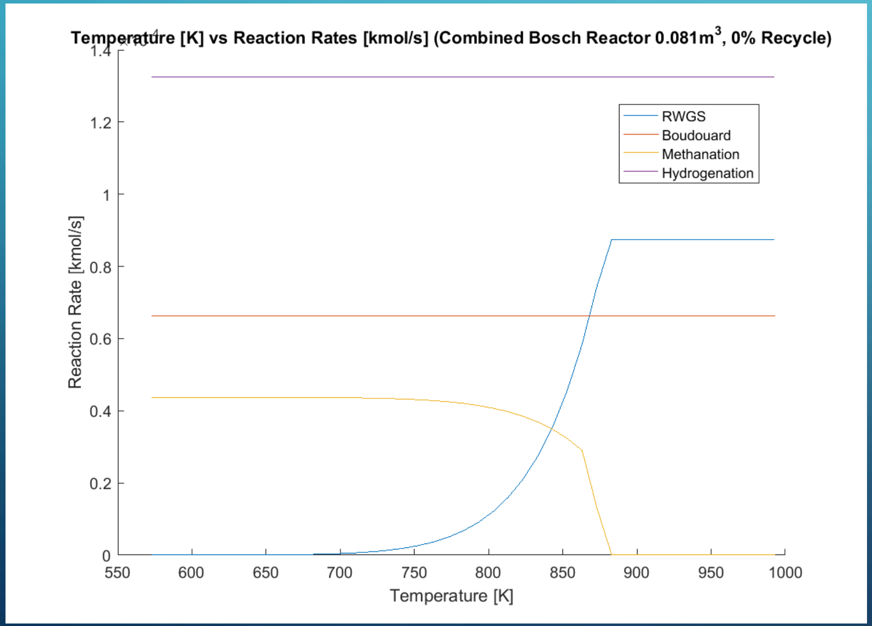
- Higher Volume → Lower Conversion
  - Lower pressure (diffuse)
  - Lower reaction rate
- Lower Volume → Higher Conversion
  - Higher pressure
  - Higher activity
  - Higher reaction rate
  - Need to minimize exit pressure



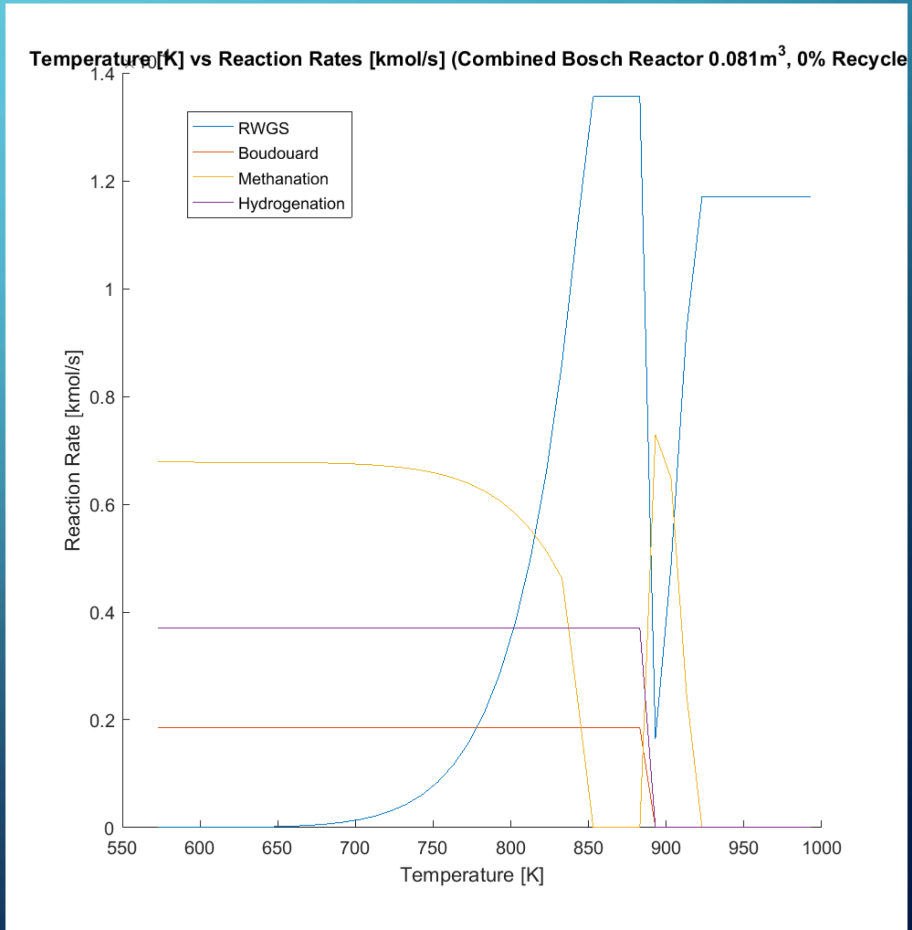
EFFECT OF TEMPERATURE (RATES)

- Directly affects reaction rate constant
  - Higher T → RWGS
  - Lower T → Methanation

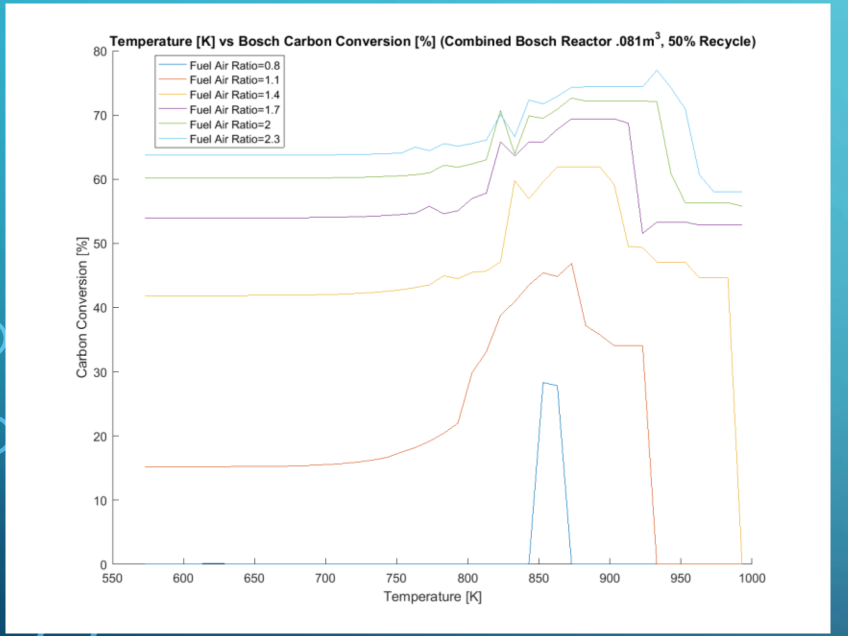
Fuel Air Ratio= 2.3

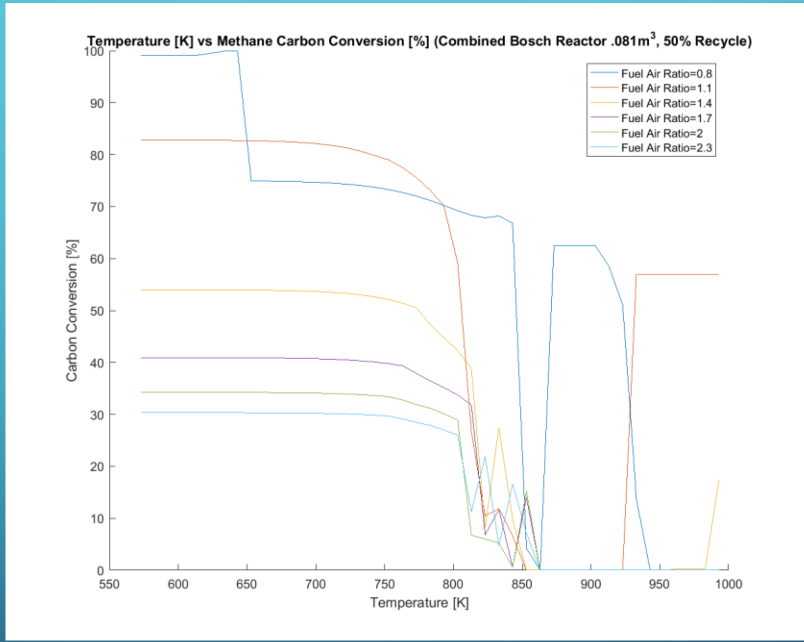


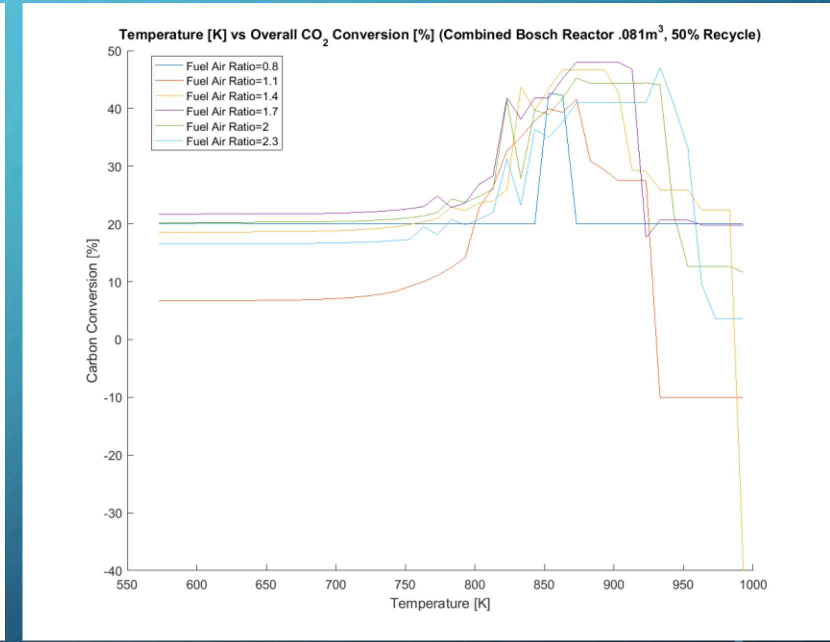
Fuel Air Ratio= 1.2



EFFECT OF TEMPERATURE (CONVERSION)

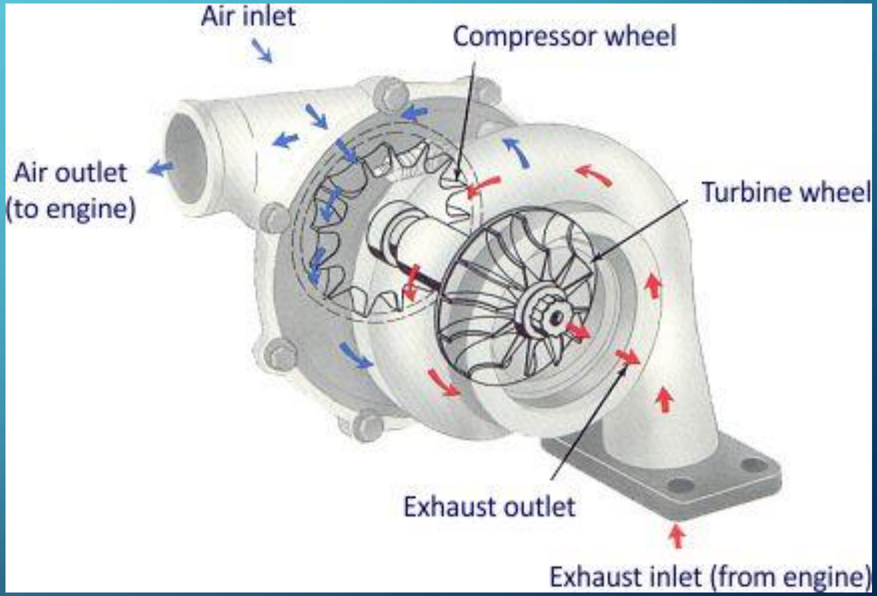






WHY INCREASE FUEL AIR RATIO?

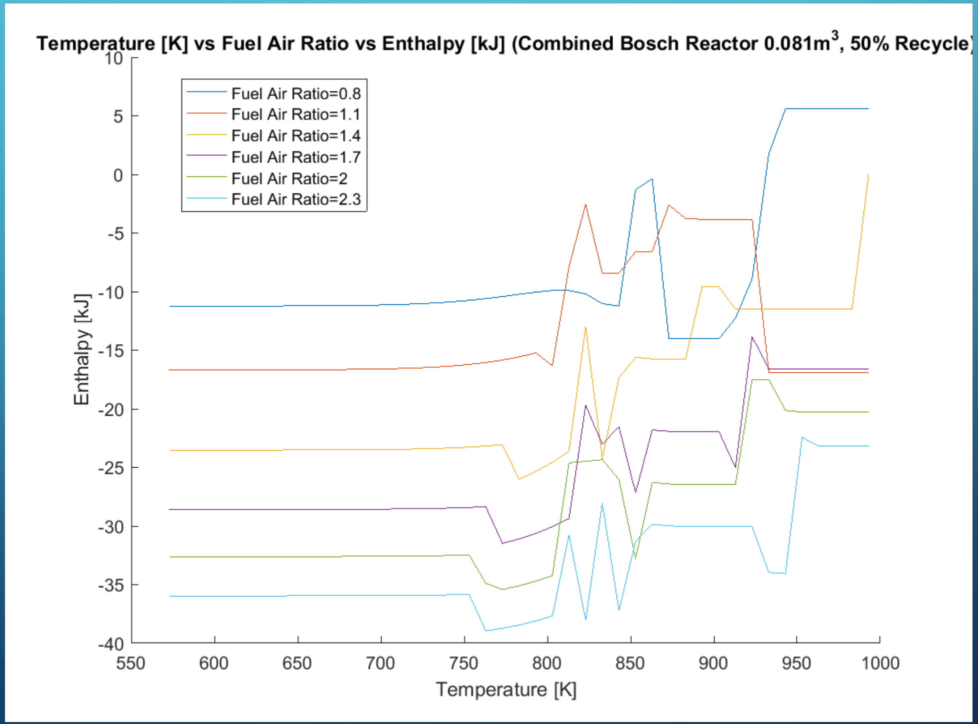
- Produce more CO and H_2 in combustion equilibrium
- Bypass RWGS reduction (endothermic)
- Increased power generation
  - Higher fuel content
  - Improved turbo-diesel operation
- One less methanation stage
- Can mitigate higher fuel use by decreasing engine size
  - Lower Volumetric Flow Rate



https://www.dieselnet.com/tech/images/air/turbo/~turbocharger.jpg

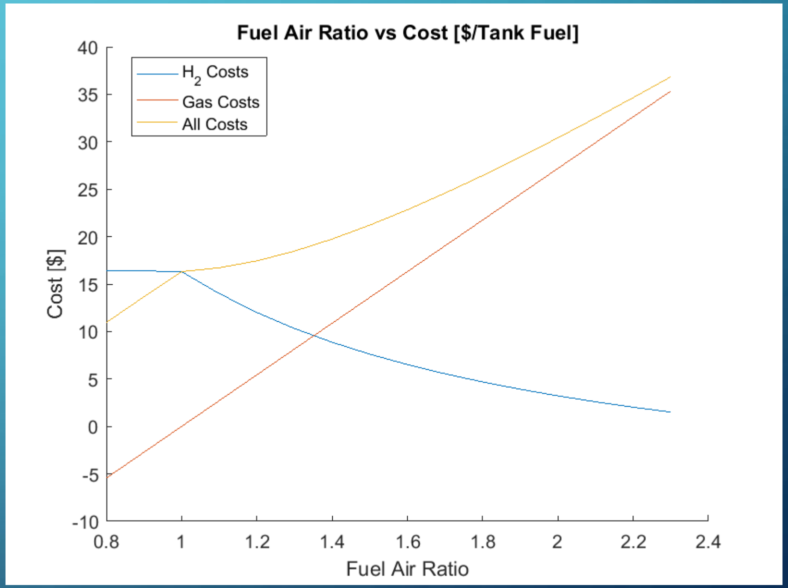
ENERGY & CARBON BALANCE

- Carbon expelled per tank ~= 74% * 30.1 kg C / tank = 22.7 kg carbon / tank



COST FACTORS

Cost Factor	Cost
H_2 Tanks	$250/tank
Reactor Cost	$1600 or $50/tank
H_2 Cost / kg	$1.80/kg
Additional Fuel Cost / gal	$2.27/gal



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