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Dynamic Modeling of a Compressed Gas Catalytic Engine Reactor

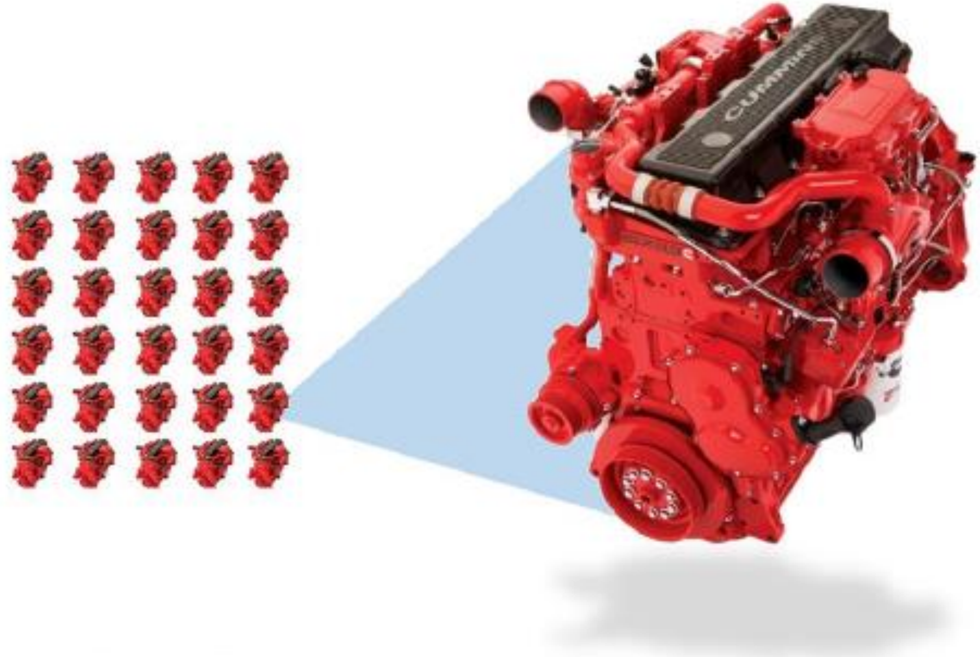
Date: 11/14/2016

Presented by: Jeff Rogers

Overview of Project

- Project Description
- Concept Selection
- Engine Reactor Design Optimization

Steam Cracker Furnace
(600 tpd ethylene)



Engine Reactor Array
(600 tpd ethylene)

Engine Reactor
(20 tpd ethylene)

tpd = tons per day

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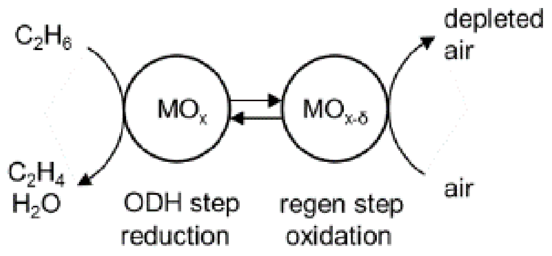
Project Description

- Internal combustion engines (ICE) are relatively inexpensive, abundant and durable. This project examines repurposing ICEs to create a high throughput, scalable gaseous chemical reactor.



- Demonstration Process: Converting ethane (C_2H_6) to ethylene (C_2H_4) using oxidative dehydrogeneration (ODH) reaction mechanism in catalyst to improve yield and reduce energy use and emissions.

- Engine Reactor Technology Potential: Efficient, low emissions, economical and scalable

Metric	State-of-the-Art Cracker	Proposed Reactor Engine
Ethylene per pass yield	60%	> 70%
Reactor volumetric productivity (GHSV)	3,000-6,000 h^{-1}	900,0000 h^{-1}
Reactor unit capacity ethylene	200-600 tpd	> 20 tpd
Process intensity	0.04 kg/m^3s	> 400 kg/m^3s
Reactor capital cost	$102/tpy	$1/tpy
Carbon dioxide emissions	1 t_{CO2}/t_{C2H4}	< 0.1 t_{CO2}/t_{C2H4}

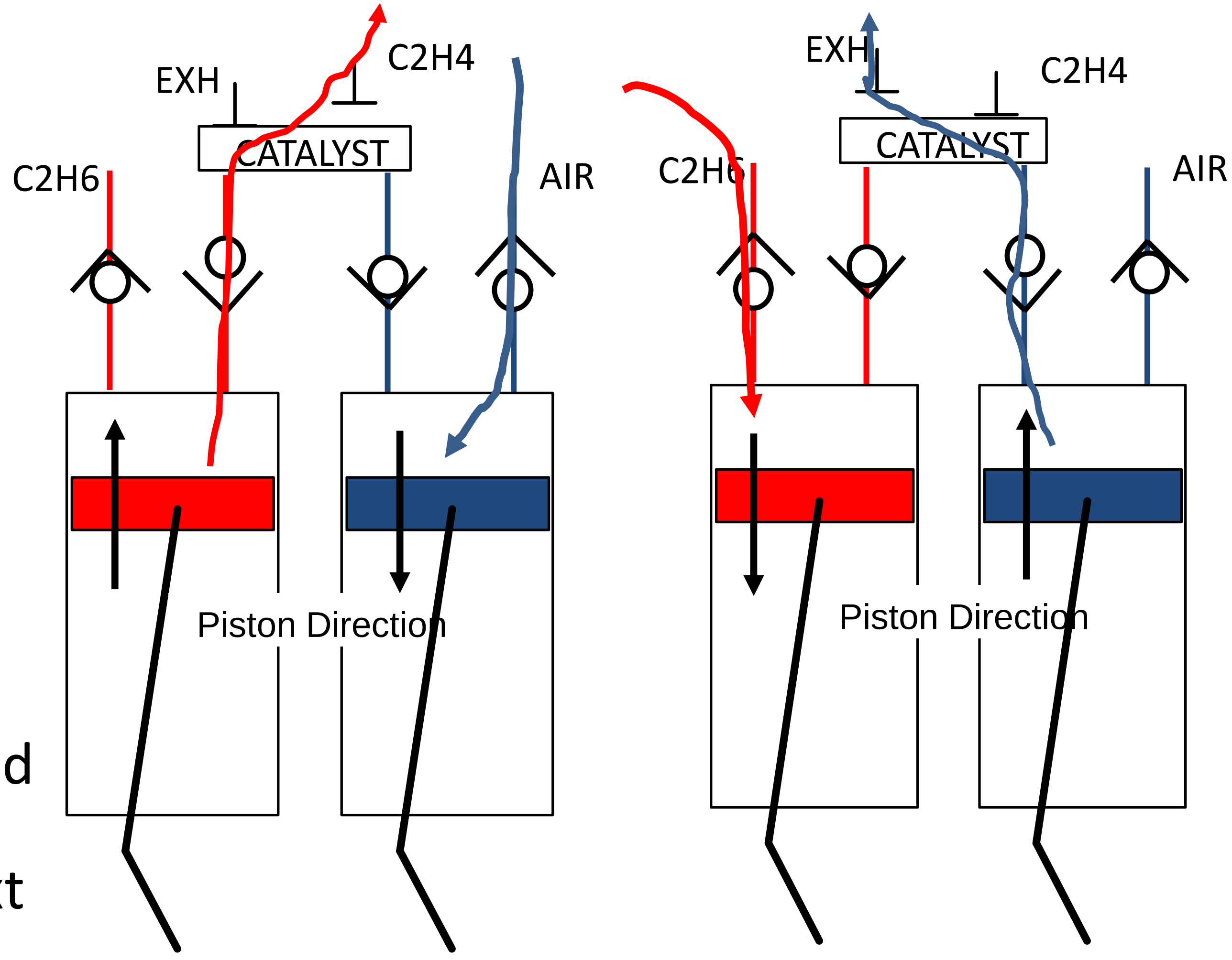
Major Performance Considerations

- Maximize mass of product output per mass of reactant input
  - Maximize volumetric efficiency for reactant flows
  - Minimize product/reactant mixing in the reaction volume

- Minimize energy used per mass of product output
  - Reduce cylinder and head heat transfer
  - Maximize conversion of ethane in reaction volume

Process Description – Dual Cylinder Example

- Feed stock (ethane) is compressed in cylinder to 850 C (1120 K) and 25 bar and passed through catalyst loaded with oxygen. Catalyst reactions strongly favor ethylene production at these conditions.
- Ethylene removed from reaction zone (catalyst) at product exit port and catalyst zone flooded with air at 650 K and 25 bar to reload catalyst with oxygen for next cycle.
- Excess air removed at exhaust gas port and catalyst zone re-flooded with feed stock stream from compression cylinder for next cycle.



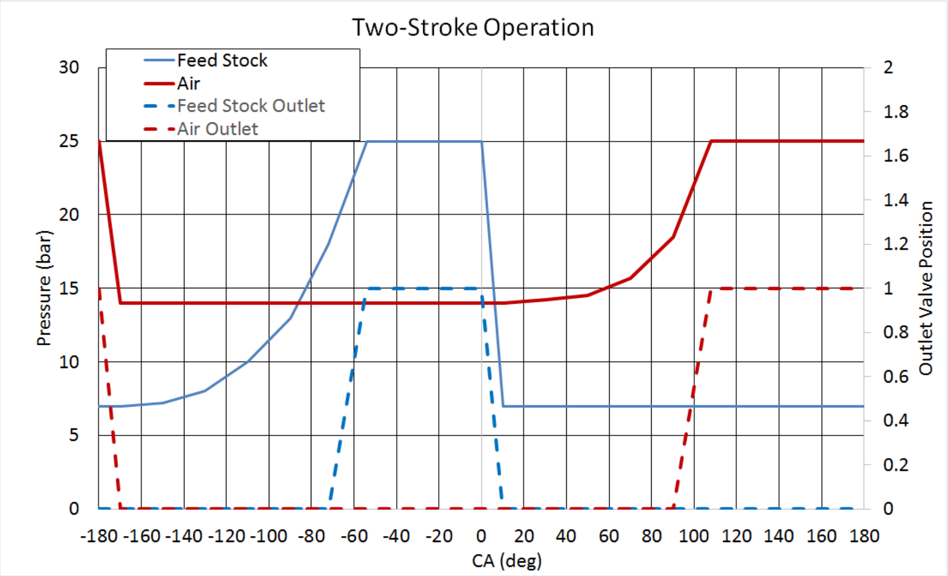
Catalyst ethylene production Catalyst regeneration with air

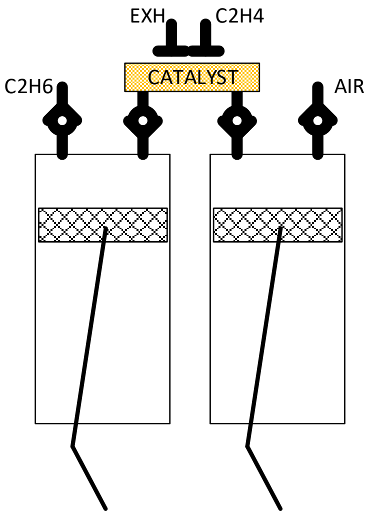
Engine Reactor Design Options

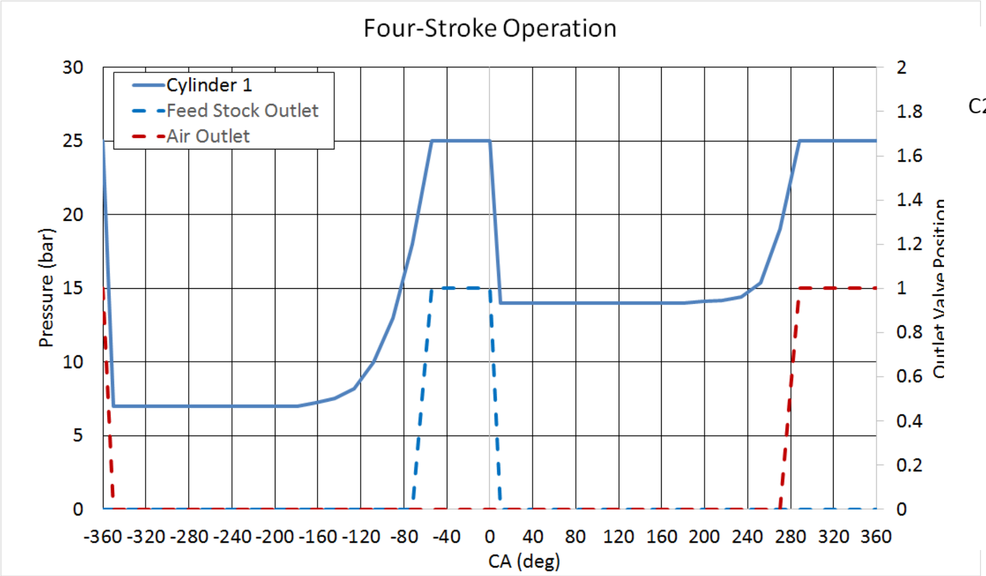
- Design options to consider:
  - Number of cylinders for reactant compression: 1 or 2
  - Catalyst location: Engine head or in cylinder
  - Catalyst flow direction: forward only vs. forward and reverse
  - Valve type: poppet, rotary or check
  - Valve operation: passive, active fixed timing, active variable timing
  - Pressure regulation: Before or after catalyst
- Initial design selections:
  - Catalyst in head with forward flow direction for both reactants
  - Active valves:
    - Valve type: rotary or poppet
    - Variable valve timing on outlet valves (phased only, no duration changes)
  - System pressure regulation performed with valves after catalyst (V3 valve)

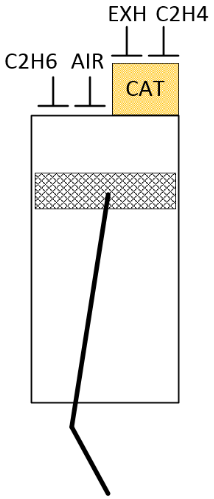
Engine Reactor Concept Selection

- Engine reactor concepts selected for further analysis
  - Single cylinder operating in 4-stroke mode, alternating between compressing feed stock and compressing air.
  - Dual cylinder engine operating in 2-stroke mode where cylinders are 180 deg out of phase. Each cylinder dedicated to compressing feed stock or air.

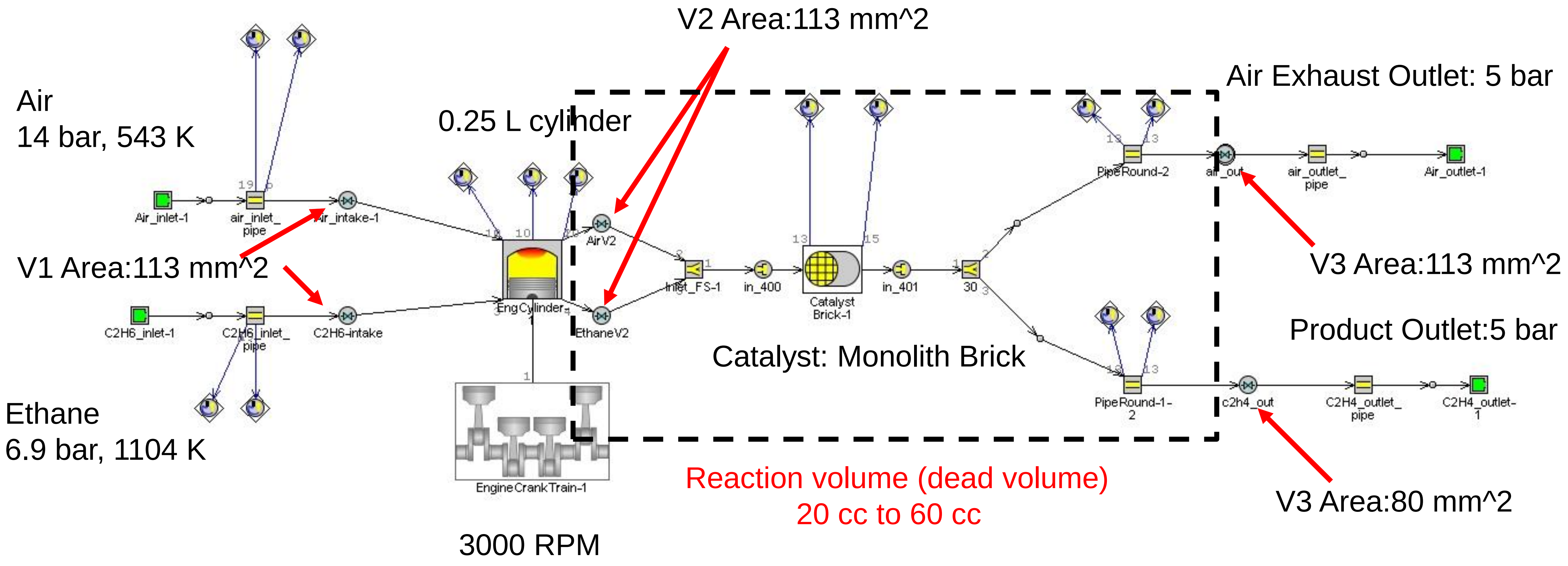




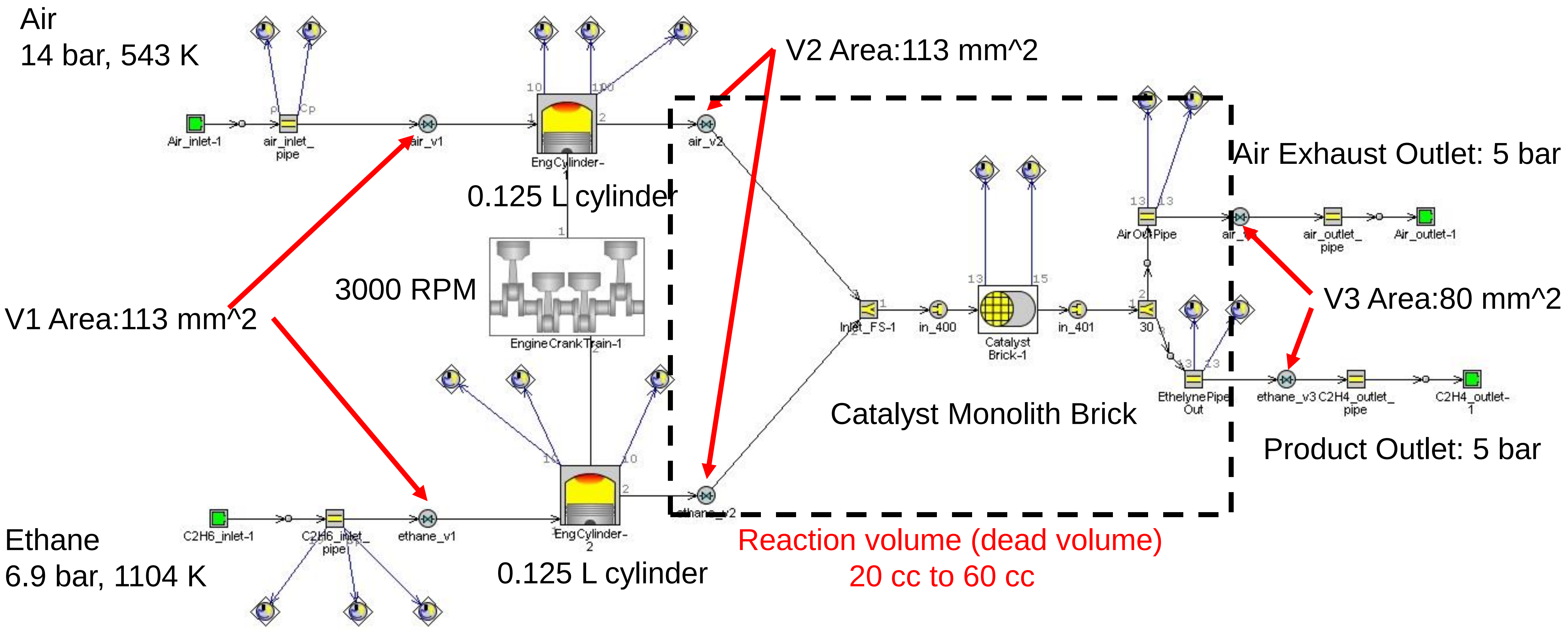




Four-Stroke Evaluation – Model Conditions



Two-Stroke Evaluation – Model Conditions



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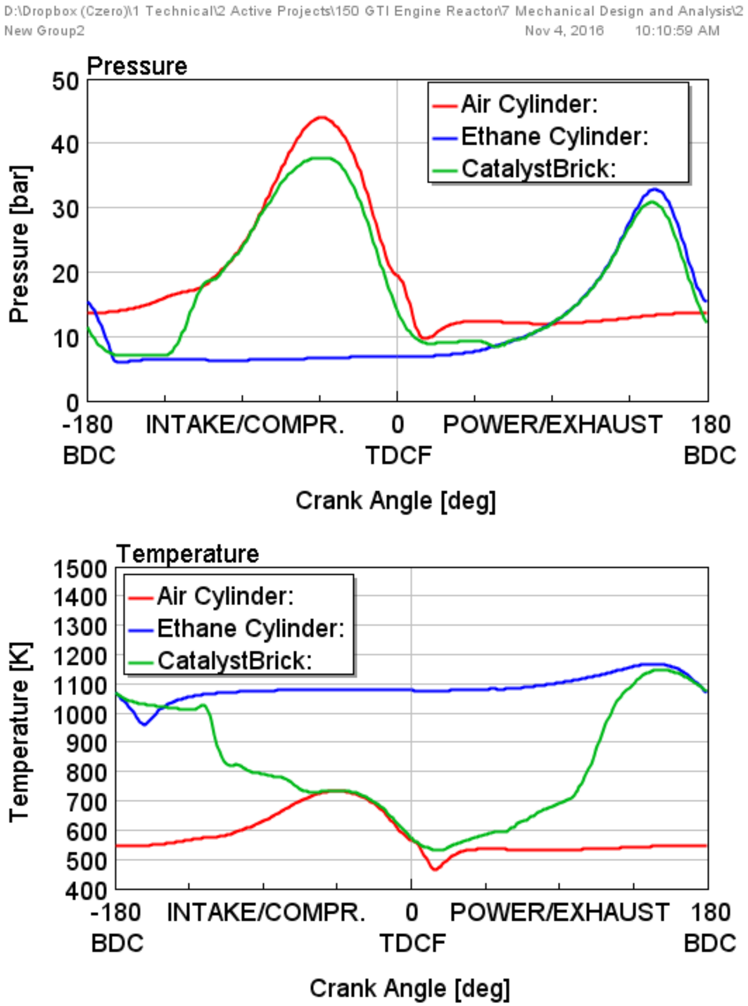
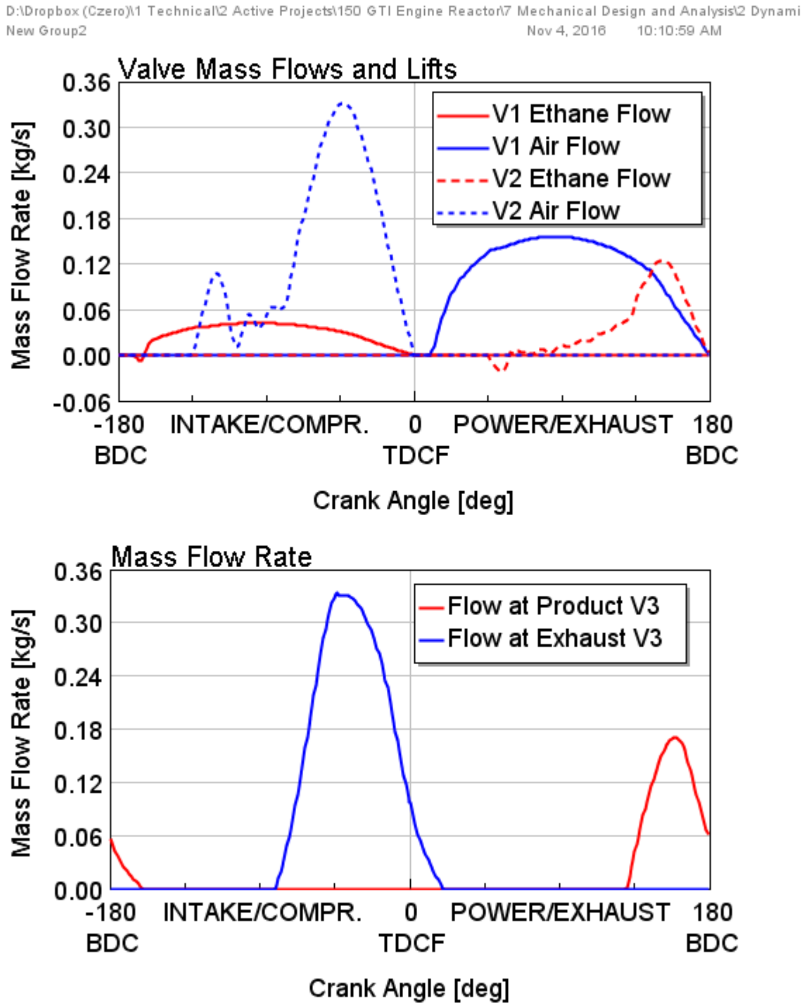
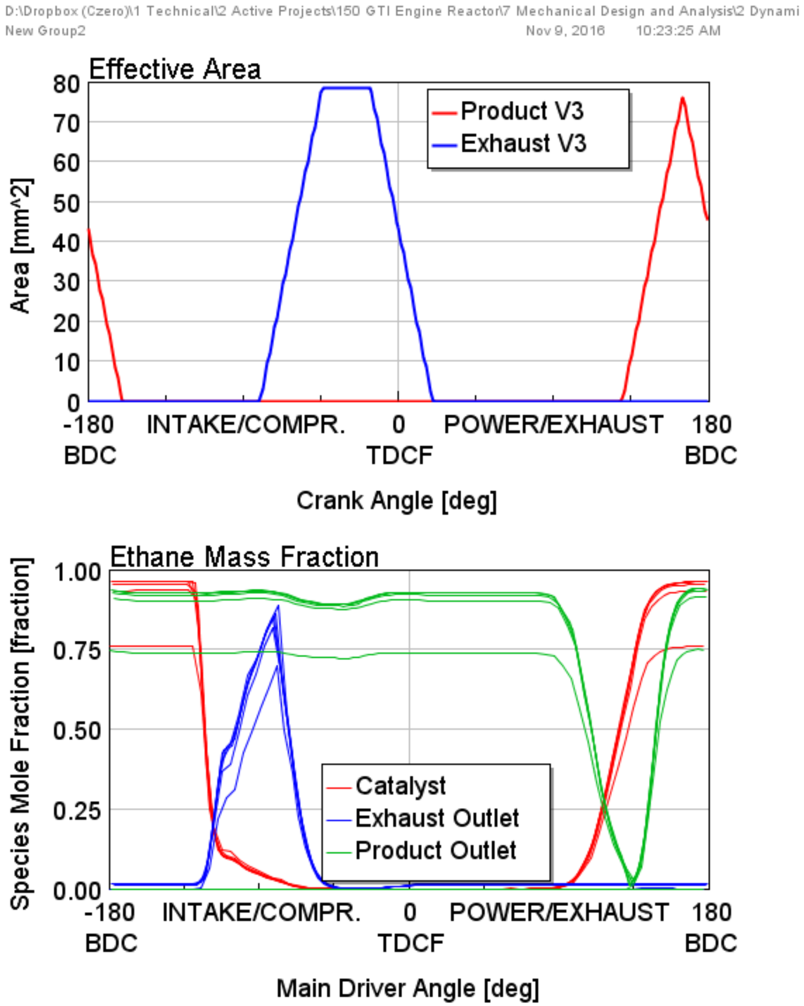
Model Output Examples – Two-Stroke Concept



Pressures and Temperatures



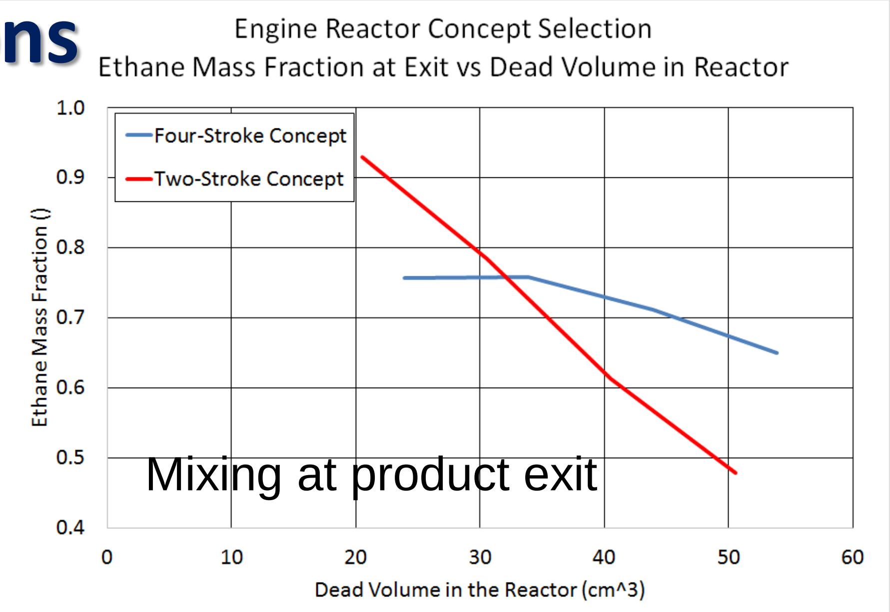
Valve Flow Rates

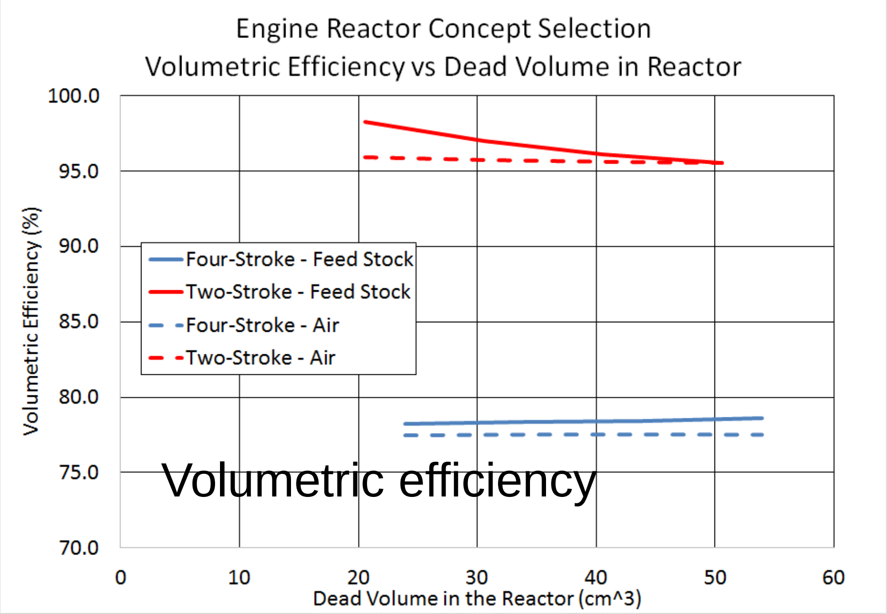


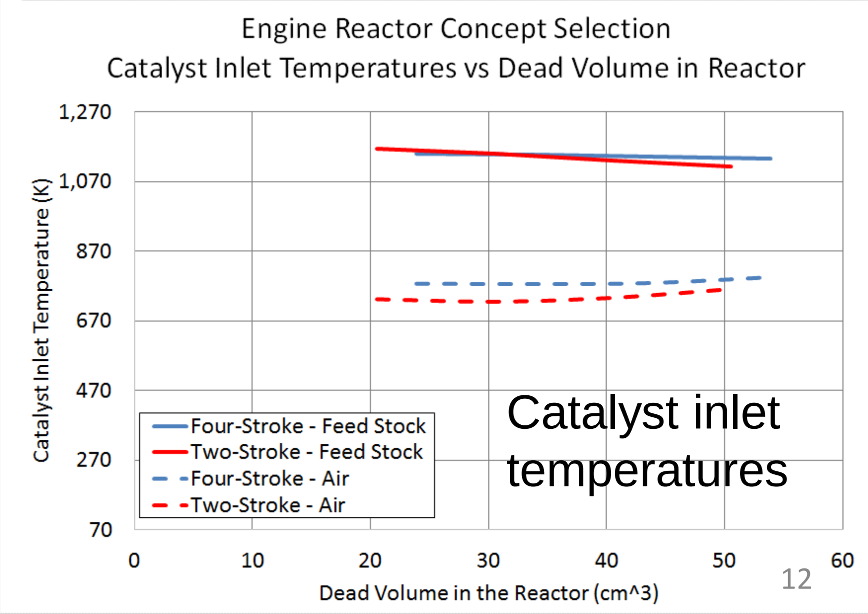
Ethane Mass Fractions

Concept Evaluation – Performance Comparisons

- Four-stroke limited to 78% volumetric efficiency due to cylinder mixing.
- Four-stroke limited to maximum of 76% product at exit, because of cylinder mixing. Less sensitive to dead volume than two-stroke.
- No significant effect on catalyst inlet temperatures.
- Two-stroke chosen as base platform.



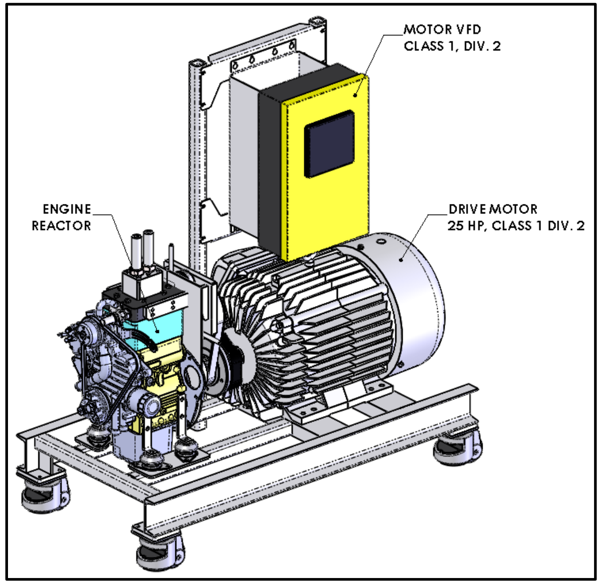


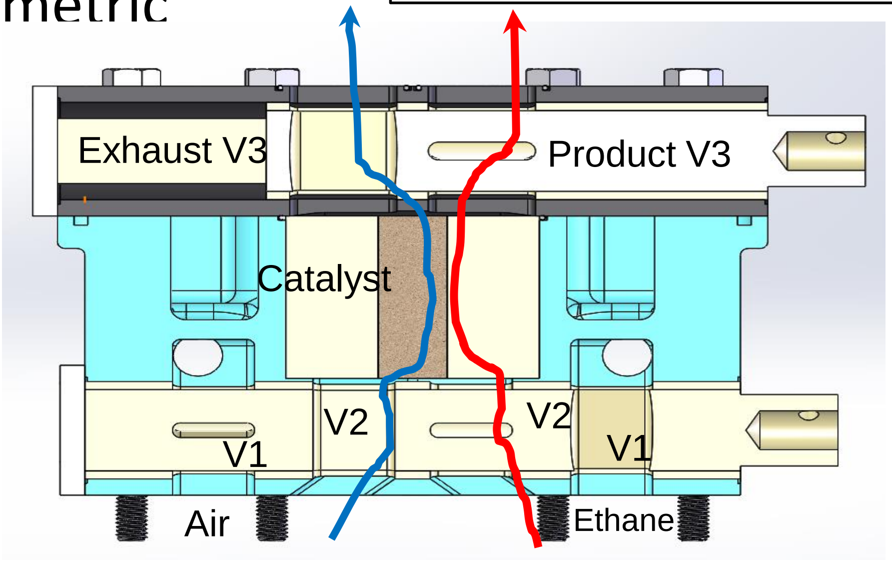


Engine Reactor Design – Key Parameters

- Minimize dead volume of reaction zone.
  - Reduces mixing of product and reactants in reaction volume zone
  - Improves blow down between reactant cycles
  - Increases temperature and pressure rise during compression event.
- Optimize V1 flow area and timing for high volumetric efficiency.
- Optimize V3 flow area and timing for:
  - Blow down
  - Catalyst pressure and temperature
- Reduce heat transfer from reactants
  - Increase coolant temperatures
  - Ceramic liner in cylinder

Pilot Engine Reactor Design

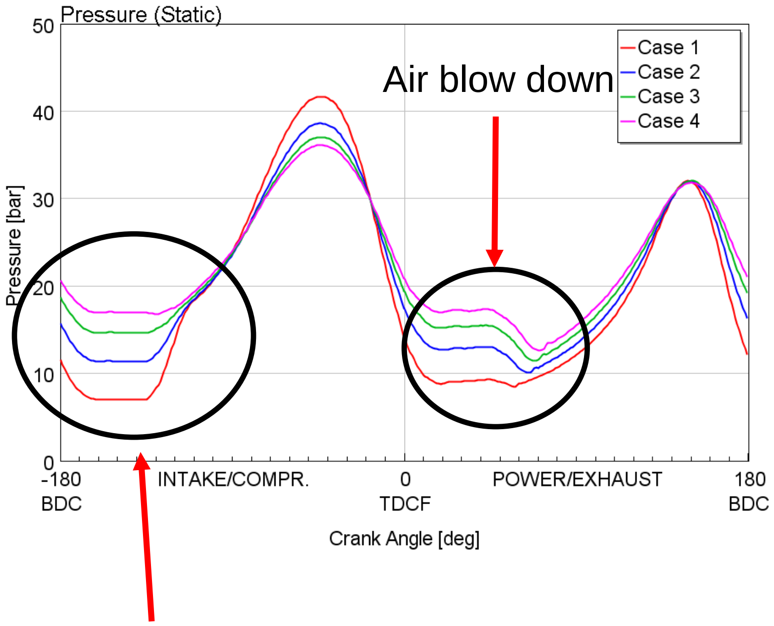




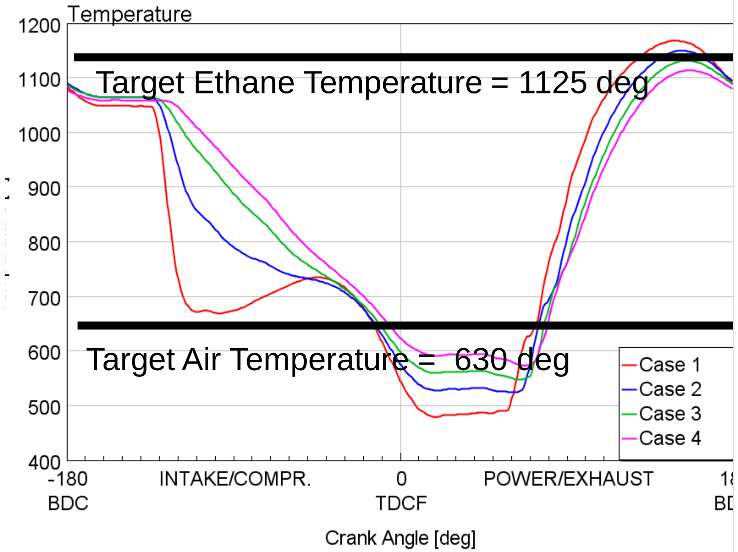
Detail of Engine Head and Reaction Zone

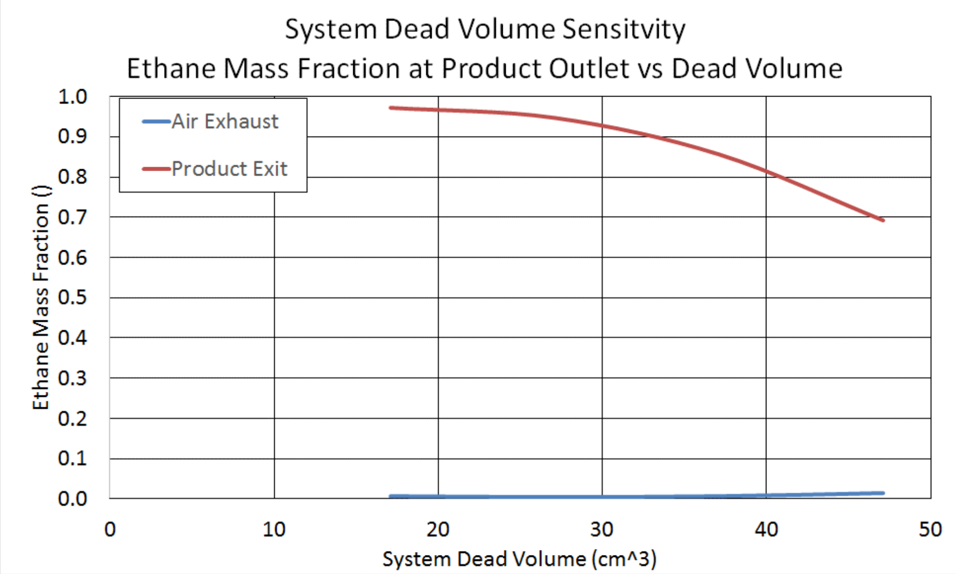
Effect of Volume in Reaction Zone on Engine Reactor Performance

- Higher dead volume results in less pressure blowdown between compression cycles
- Higher dead volume results in slightly lower catalyst temperatures during compression
- Higher dead volume results more dilution at the product exit



product blow down

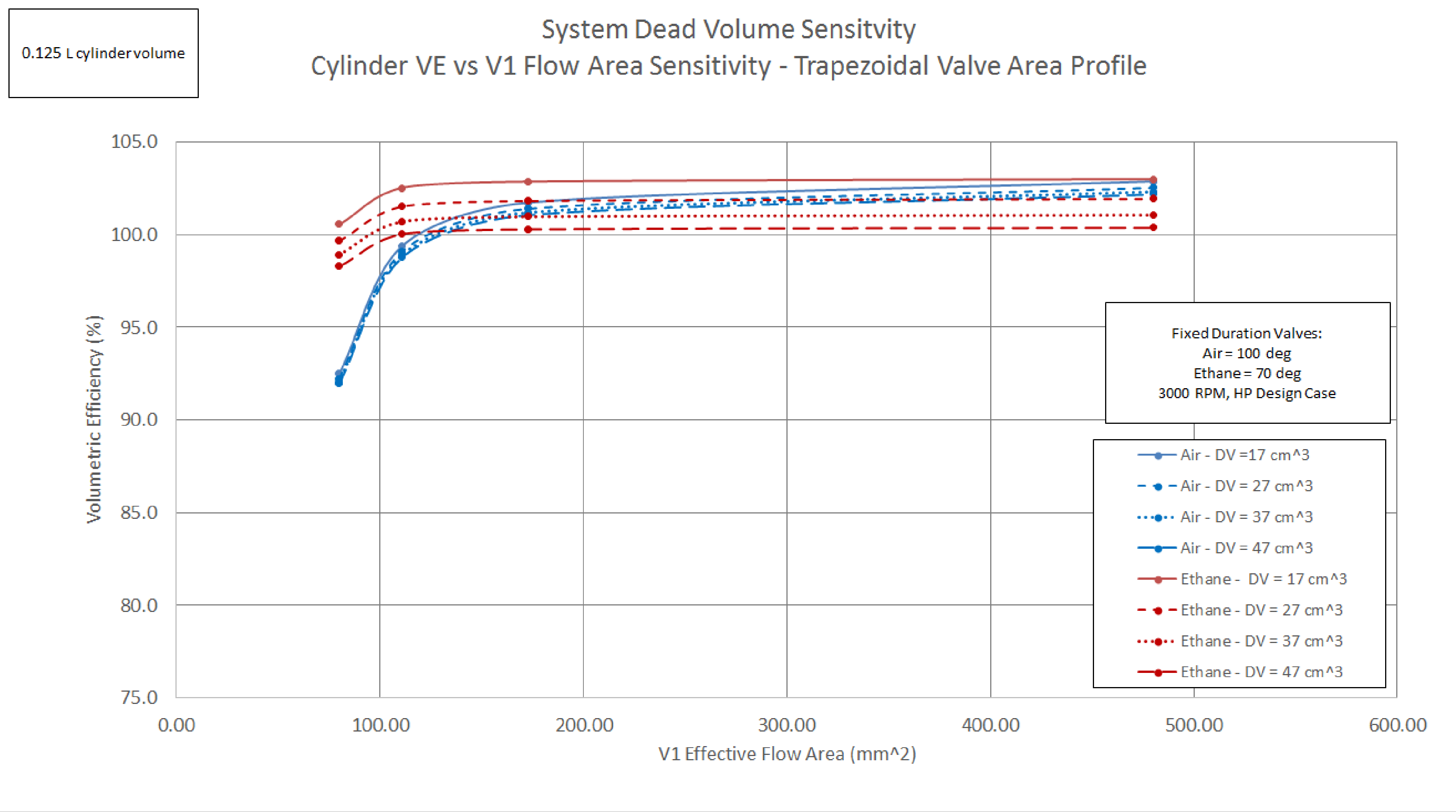




- Case 1: DV = 17 cm^3, CR = 8.22
- Case 2: DV = 27 cm^3, CR = 5.56
- Case 3: DV = 37 cm^3, CR = 4.33
- Case 4: DV = 47 cm^3, CR = 3.62

Effect of V1 Effective Flow Area on Volumetric Efficiency

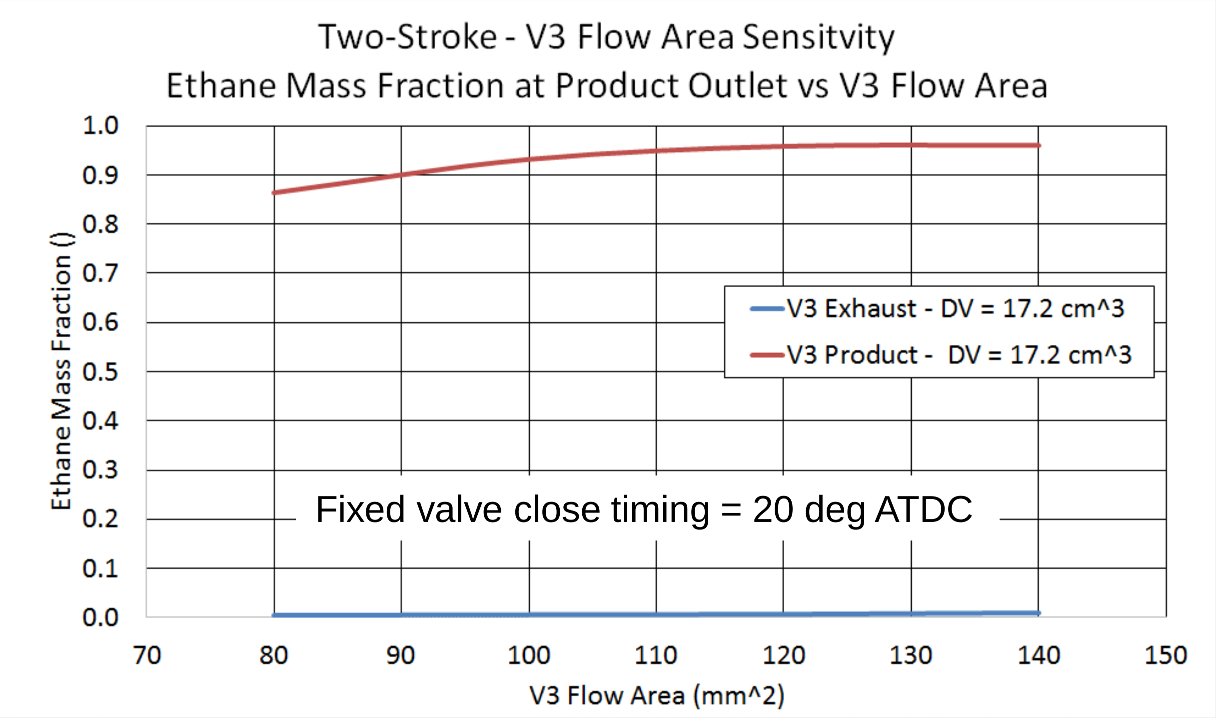
- Effective flow areas below 100 mm^2 significantly reduce volumetric efficiency, especially for air cylinder

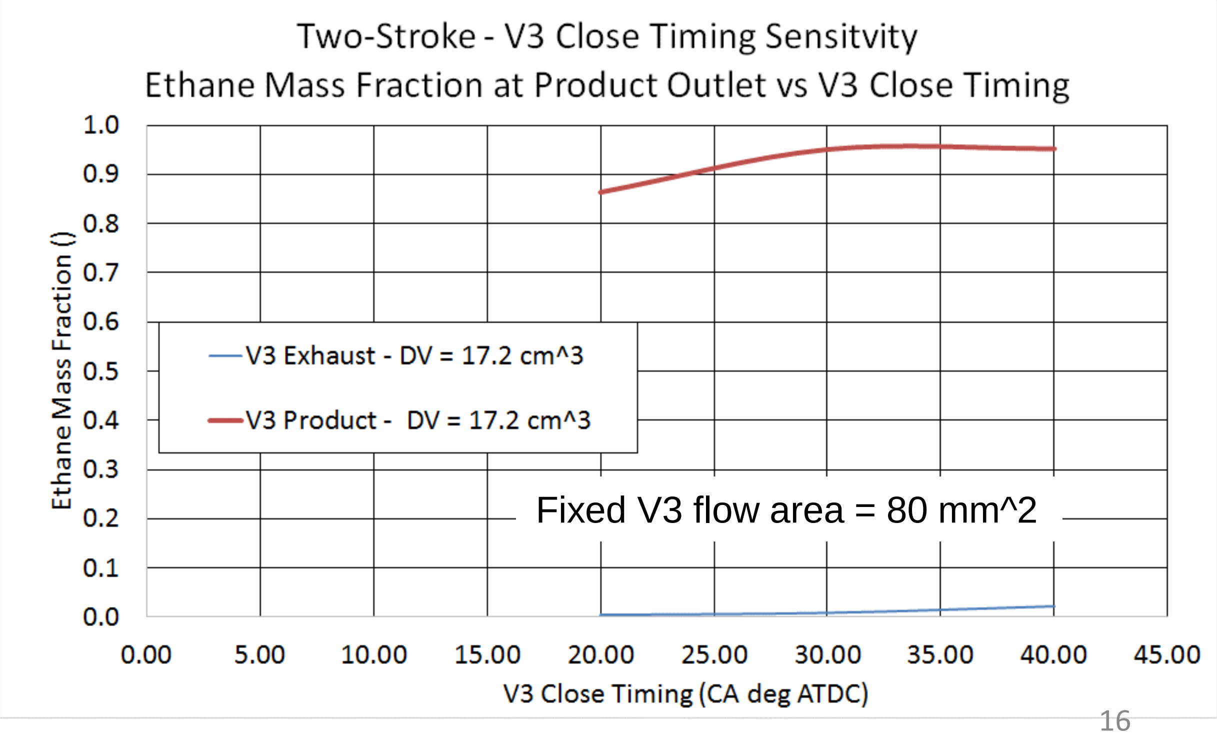


Effect of V3 Area and Timing on Dilution at Reactor Exit

- Increased V3 effective flow area improves blow down and reduces dilution at product exit

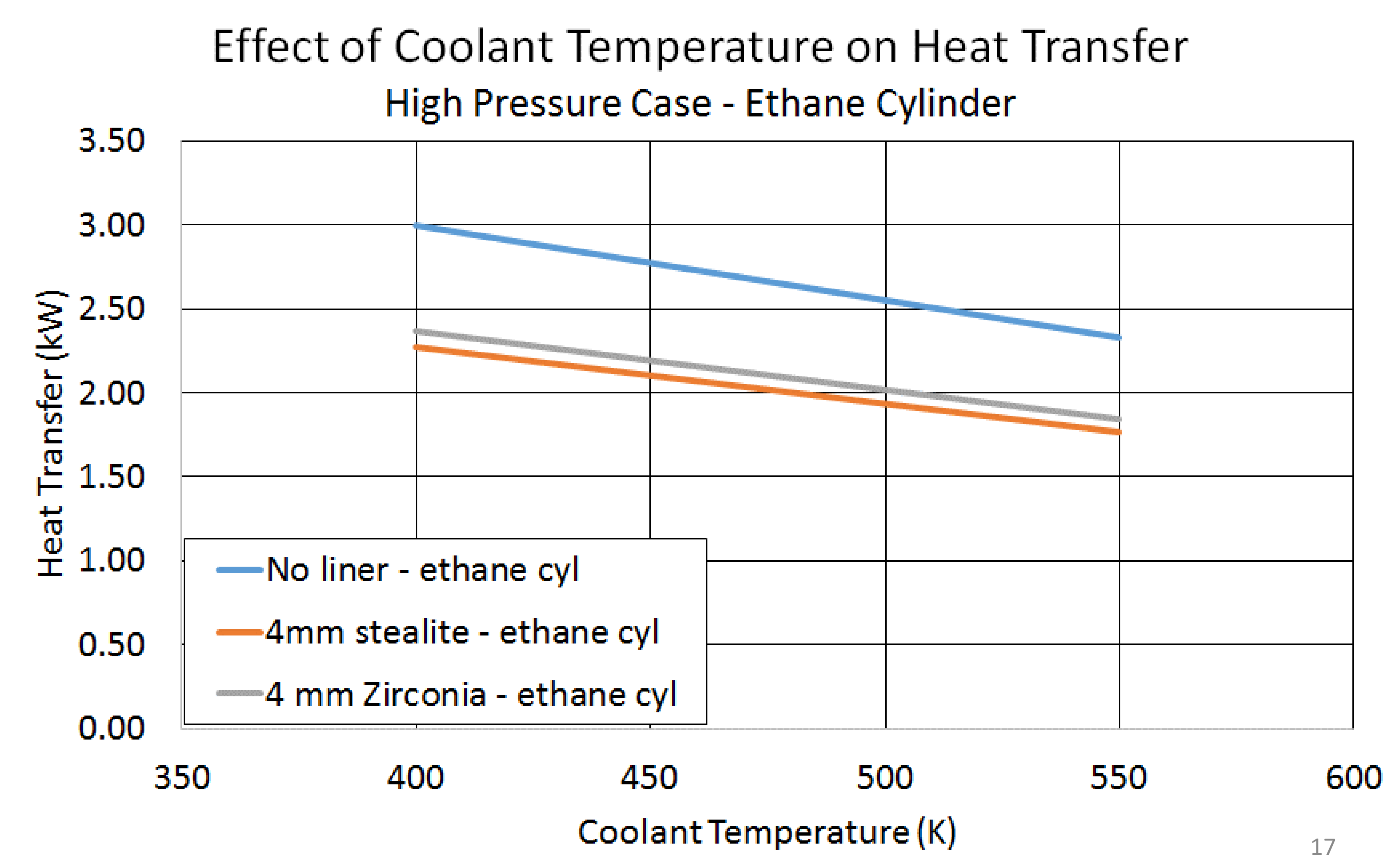
- Later valve close timing improves blow down and can compensate for reduced V3 flow area





Heat Transfer in Reactant Compression Cylinder

- Heat transfer at 400 K cylinder wall temperature is 60% of the isentropic compression work.
- Increasing coolant temperature and adding cylinder liner are needed to significantly reduce heat transfer in the ethane reactant cylinder



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Final Design: System Performance Predictions - Summary

Catalyst							
Ethane Compression				Air Compression			
Temperature		*Pressure*		*Temperature*		*Pressure*	
Target (K)	Final Design (K)	Target (bar)	Final Design (Bar)	Target (K)	Final Design (K)	Target (bar)	Final Design (Bar)
1123	1157	25	28	630	684	25	26

Air Cyl.			Ethane Cyl.		
Mass Flow Rate (kg/s)	*VE* (%)	*Heat Transfer* (kW)	*Mass Flow Rate* kg/s)	*VE* (%)	*Heat Transfer* (kW)
5.20E-02	92.8	0.641	1.28E-02	91.3	2.54

Ethane Mass Fractions			Blow Down Pressure	
Catalyst	*Product Exit*	*Exhaust*	*Air* (bar)	*Ethane* (bar)
0.972	0.953	2.70E-04	6.5	7.5

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Questions?