Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes

Project ID: ACE015

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Project Overview

BARRIERS (MYPP, SECTION 2.4, CHALLENGES AND BARRIERS C.)

Lack of fundamental knowledge of advanced engine combustion regimes.

…inadequate understanding of the fundamentals of thermodynamic combustion losses

…inadequate capability to accurately simulate these processes

BUDGET

- FY14: $300k
- FY15: $300k
- FY16: $300k

PROJECT TIMELINE

- ***Stretch Efficiency research program started at ORNL in 2005***
  - ***Initiated current focus on thermochemical recuperation in 2011***
- ***Project will conclude in it's current form at end of FY16***
- ***Proposing to continue work through Combustion Lab Call FY17-FY20***

INDUSTRIAL PARTNERSHIPS AND COLLABORATION

- ***AEC working group led by SNL***
  - ***Mechanism for industry feedback***
- ***Aramco Services – Related Funds-In Project***
- ***ANSYS (formerly reaction design) – CFD model development***
- ***Umicore – Catalyst coatings***
- ***SNL – Isaac Ekoto***

Universities

- ***University of Michigan - Galen Fisher***
- ***University of Michigan – Yan Chang***
- ***University of Minnesota – Will Northrop***

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Pursuing Strategies that Show Potential of Higher Thermodynamic Efficiency

- This project is focused on high risk/high reward technologies that could have a real world impact on longer-term timeframe (as defined by the 2010 Transportation Combustion Engine Efficiency Colloquium held at USCAR)

http://feerc.ornl.gov/pdfs/Stretch_Report_ORNL-TM2010-265_final.pdf

- The path that is currently being pursued is focused on high EGR dilution SI combustion and thermochemical recuperation
  - High EGR dilution SI combustion: Improved efficiency through higher γ, reduced heat losses, improved resistance to knock
  - Thermochemical recuperation: Waste heat recovery by converting thermal energy to chemical energy through endothermic reactions

This Project has Two Tracked Milestone for FY16

Second Quarter, FY2016

Complete a sweep of operating conditions with the in-cylinder reforming strategy to determine the equivalence ratio for maximum H_2 production.

Status: Complete

Fourth Quarter, FY2016

Complete a quantification of the brake thermal efficiency and the reforming thermodynamic cost or TCR benefit for the in-cylinder reforming strategy and the catalytic reforming strategy at 2000 rpm, 4 bar BMEP.

Status: On-track

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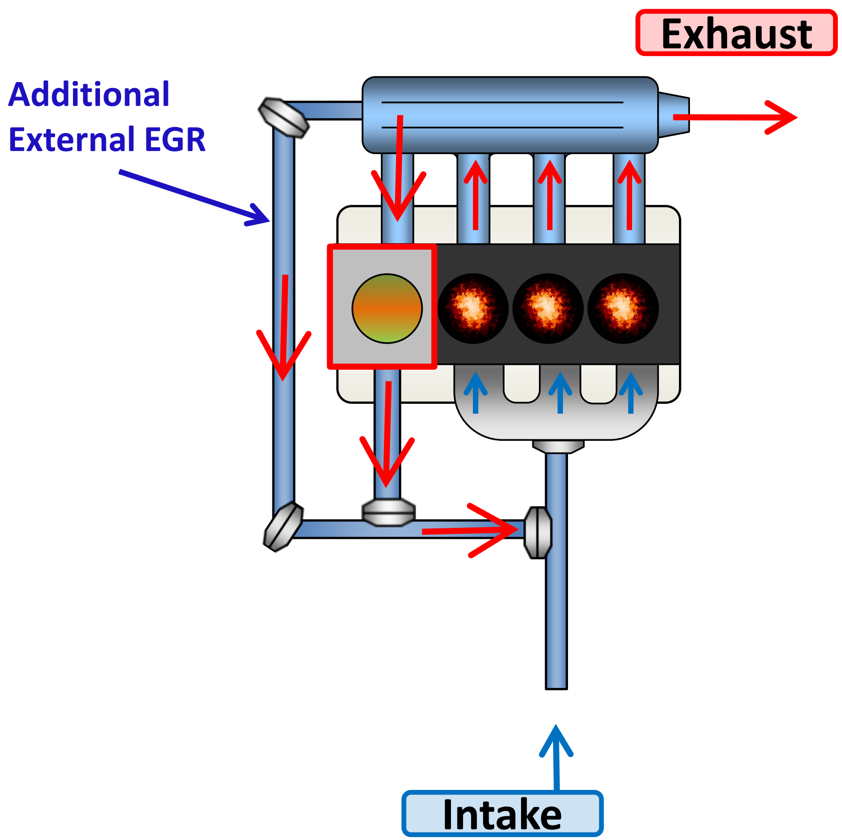
Pursuing Reformate-Assisted Dilute SI Combustion through Two Parallel Strategies

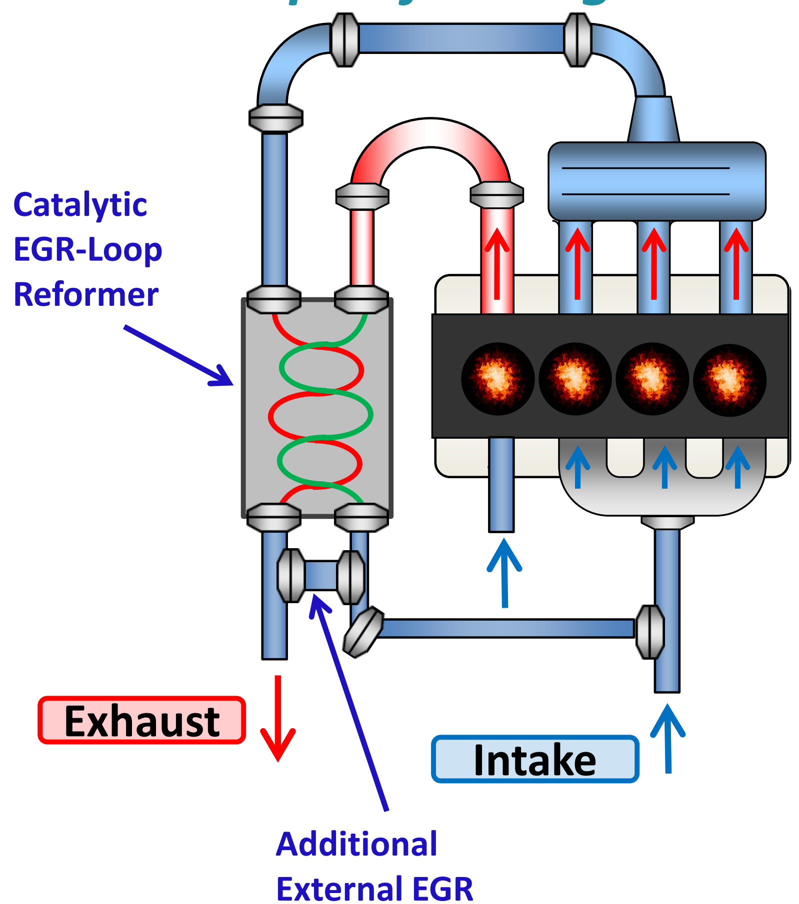
Approach (1/2)

Both Strategies Start with a Multi-Cylinder Engine

In-Cylinder Reforming

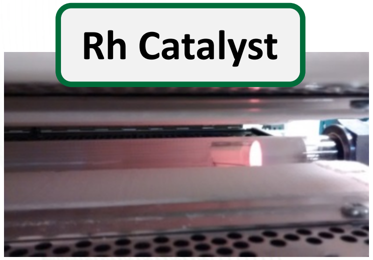


EGR-Loop Reforming



Flow Reactor Used to Evaluate Catalyst Performance and Durability Prior to Engine Experiments

- EGR operating environment varies significantly from typical industrial steam reforming applications
  - water concentration fixed by engine stoichiometry, dilution
  - lower operating temperatures and pressures
  - sulfur from fuels and lubricants
- Currently focused on a pre-commercial Rh-based catalyst
  - Galen Fisher (University of Michigan) advising on catalyst formulation and operating conditions through subcontract
- Flow reactor experiments designed to mimic engine operation
  - holding flows of H_2O, CO_2, N_2 fixed (synthetic EGR mix)
  - investigating effects of:
    - gas temperature: use tube furnace to heat gas feed, but not catalyst
    - equivalence ratio: add varying amounts of air to EGR mix
    - fuel feed rate: add varying amounts of fuel to EGR mix
    - fuel composition: iso-octane, ethanol, gasoline



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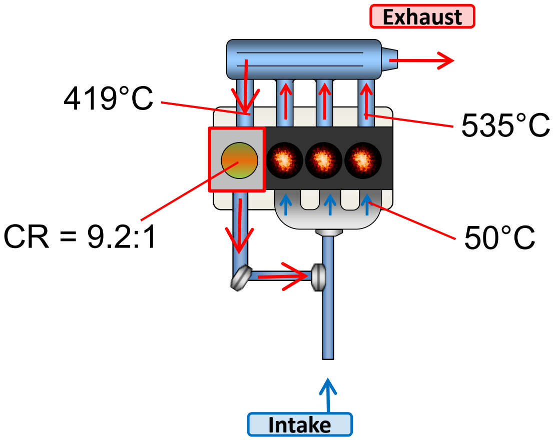
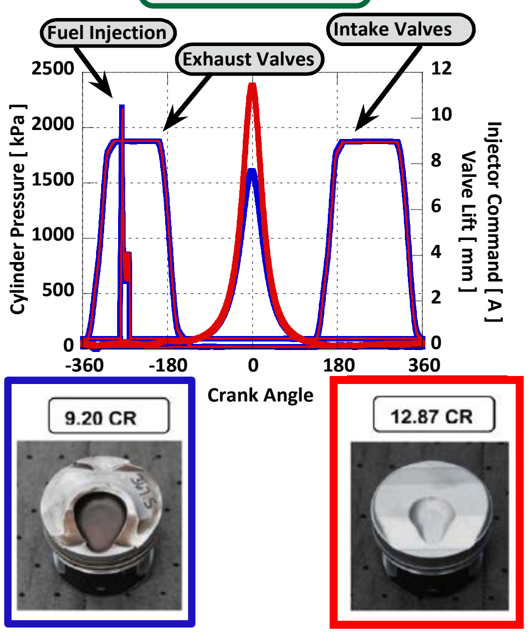
FY16 In-Cylinder Reforming Activities Pursued Enhancements Identified at FY15 AMR

Accomplishments (1/11)

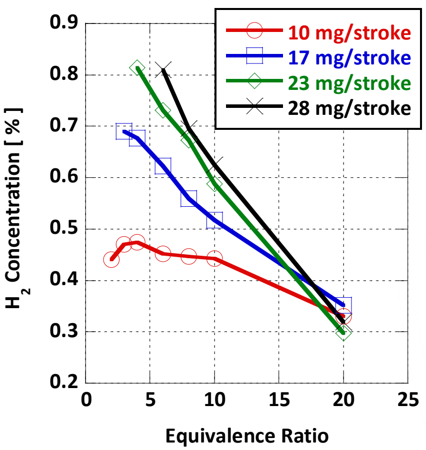
- Low fuel conversion encountered previously
- Hypothesis: in-cylinder temperatures were insufficient for reforming due to high heat losses
  - Solution 1: Higher reforming cylinder compression ratio
  - Solution 2: Exothermic reactions to drive reforming
  - Solution 3: Redesigned exhaust manifold



Solution 1

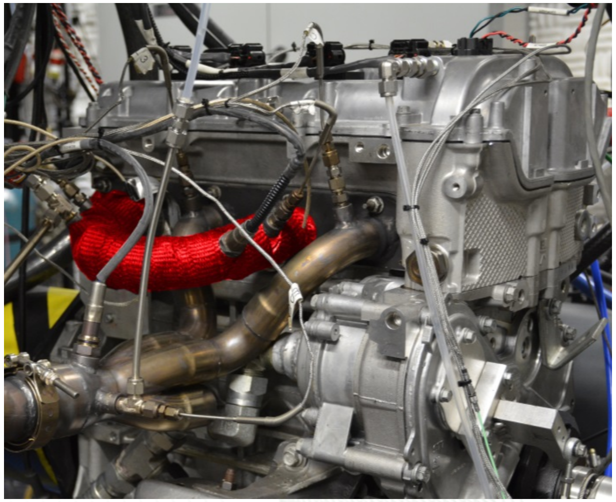


Solution 2



- Φ as low as 2.0 in reforming cylinder

Solution 3



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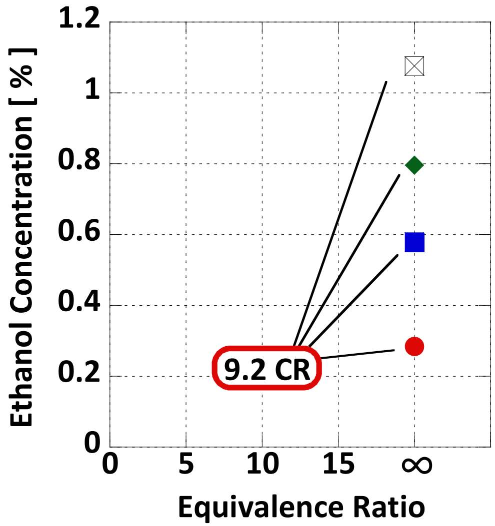
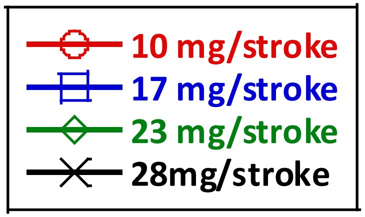
Fuel Conversion and Reformate Yield Doesn't Increase with CR, Sharply increases with Air Addition





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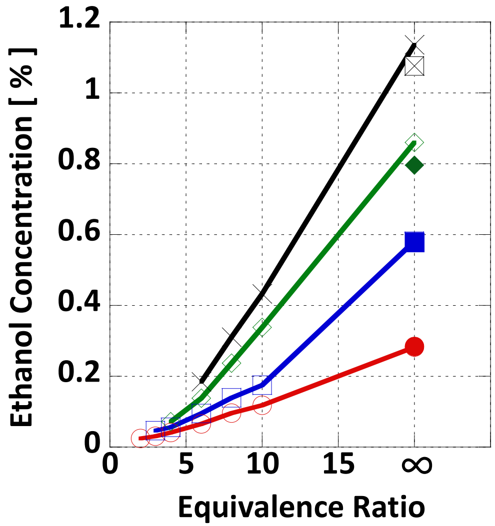
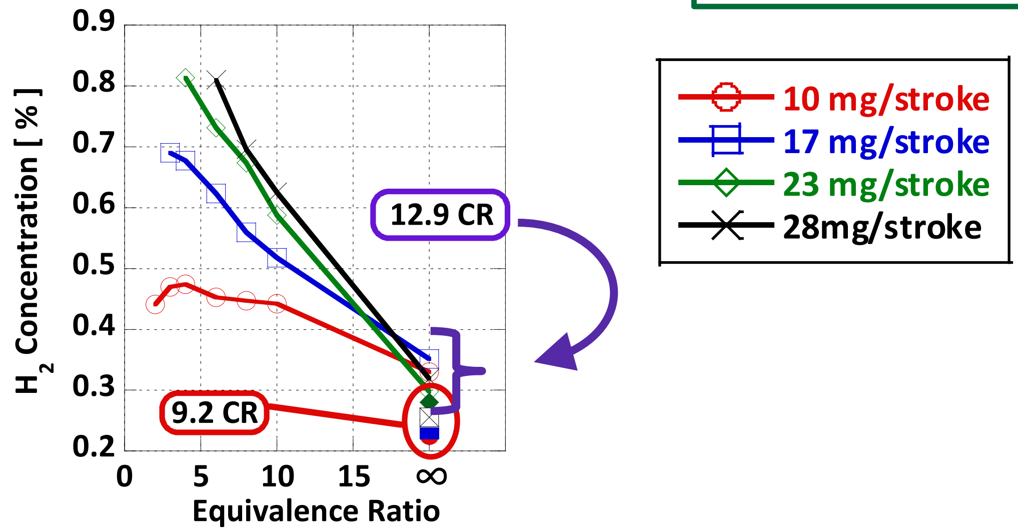
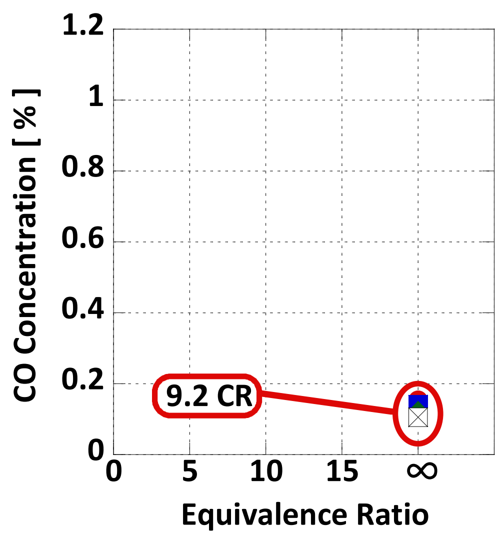
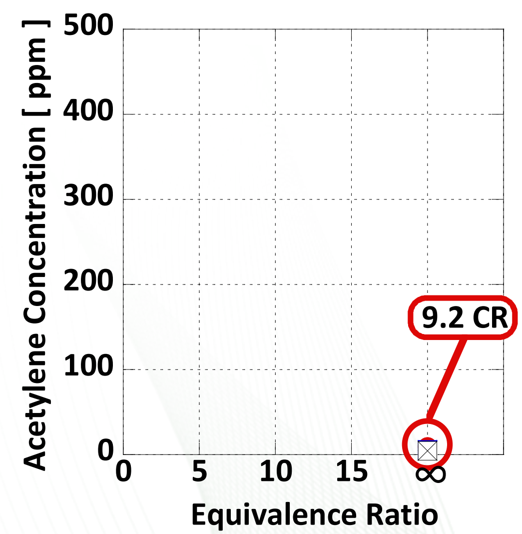




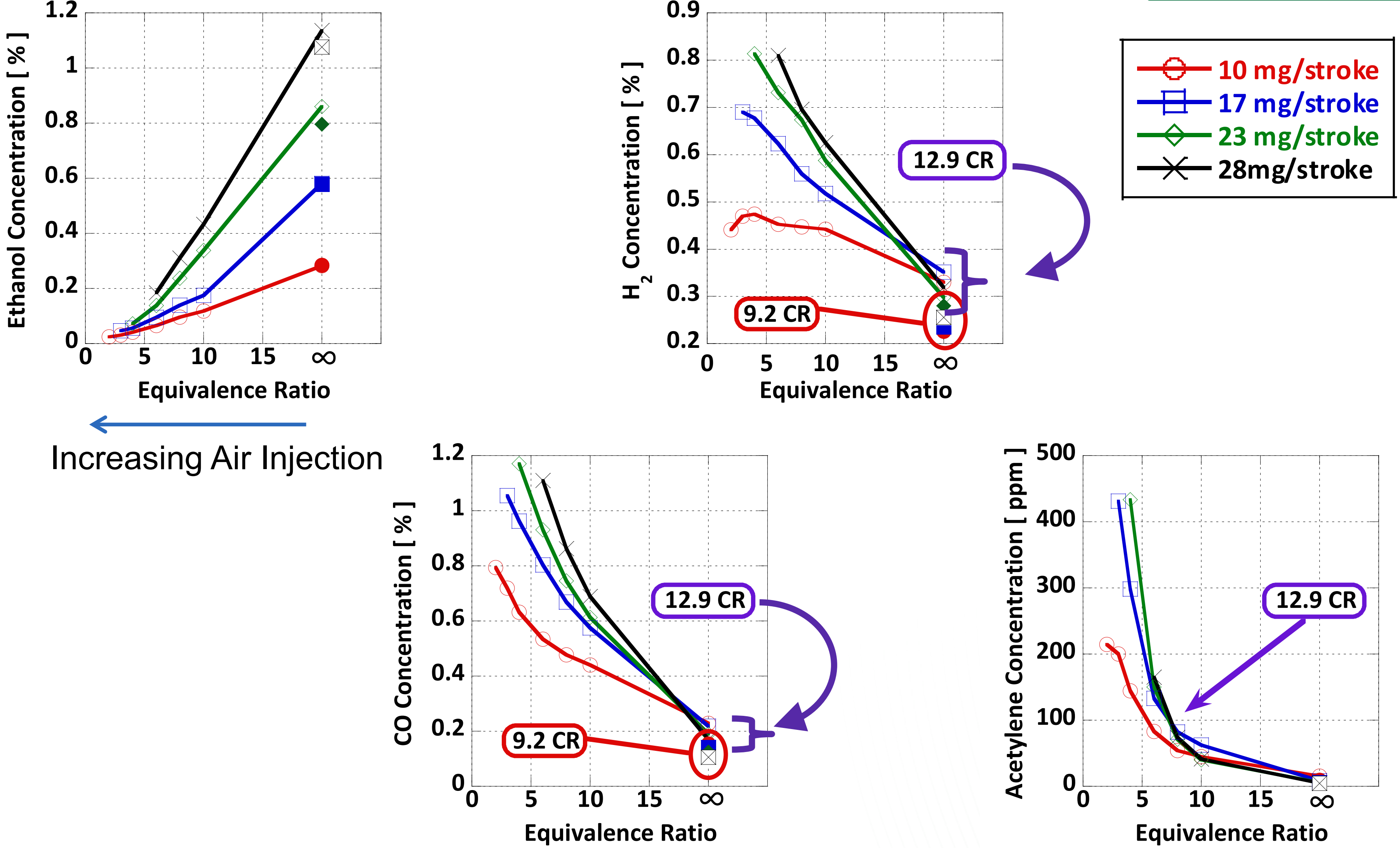
Increasing Air Injection





Fuel Conversion and Reformate Yield Doesn't Increase with CR, Sharply increases with Air Addition

Accomplishments (2/11)



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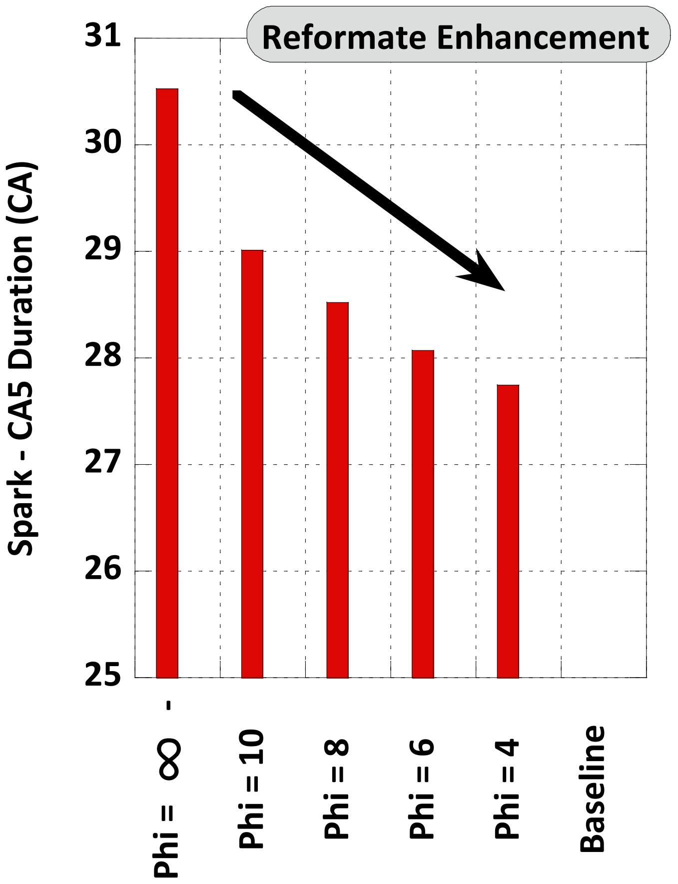
Despite Increased Fuel Conversion with PO_x Reforming, Little Change was Observed in the SI Combustion Event

- Fuel conversion in reforming cylinder increases as Φ decreases
- Measurable decrease in spark-CA5 duration in SI cylinders
  - Spark-CA5 duration is a key indicator of combustion stability
  - EGR dilution tolerance is limited by combustion stability
- Decrease in spark-CA5 is relatively minor compared to baseline case (0% EGR)
  - Nearly a factor of 2 increase



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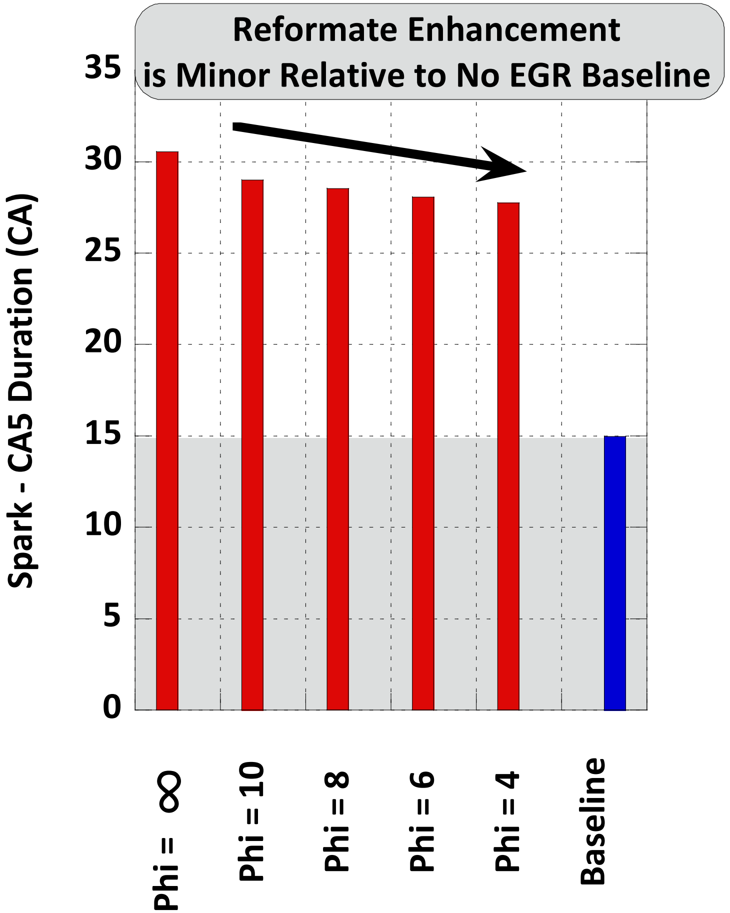
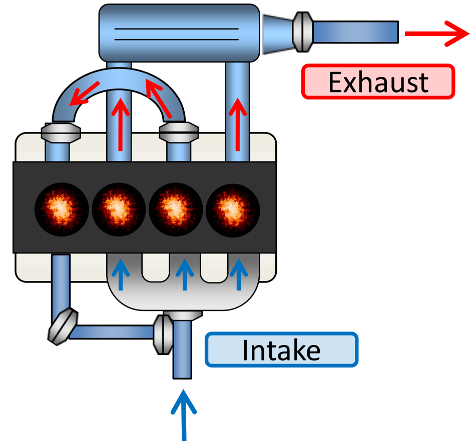
➢ <u>Conclusion: The level of reformate being generated from this strategy is insufficient to substantially change SI combustion</u>

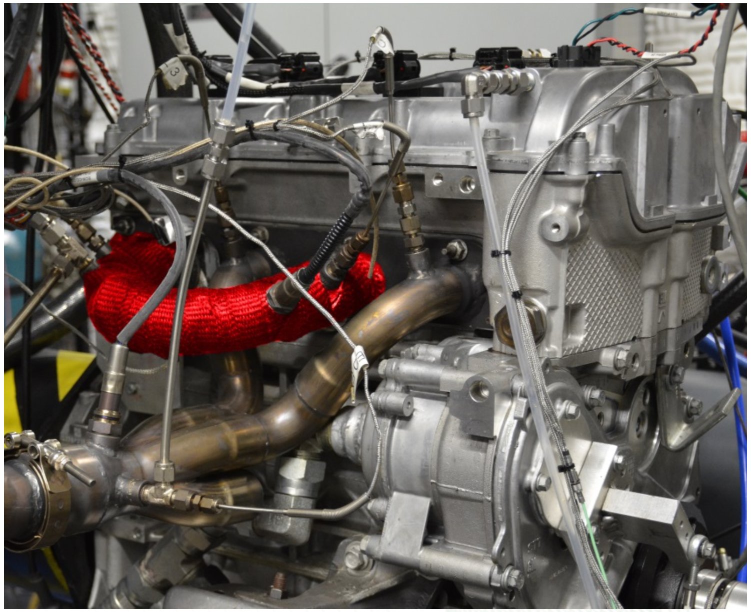


Re-Designed Exhaust Manifold with Heating Minimized Heat Loss, but Provided Little to No Benefit for Reforming Process

Accomplishments (4/11)

- Custom exhaust manifold to minimize heat loss coincided with operating strategy adjustment
  - O_2 in reforming cylinder required for fuel conversion
  - Desire for stoichiometric exhaust
  - Short-circuit exhaust of cylinder 2 (lean combustion) to feed cylinder 4
- Exhaust manifold minimized heat losses
  - Previous temperature loss: >100°C
  - New temperature loss: 30-40°C
- Parametric sweeps of engine operation
  - Fuel (iso-octane, ethanol, gasoline), Φ in reforming cylinder, reformate fueling, engine speed
- Engine was nearly in-operable with this strategy
  - No significant increase in reforming activity
  - EGR dilution in cylinders 1-3 increased substantially, leading to very poor combustion stability





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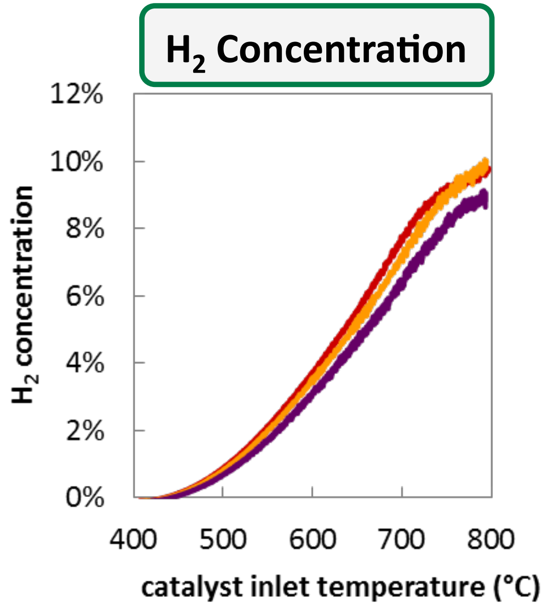
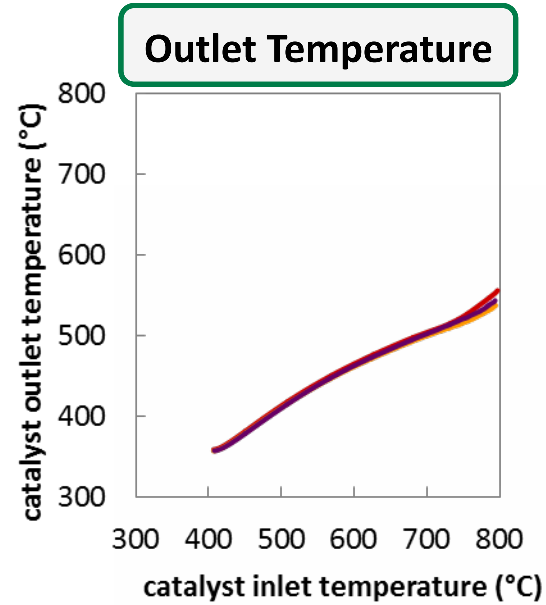
Summarizing Results from the In-Cylinder Reforming Strategy

- Low fuel conversion for in-cylinder reforming using stoichiometric exhaust
  - Changes in compression ratio of reforming cylinder made no substantial difference
- Higher fuel conversion when air was injected into inlet of reforming cylinder
  - More significant levels of H_2 and other reformed products
  - Presence of reformate at these concentrations made only minor differences on the SI combustion performance
- **Impact of the in-cylinder reforming work was significantly lower than anticipated**
  - Fully confident that additional measures could be taken to make incremental improvements
  - No results to-date indicate that the reformate has provided a substantive expansion of the EGR dilution limit
  - Completion of the data analysis and reporting of experiments done to-date
  - Additional experiment representing a minor effort is possible for the sake of completeness
- **Primary focus moving forward is on the catalytic reforming strategy**

EGR Loop Reforming: SI Exhaust Conditions Not Conducive to Steam Reforming

fuel flow (as fraction of fuel fed to EGR):
26%
17%
13%



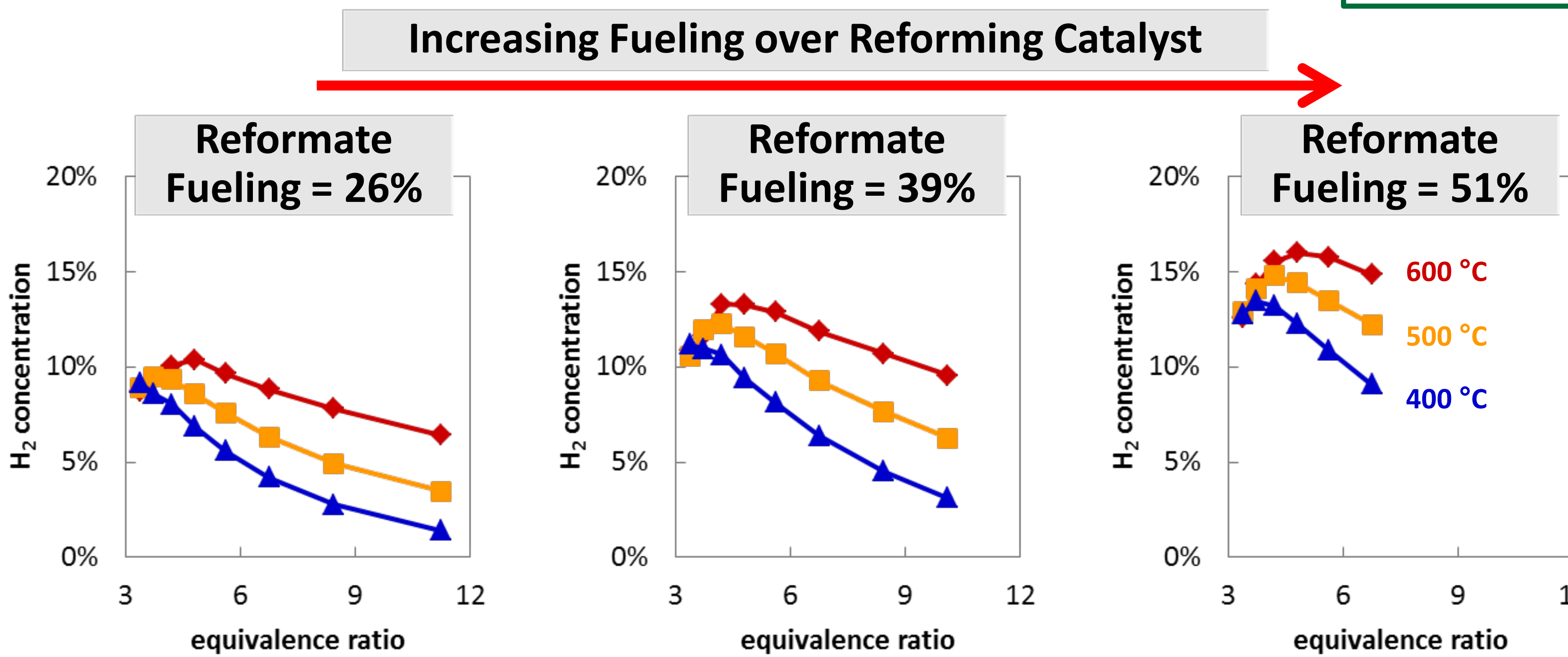


reforming conditions:
2 wt% Rh/Al_2O_3
GHSV: 40000 h^{-1}
inlet T: 400-800 °C
i-C_8H_{18}: 0.74 - 1.48%
no O_2
H_2O: 12%
CO_2: 14%

- Endothermic steam reforming is thermodynamically advantageous (thermochemical recuperation), but practically difficult to implement
- Significant H_2 production from steam reforming requires EGR temperatures >700 °C
- Steam reforming activity is limited by heat available in the EGR gas stream
  - endothermic reactions decrease catalyst temperature until reforming shuts down
  - adding fuel does not significantly increase H_2 or change catalyst outlet temperature

Partial Oxidation Reforming of Iso-Octane Generates Significant H_2 Concentrations

Accomplishments (7/11)



- Adding air to the EGR mix upstream of the reforming catalyst generates significant H_2 concentrations over a fairly wide range of operating conditions
- H_2 production increases with T and fuel feed rate, decreases at low Φ
- <u>H_2 production is an order of magnitude higher than for the in-cylinder reforming strategy!</u>

reforming conditions:
2 wt% Rh/Al_2O_3
GHSV: 41000-65000 h^{-1}
inlet T: 400-600 °C
$i\text{-}C_8H_{18}$: 1.2- 2.3%
O_2: 0.6-7.5%
H_2O: 7.5-11.5%
CO_2: 8.7-13.4%

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Energetic Differences Between Steam and POx Reforming. Our Approach Uses a Combination of These Processes.

- Energy balance highly fuel-dependent (C/H/O)
- POx consumes fuel energy (ethanol is an exception)

$$C_8H_{18} + 4*(O_2 + 3.76\ N_2) \rightarrow 8\ CO + 9\ H_2 + 15.04\ N_2$$

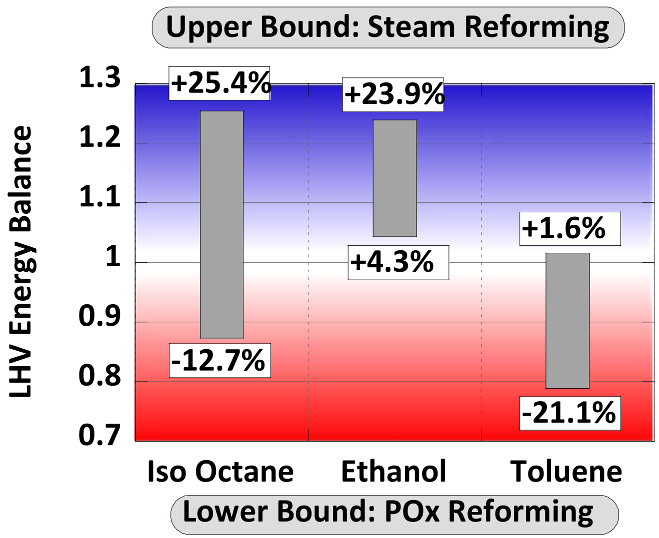
POx reforming with iso-octane, C:O = 1

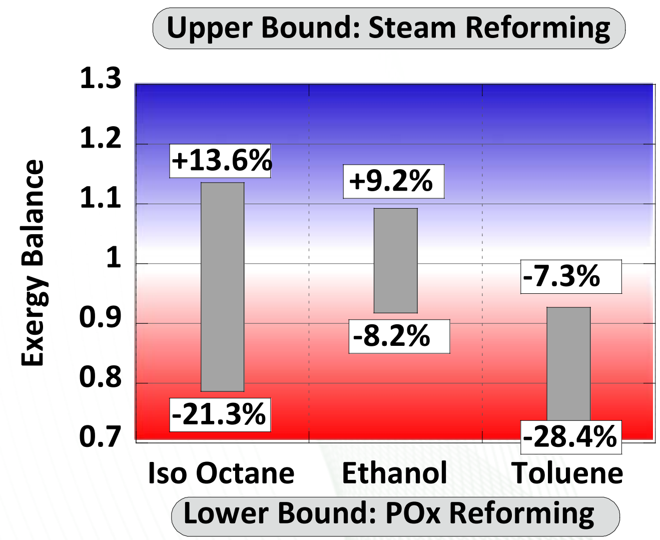
- Steam reforming is the route to thermochemical recuperation

$$C_8H_{18} + 8\ H_2O \rightarrow 8\ CO + 17\ H_2$$

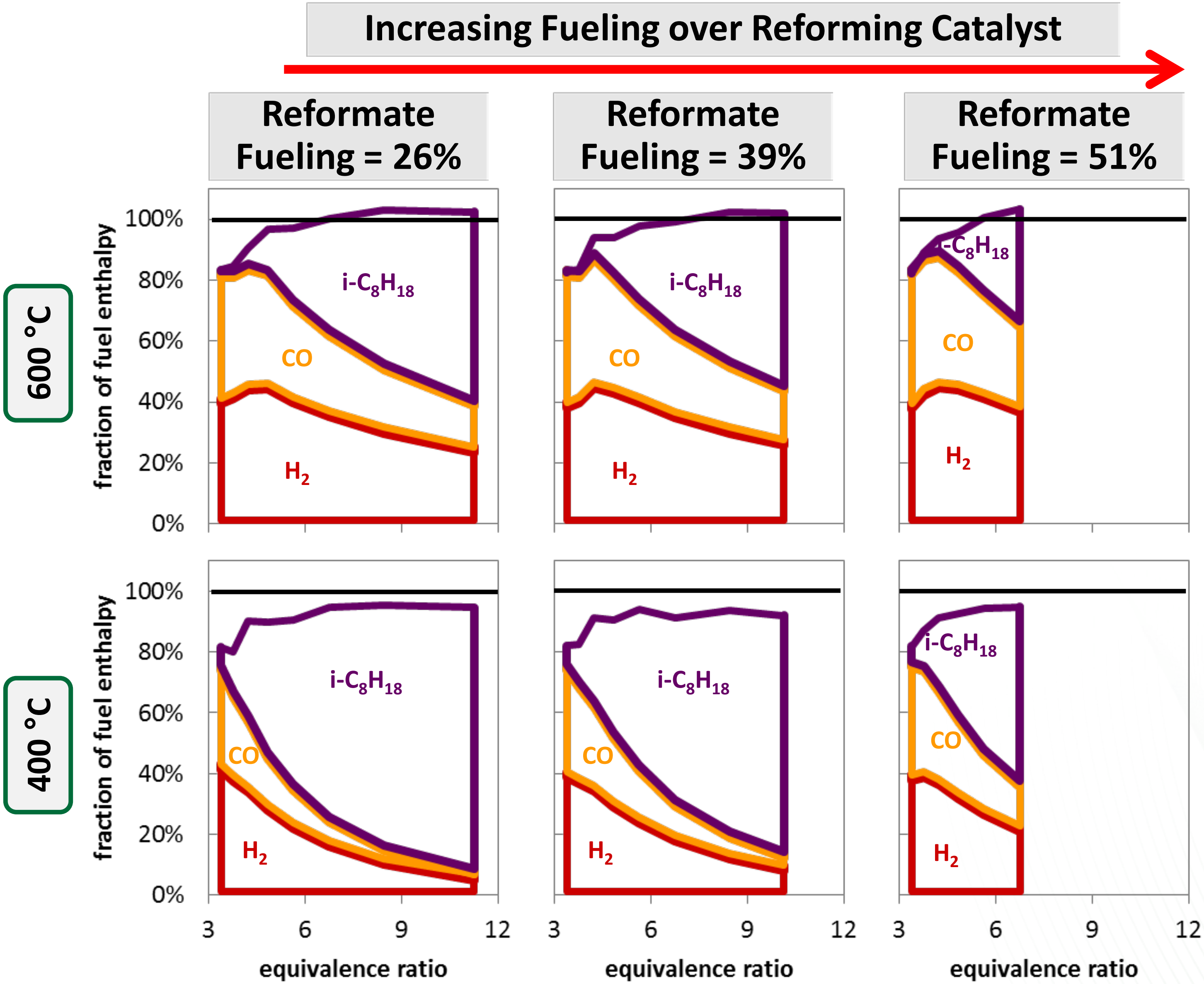
Steam reforming with iso-octane

- Optimal reforming conditions may differ based on desired outcome – highly dependent on engine response
  - Highest H_2 yield
  - Most favorable reforming energetics
  - **Best overall engine efficiency**





TCR at High Φ, Accompanied by Low Reformate Yield; Highest Reformate Yield when Energy Balance is Unfavorable

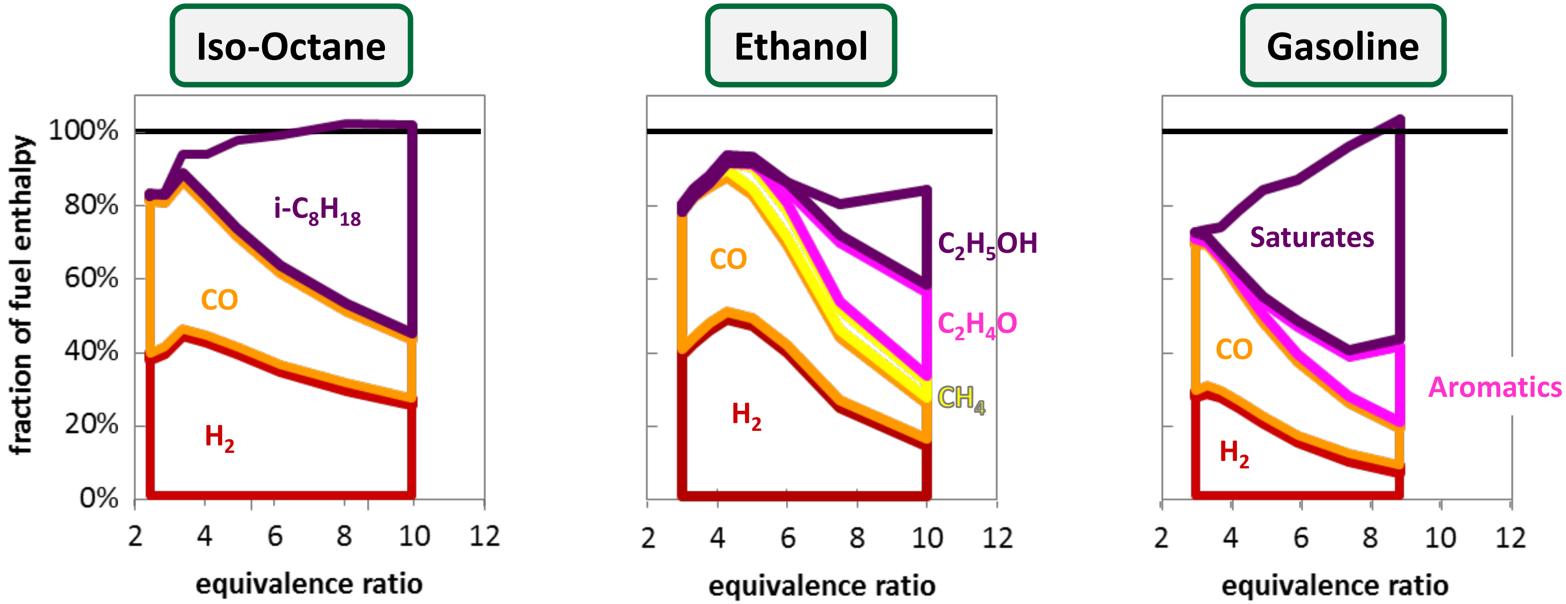


Tradeoff between H_2 yield (dilution tolerance) and fuel energy retention

reforming conditions:
2 wt% Rh/Al_2O_3
GHSV: 41000-65000 h^{-1}
inlet T: 400-600 °C
i-C_8H_{18}: 1.2- 2.3%
O_2: 0.6-7.5%
H_2O: 7.5-11.5%
CO_2: 8.7-13.4%

Yield and Energetics Vary with Fuel Composition as Well

Accomplishments (10/11)



- Iso-octane demonstrated the most readily quantifiable behavior
- Ethanol reforming yields significant concentrations of acetaldehyde and methane
  - Calculations showed that acetaldehyde is not an equilibrium product
  - Acetaldehyde is unfavorable for reforming energetics
- Gasoline speciated as mixture of iso-octane and toluene using a combination of FTIR and mass spectrometry, results in lower energy balance than iso-octane (lower H/C)
- Yield and energetics also depend on the temperature and fueling rate

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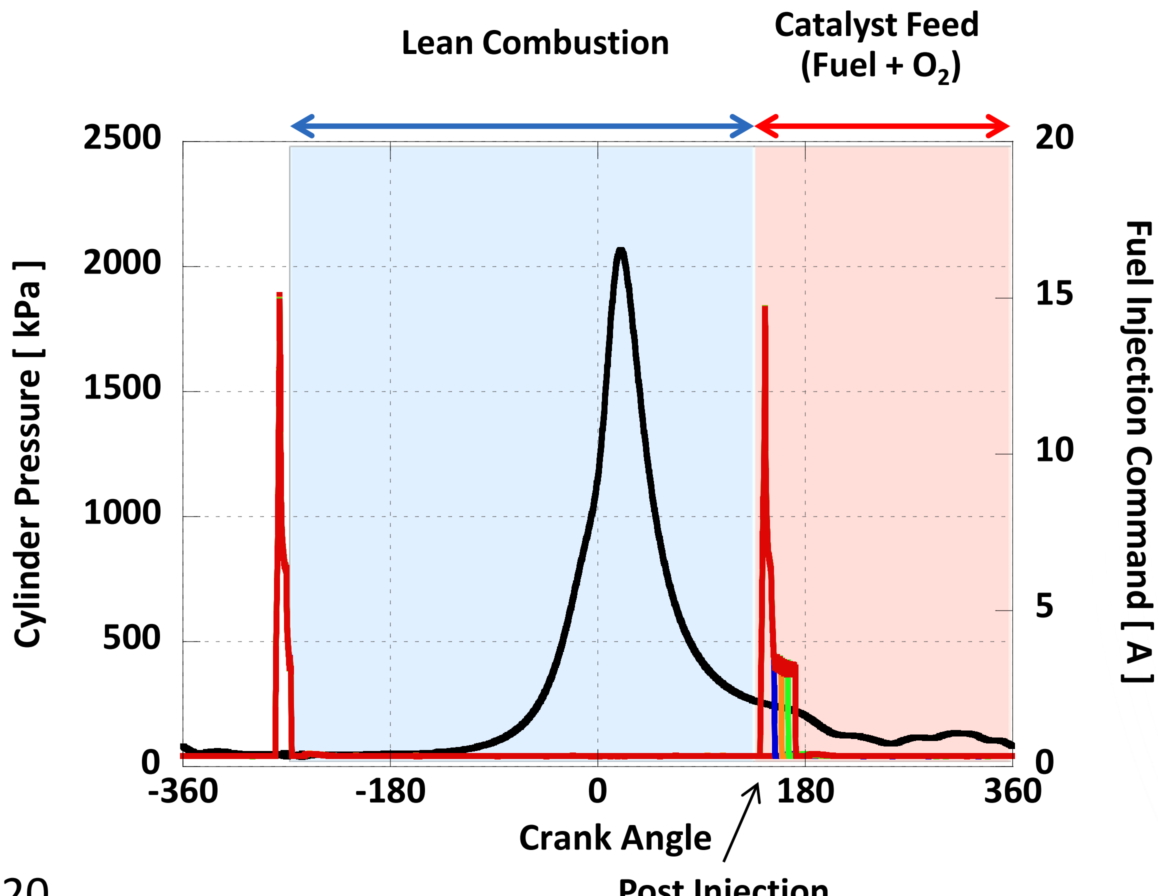
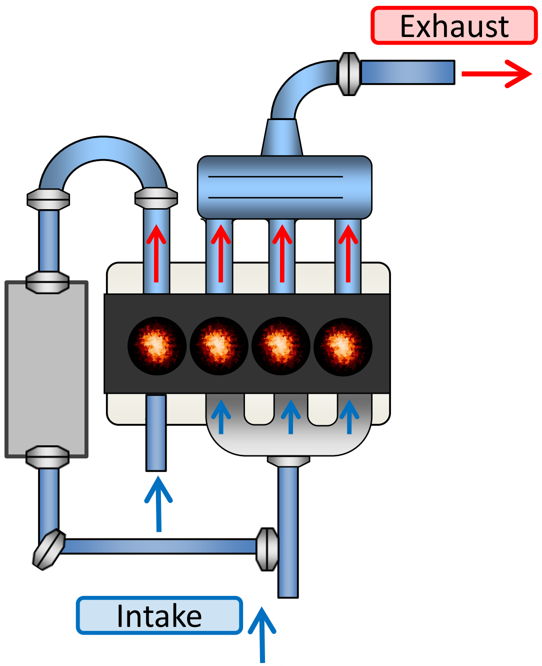
Implementation of the EGR Loop Reforming on an Engine: Providing Oxygen to the Catalyst will Require Lean Operation

- Lean combustion by one cylinder to feed oxygen to catalyst
  - Allows stoichiometric exhaust for 3-way catalyst compatibility
  - Allows lean cylinder to be at a higher MAP, match load
- Fuel provided to catalyst through post injection event





Example Case:
2000 rpm, 4.5 bar BMEP

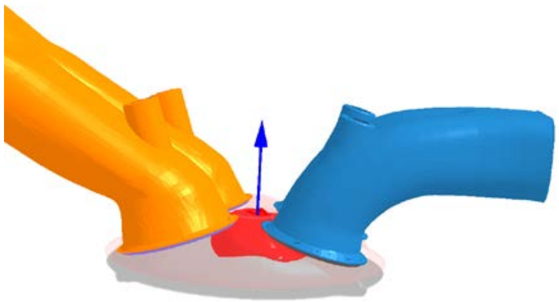
Post Injection: 50% of fuel for Cylinders 1-3

- Combustion $\Phi = 0.74$
- Catalyst $\Phi = 4.2$
- Predicted H_2: 12% reformer out
- Predicted H_2: 3% intake manifold

Five Reviewers Evaluated This Work in 2015 (ACE015) Overall Positive Comment with Room for Improvement

Several reviewer comments on including CFD modeling to assist development, add insight

At the 2015 AMR we demonstrated an expanded use of modeling through collaborations. CFD modeling capability for this project is being developed by leveraging another ORNL project (reviewed during FT038 and FT039). A mesh of this engine has been developed using FORTE modeling software and is currently being validated. We expect to have results using CFD next year.



FORTE CFD simulation.

Comment that the heat losses in the exhaust manifold should have been addressed quickly through aggressive insulation.

This was the initial attempt, but the length of the gas passage made this ineffective. An attempt was also made to counter the heat losses using heating tapes. However, with the custom valve cover and the Sturman HVA system hybrid configuration used in 2015, oil leaks from the valve cover area were common. With this issue, aggressive use of heating tapes posed a safety issue. The engine was reconfigured to run on custom cams to eliminate the oil leaks, and the work in 2016 did include aggressive use of heating tapes.

Several comments that additional industry collaboration would be beneficial.

We agree, and in the last year a collaboration on the catalytic reforming was initiated with Aramco Services Co. Additional OEM collaboration is being sought.

Custom cam shafts for the in-cylinder reforming strategy used in 2016. This engine configuration replaced the HVA configuration to eliminate oil leaks so that aggressive exhaust manifold insulation and heating could be pursued.

Collaborations

- Project was born out of a 2010 USCAR Colloquium

http://feerc.ornl.gov/pdfs/Stretch_Report_ORNL-TM2010-265_final.pdf

- Umicore – Catalyst coatings
- ANSYS (formerly reaction design) – CFD model development
- University of Michigan: Yan Chang is a UM student working on the project at ORNL for 2016, advised by Stani Bohac and André Boehman
- AEC Working Group bi-annual meetings
  - Mechanism for industry feedback
- Joint effort with SNL on in-cylinder chemistry (ACE 006)
  - 2014 SAE paper (ORNL lead, Dick Steeper)
  - 2015 SAE paper is in manuscript form (SNL lead, Isaac Ekoto)
- University of Minnesota: Will Northrop is collaborating with SNL and ORNL, performing kinetic and thermodynamic simulations of in-cylinder reforming
- University of Michigan: Galen Fisher advising on catalyst formulation and operating conditions through subcontract
- Related funds-in project with Aramco Services Co.

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Future Work: Focus on Catalytic Reforming for the EGR Loop using Engine Experiments

Lower Priority of In-Cylinder Reforming Work

- Data shows that results are not sufficiently promising to continue to pursue this pathway in its current form, conclude with reporting

EGR Loop Engine Experiments Beginning in FY16

- Six 4" x 6" monoliths of pre-commercial Rh-based catalysts are being acquired
  - Zirconia mullite substrates for durability at high temperature procured from CTI
  - Umicore is currently coating the substrates with a pre-commercial Rh-based catalyst
- Initial engine experiments will focus on engine efficiency and dilution tolerance at the ACEC Tech Team part-load efficiency point (2000 rpm, 20% load)
  - Initial experiments will use low sulfur fuels (lube certification gasoline, iso-octane, ethanol)
  - Model engine operation with and without reformate at this condition

Bench Flow Reactor Reforming Activities Continuing

- Evaluate catalyst durability under reforming conditions
  - Determine stability of H_2 production over long operating times and measure sensitivity to SO_2
  - Identify strategies for mitigating any performance loss

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Summary

Relevance

Investigate high risk combustion strategies with a thermodynamic potential for large efficiency increases

Approach: Dilute Combustion and TCR for Increased Efficiency

- Strategy 1- In-cylinder reforming in a low oxygen environment
- Strategy 2- Catalytic EGR-loop reforming

Accomplishments

- Pursued three strategies to improve performance of in-cylinder reforming that ultimately made minimal difference to engine performance (higher CR, oxygen availability, and exhaust manifold)
- Bench flow reactor configured to replicate engine-conditions, results show potential for order-of-magnitude higher H_2 from catalytic reforming
- Data-based decision to switch engine focus from in-cylinder reforming to EGR loop reforming

Collaborations

- Industry (Aramco Services Co., Umicore, Ansys), University (U Mich, U Minn), National Laboratories (SNL)

Future Work

- Implement EGR loop reforming in engine experiments, focus on ACEC tech team efficiency point
- Investigate catalyst durability during long durations and with SO_2 exposure on flow reactor
- Complete development of CFD model, to add insight to experiments and aid development

Technical Backup Slides

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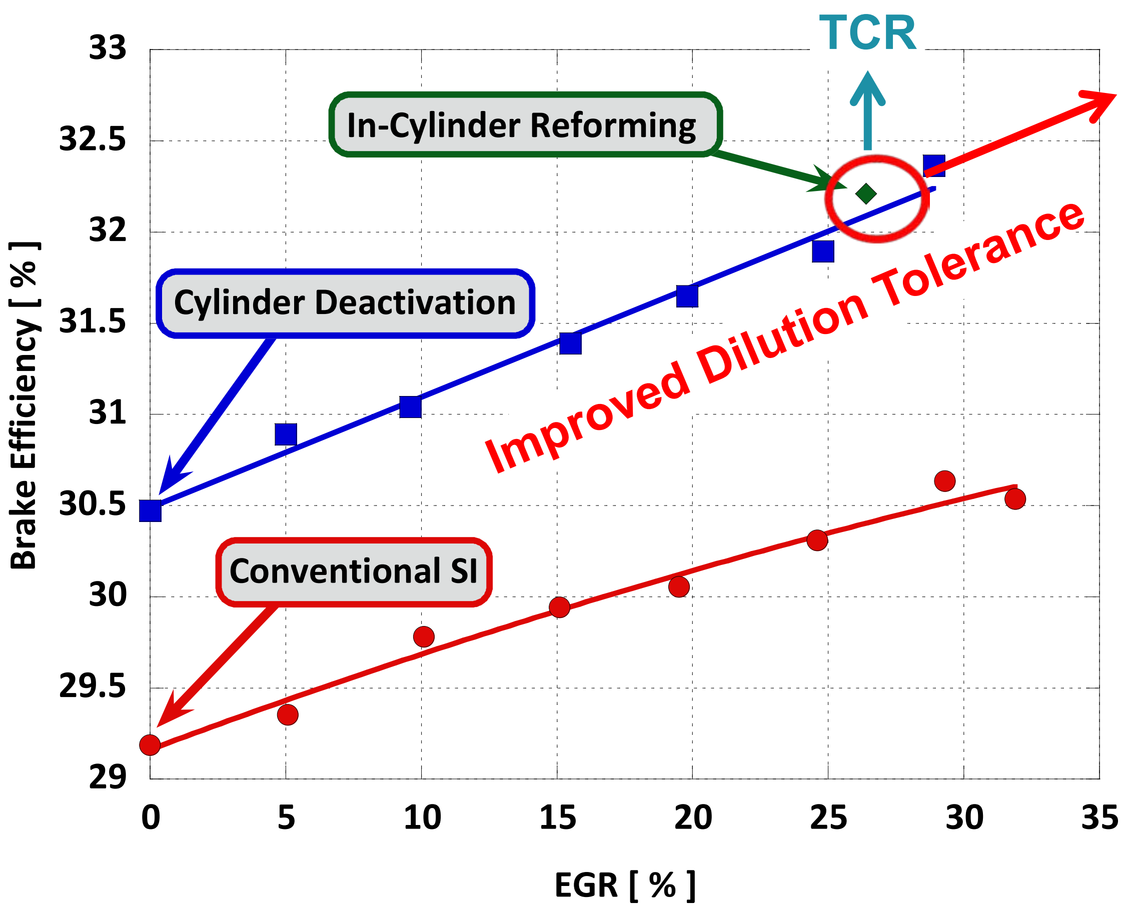
Efficiency Increase can be Primarily Attributed to Cylinder Deactivation and EGR Dilution rather than In-Cylinder Reforming

BACKUP 1

Stoichiometric Combustion with CR = 9.2:1
2000 rpm, 4 bar BMEP, CA50 = 8 CA $aTDC_f$



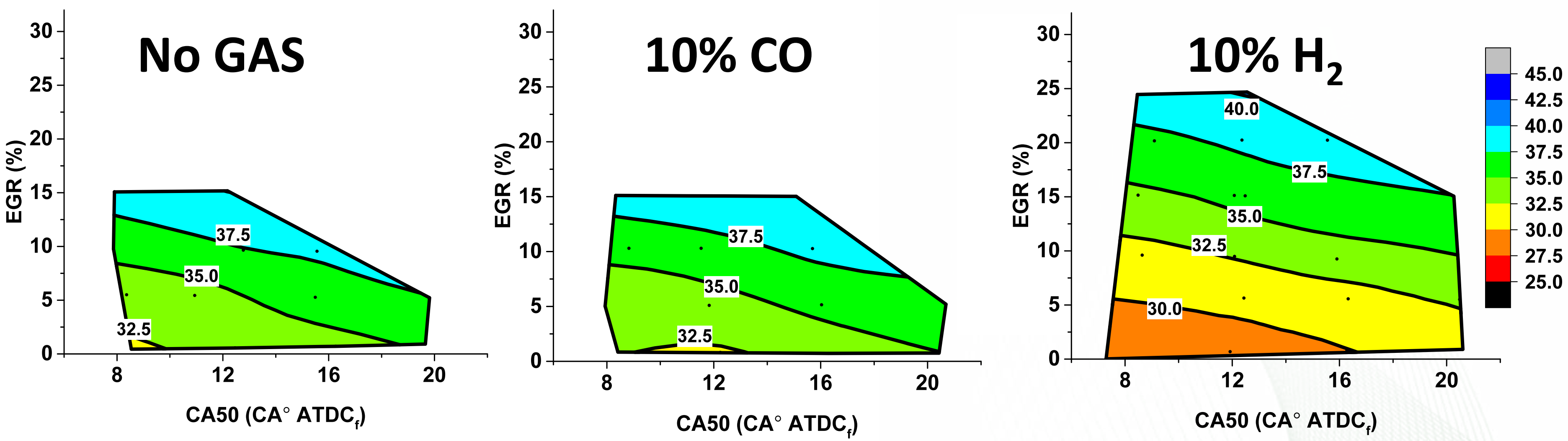
- BTE improvement with valve deactivation is substantial
  - Fuel consumption decrease of 4.2%
- BTE improvement with in-cylinder reforming is higher
  - Fuel consumption decrease of 9.4%
- EGR increases efficiency for both valve deactivation and conventional SI
- Valve deactivation with EGR matches efficiency from in-cylinder reforming
- Future work will focus on maintaining improving reforming so that dilution limit can be extended

Based on Previous Work, H_2 at 10% of the Fuel Energy is Expected to Significantly Increase the EGR Dilution Tolerance

BACKUP 2

- Same SI engine used for this project (GM LNF engine)
  - Work presented at the AEC Program Review Meeting, Feb. 2015
- CO as 10% of fuel energy provides a modest increase in dilution tolerance
- H_2 as 10% of fuel energy provides a much larger increase in dilution tolerance

H_2 as 10% of fuel energy is the concentration expected for the EGR loop catalytic reforming strategy

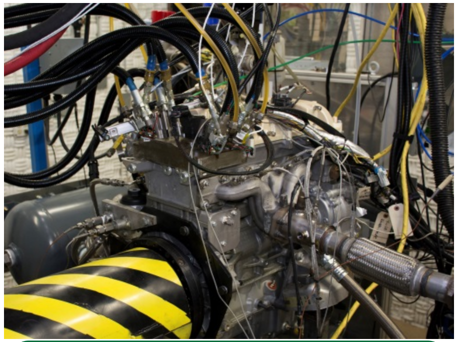


Contours indicate 10-90% combustion duration

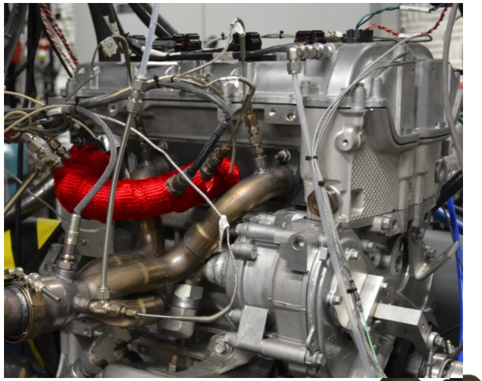
Experimental Details

BACKUP 3

- Highly modified 2007 GM LNF engine
  - 2.0 L Displacement (bore x stroke: 86 mm x 86 mm)
  - Direct injection (constant rail pressure of 85 bar for this study)
  - Stock pistons and compression ratio (9.2:1)
  - Early data taken with Sturman HVA system, 2016 data used custom cams to enable the in-cylinder reforming strategy
- Single operating point study: 2000 rpm, 4 bar BMEP
- All data collected at a CA50 combustion phasing of 8 CA $aTDC_f$
- Engine-out emissions measured with a 5-gas emissions bench
- Additional analyzers used to speciate reformate and exhaust
  - FTIR to speciate hydrocarbons
  - Magnetic sector mass spectrometer used to measure H_2
- Ethanol, iso-octane, and certification gasoline used
  - Ethanol has low sooting tendency
  - Pure components enable speciation, closure of carbon balance
  - All 3 fuels have low sulfur, helpful for catalytic reforming work



Engine assembly and installation complete



Configuration with Custom cams for 2016