Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes

Project ID: ACE015

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Project Overview

Barriers (MYPP 2011-2015, 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

- FY12: $250k
- FY13: $350k
- FY14: $300k

Project Timeline

- ***Stretch Efficiency research program started at ORNL in 2005***
  - ***Initiated current focus on thermochemical recuperation in 2011***
- ***Investigations have evolved based on comments from previous AMR reviews and will continue to evolve with emerging needs***

Industrial Partnerships and Collaboration

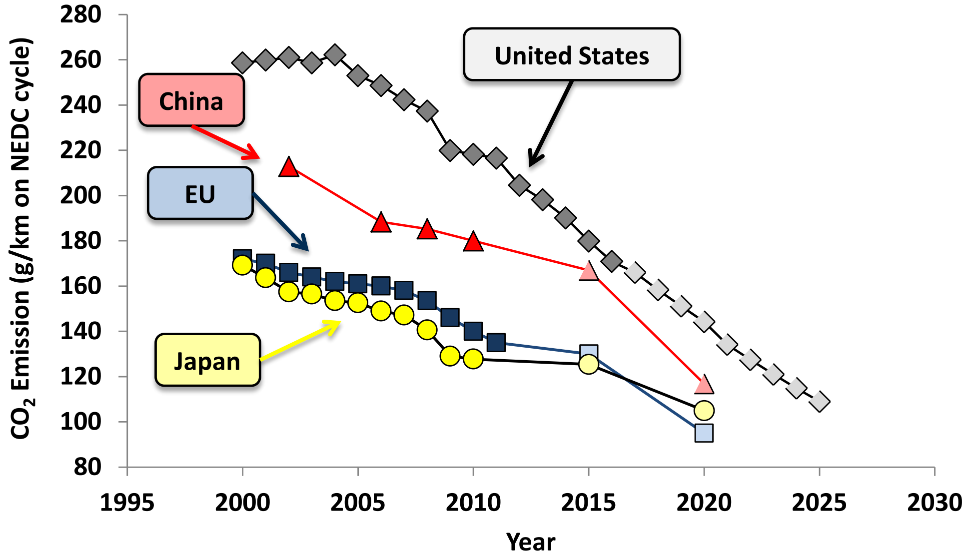
- ***AEC working group led by SNL***
  - ***Mechanism for industry feedback***
- ***SNL – Dick Steeper***
- ***Gas Technology Institute***
- ***Cummins***

Universities

- ***University of Michigan***
- ***Penn State University***

Objective: Increase Efficiency through Major Changes to Combustion Processes and Engine Architecture

Motivation: Legislation in U.S. and worldwide to reduce vehicle CO_2 emissions



Data from the International Council on Clean Transportation http://www.theicct.org/info-tools/global-passenger-vehicle-standards

Pursue thermodynamic strategies and implementation methods that could provide an increase in efficiency that is revolutionary rather than evolutionary

- Evolutionary technologies are defined as the current major paths forward, with room to grow (downsize and boost)
- This project is focusing 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

THIS PROJECT HAS A TRACKED MILESTONE FOR EACH QUARTER OF FY14

FIRST QUARTER, FY2014

Complete major hardware modifications for modified engine system to operate with one cylinder driven by the Sturman hydraulic valve actuation system

Status: Complete

SECOND QUARTER, FY2014

Complete shakedown in conventional SI combustion mode with modified valvetrain

Status: In-Progress

THIRD QUARTER, FY2014

Operate the unique ORNL in-cylinder reforming strategy with reformate recirculated back to the remaining 3 cylinders

Status: On-track

FOURTH QUARTER, FY2014

Complete a parametric study of engine operating parameters on in-cylinder reforming

Status: On-track

Emphasis on Reformate-Assisted Dilute Combustion through Thermochemical Recuperation (TCR)

Thermal Efficiency of Stoich SI Engines Improves with EGR Dilution

- Thermodynamics of efficiency improvement are well-understood
  - Improved working gas properties (**higher γ**) from composition change
  - Lower temperature results in **reduced heat loss** and further improvements to the working gas properties (**higher γ**)
  - EGR reduces knock tendency, allows **higher compression ratio** for improved efficiency

EGR Dilution Limit can be Extended with H_2-rich Reformate

- High flame speed and low ignition energy of H_2 are well-known to stabilize dilute combustion, allowing higher EGR

TCR Approach to Reforming to Maximize System Efficiency

- TCR through steam reforming to increase heating value and exergy of the fuel
  - Exhaust heat drives endothermic steam reforming reactions to increase chemical energy
  - **Waste heat recovery with a single work conversion device!**

	Reforming Reaction	LHV Increase	Exergy Increase
Octane	$C_8H_{18} + 8H_2O \rightarrow 8CO + 17\ H_2$	25%	14%
Ethanol	$C_2H_5OH + H_2O \rightarrow 2\ CO + 4H_2$	24%	9%
Methanol	$CH_3OH \rightarrow CO + 2H_2$	20%	3%

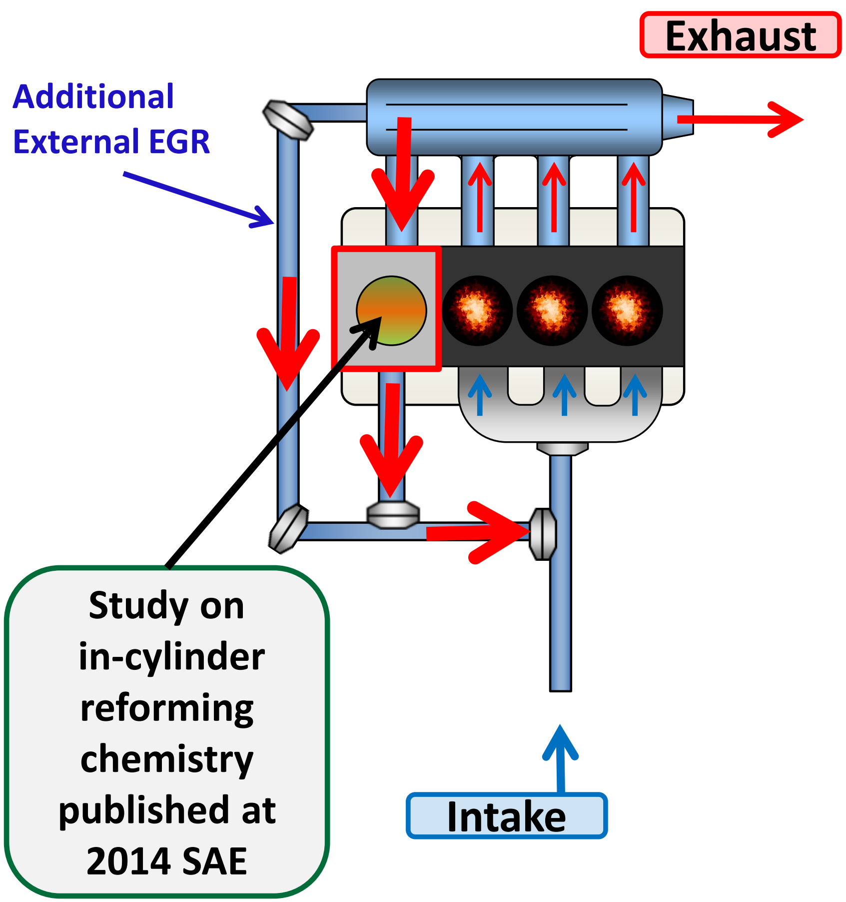
Dilute combustion and TCR are not new ideas. We are pursuing novel approaches to make implementation more feasible in an engine.

Pursuing Reformate-Assisted SI Combustion through Two Parallel Strategies

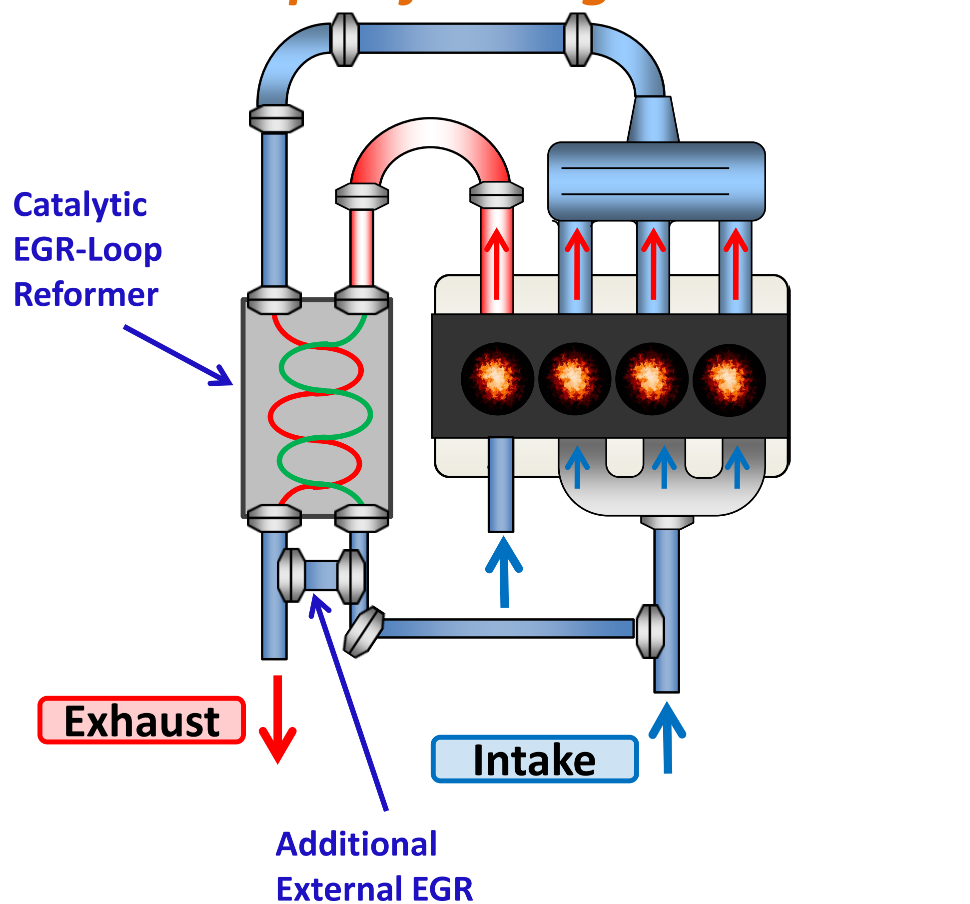
Approach (2/3)

Flexible Hydraulic Valve Actuation for Cylinder 4 Enables Both Strategies to be Investigated on the same Experimental Engine Platform

In-Cylinder Reforming



EGR-Loop Reforming

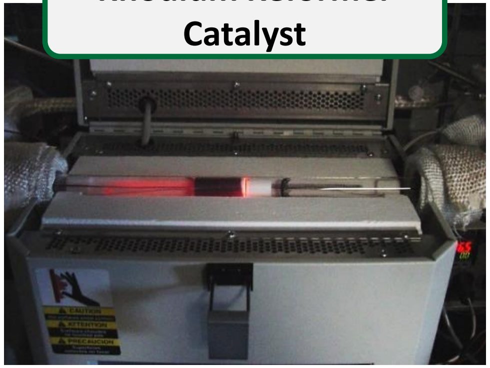


Prior to Engine Experiments, Catalyst Performance and Durability Being Studied on Bench Flow Reactor

- EGR TCR conditions vary from typical steam reforming applications
  - Low steam to carbon ratios (limited to steam in exhaust)
  - Significantly lower temperature available compared to industrial applications
  - Sulfur from fuels and lubricants
- Previous catalyst sample from GTI used a Ni-based catalyst and evaluated it on a Cummins natural gas engine in a CEC funded project*
  - Formulation extremely sensitive to sulfur (2 ppm, presented at 2013 AMR)
- Currently pursuing Rh-based catalyst for improved sulfur tolerance
  - Galen Fisher from University of Michigan advising on catalyst formulation and operating conditions through subcontract
- Various reforming conditions are being considered
  - TCR through steam reforming is primary goal
  - Also considering auto-thermal reforming to achieve sufficiently high temperature when engine exhaust temperature is too low

Bench Flow Reactor

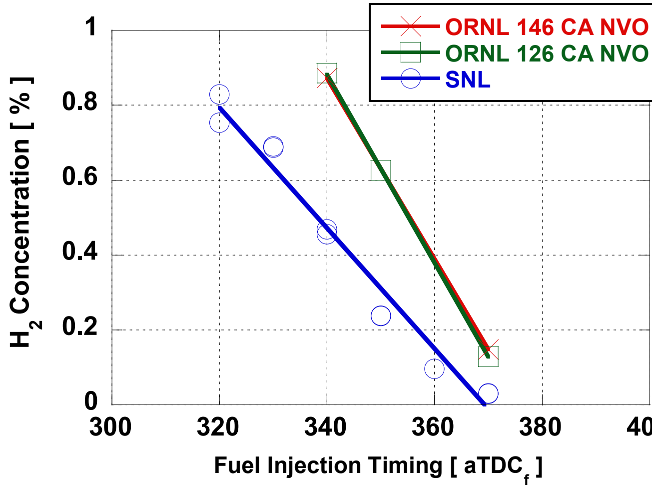
Rhodium Reformer Catalyst

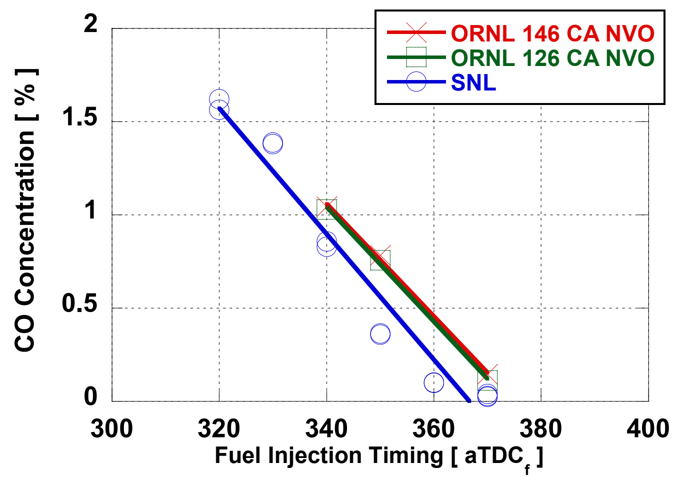


*California Energy Commission Report Publically Available At:
http://www.energy.ca.gov/2009publications/CEC-500-2009-011/CEC-500-2009-011.PDF

Published Collaborative Study with SNL on NVO Chemistry in Oxygen Deficient Environments

- ORNL experimental results from single-cylinder 6-stroke investigation presented at 2013 AMR
  - Results were "hot off the press" and required a significant amount of additional data analysis and reporting
  - Invited talks based on these experiments given at SAE High Efficiency Symposium and SWRI HEDGE consortium
- NVO sampling on a subset of ORNL conditions by D. Steeper at SNL to assess universality of major findings
  - Major differences experimental configuration and methodology between ORNL and SNL (technical backup #1)
  - ORNL and SNL results for H_2 and CO production are in excellent trend-wise agreement for iso-octane
  - Confirms ORNL conclusion that non-catalytic in-cylinder reforming is a kinetically-limited process – timescales dominate
  - Excellent trend-wise agreement also observed for small-chain HC species (technical backup #2)



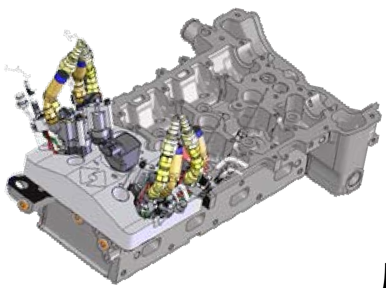


Reformate rich in H_2 and CO can generated using an in-cylinder process, then used to enable highly dilute combustion in SI engines

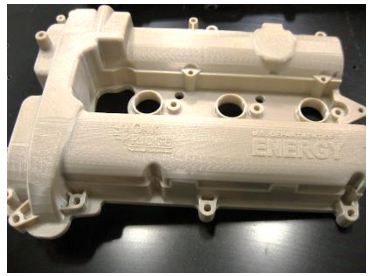
Major Hardware Modifications are Complete for Flexible TCR Research Engine, Currently Installed at ORNL

Accomplishments (2/7)

Cylinder head design for 3 cam-based cylinders and 1 HVA cylinder



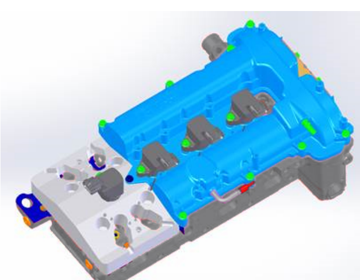
Custom valve cover fabricated with 3D printing at ORNL's MDF



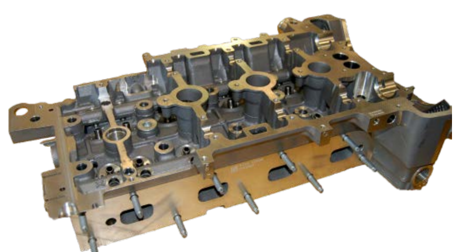
Major hardware modifications complete

Begin Engine Troubleshooting and Break-in

July | Aug. | Sept. | Oct. | Nov. | Dec. | Jan. | Feb. | Mar. | April

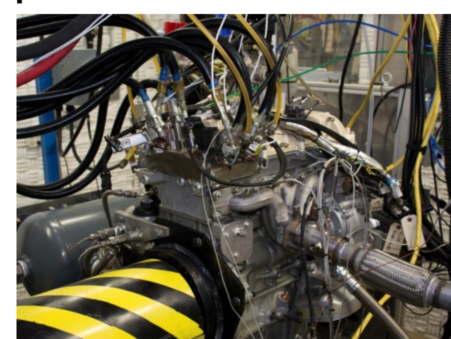


Design of custom valve cover complete



Machining of cylinder head and HVA transfer plate

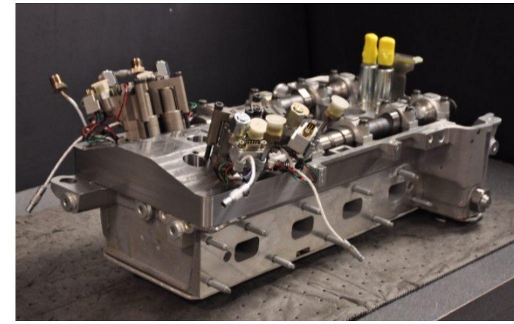
High pressure fuel cart completed and tested

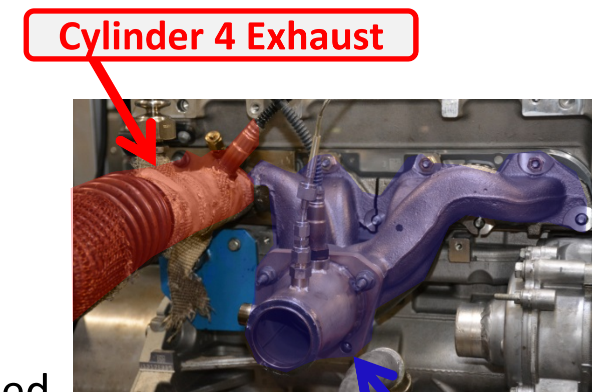


Engine assembly and installation complete

Flexible TCR Research Engine can be Configured for Conventional SI Combustion and Several Reforming Strategies

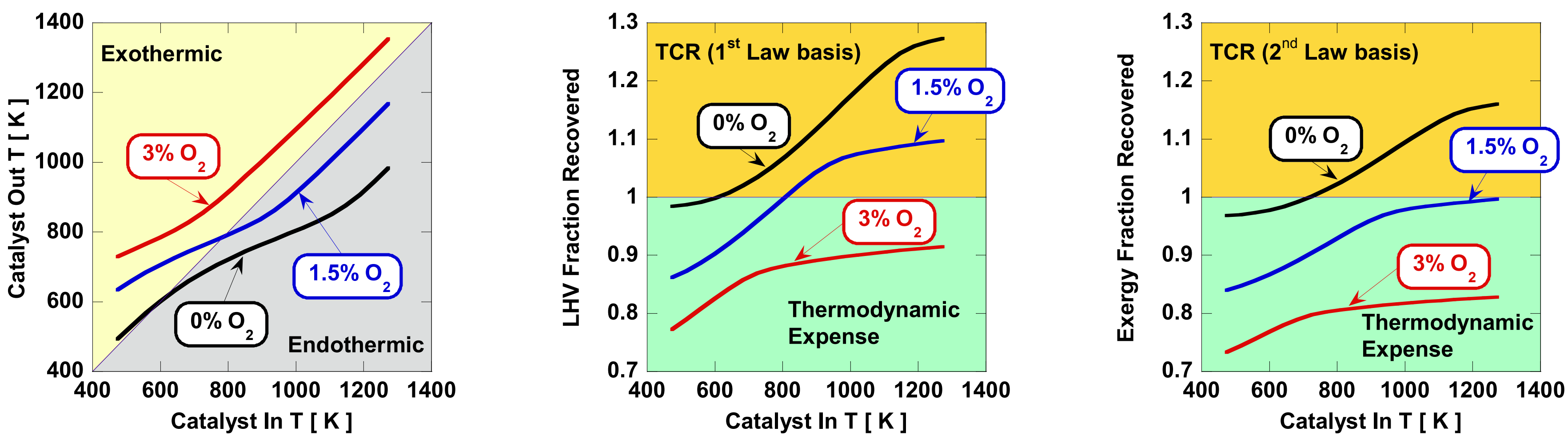
- Three cam-controlled cylinders, one cylinder controlled with Sturman HVA system
  - Cylinder 4 does not have to be operated in the same manner (i.e., in-cylinder reforming or different SI dilution)
  - HVA control minimizes hardware swaps (i.e., camshafts)
- Intake and exhaust manifold designs can be installed to isolate the intake and/or exhaust from cylinder 4
  - Required for both in-cylinder reforming and EGR-loop reforming
- External cooled EGR loop allows total EGR to be varied independent of reforming strategy
  - Static mixer in intake for homogeneous charge to all cylinders
  - Thermal management of intake manifold, regardless of EGR level
- Dual independent cam phasing of base engine has been retained
  - Control of external vs. internal EGR
- Independent control of fuel rail pressure with high pressure fuel cart
- Two different compression ratio pistons available (9.2:1 and 11.85:1) plus piston blanks
- NI/Drivven engine controller and Sturman HVA controller provide full authority





Thermodynamic Modeling of Catalyst Performance to Guide Experimental Efforts in Constrained Operating Space

- University of Michigan is using Aspen thermodynamic modeling software to guide the "thermodynamic expense" of reforming under equilibrium conditions
- Engine exhaust conditions constrain reforming chemistry
  - Steam mass is fixed by combustion, so less control of steam/carbon ratio
  - Exhaust temperatures are low compared to industrial steam reforming temperatures
- A small amount of oxygen at catalyst inlet may be required for catalyst performance and operability (to inhibit coking and promote sulfur tolerance)
- Flexible TCR research engine expands the research parameter space for EGR-loop reforming



Dilute combustion may allow for a net efficiency benefit even if there is an exergy penalty

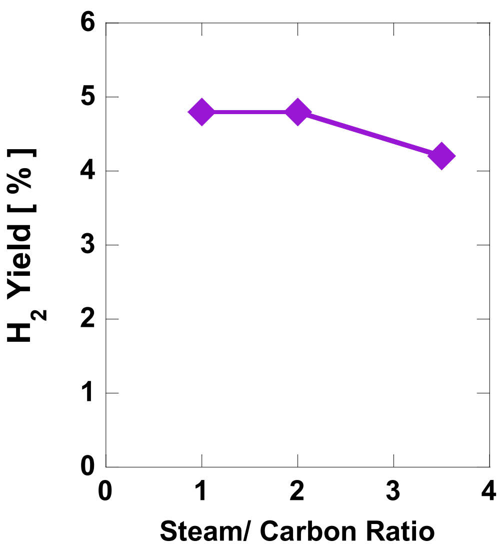
Bench Flow Results Highlight Challenging Parameter Space for Reforming Without O_2

Accomplishments (5/7)

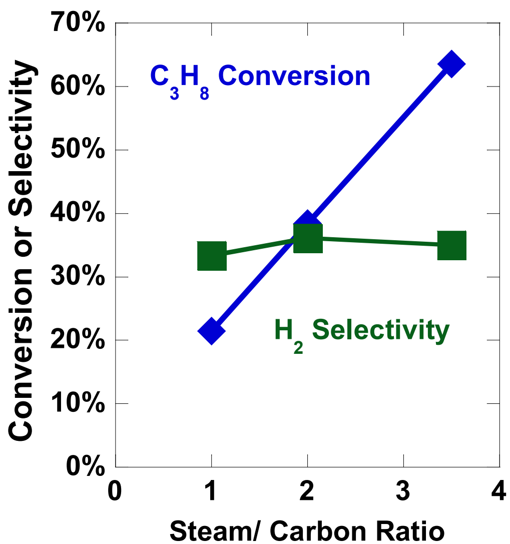
- Bench flow reactor results confirm the thermodynamic modeling results
  - Bench conditions investigated at: Exhaust T 600 °C, H_2O 10-12%, O_2 0-4%
- H_2 yield from steam reforming at 600 °C limited to about 5%
  - Increasing steam/carbon improves C_3H_8 conversion, but...
  - Fixed exhaust H_2O concentration requires that less fuel be reformed to increase steam/carbon
- Steam reforming not sufficiently active for high H_2 yields at 600 °C

reforming conditions:
2 wt% Rh/Al_2O_3
GHSV: 50000 h^{-1}
inlet T: 600 °C
1.14%, 2.0%, or 4.0% C_3H_8
12% H_2O, 14% CO_2

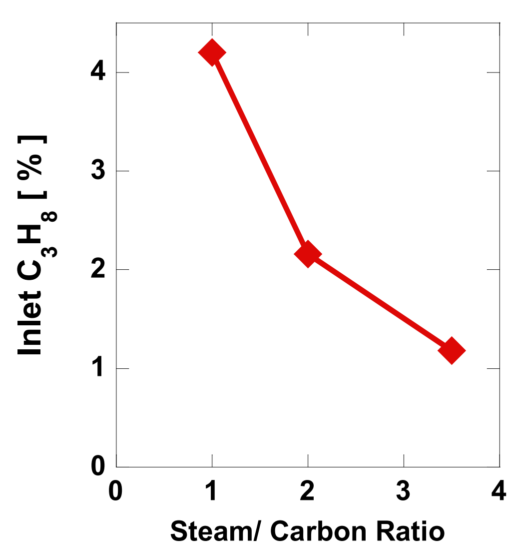
H_2 Yield



C_3H_8 Conversion & H_2 Selectivity



Inlet C_3H_8 Concentration

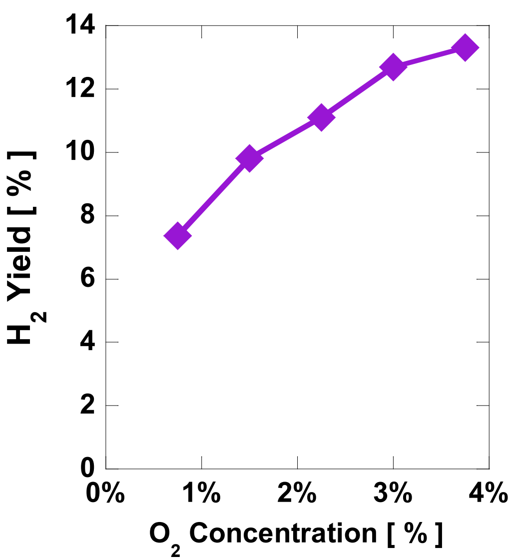


Partial Oxidation Reforming Enables Higher H_2 Yields by Increasing Catalyst Temperature

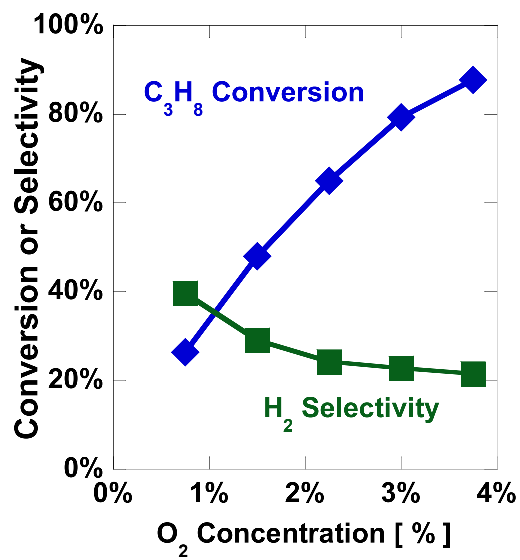
- Higher reactivity (and higher H_2 yields) requires higher catalyst T
  - Typical engine exhaust temperature is ~600 °C
  - Heat generation possible through partial oxidation reforming
- Adding O_2 boosts H_2 yield and C_3H_8 conversion by increasing T
  - Decreases H_2 selectivity (starting to oxidize to H_2O)
  - Limited by attainable engine out O_2 concentration before reaching peak H_2 yield
- **Thermodynamically undesirable because fuel energy is consumed in catalyst**

reforming conditions:
2 wt% Rh/Al_2O_3
GHSV: 50000 h^{-1}
inlet T: 600 °C
4% C_3H_8, 12% H_2O, 14% CO_2
0-4% O_2

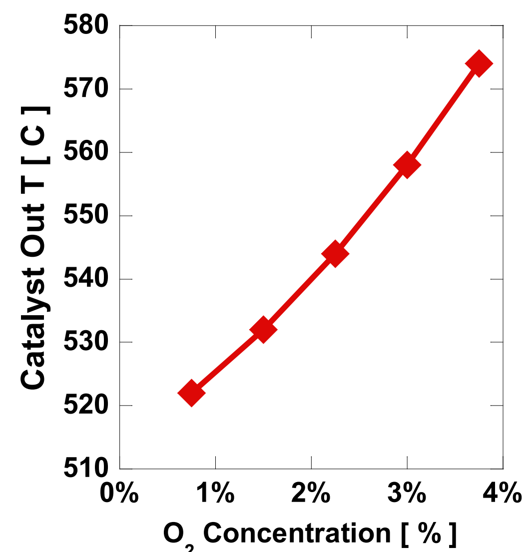
H_2 Yield



C_3H_8 Conversion & H_2 Selectivity

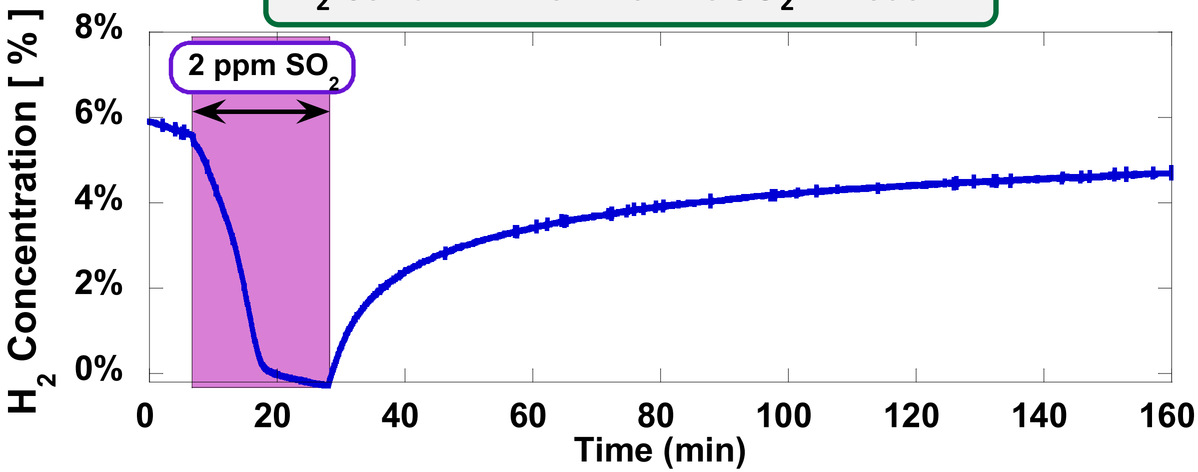


Catalyst Outlet Temperature



Rhodium Catalyst is More Sulfur Tolerant, but Sulfur Sensitivity Remains a Challenge

H_2 Concentration During SO_2 Exposure



reforming conditions:
2 wt% Rh/Al_2O_3
GHSV: 50000 h^{-1}
inlet T: 600 °C
2% C_3H_8,
3% O_2
12% H_2O,
14% CO_2
0 or 2 ppm SO_2

- Prior Ni-based formulation irreversibly deactivated in presence of 2 ppm SO_2 under methane EGR reforming conditions (presented at 2013 AMR)
- Rh catalyst also deactivates when exposed to SO_2, but H_2 production recovers after SO_2 removal under partial oxidation reforming of C_3H_8
- Tolerance to sulfur is highly dependent on operating conditions
  - Performance does not recover when sulfur is removed if oxygen is not present at 600 °C
- Further experiments will evaluate impact of SO_2 concentration
- The search for more sulfur tolerant operating conditions continues...

ORNL's catalysis expertise positions us well to continue to make progress in this area

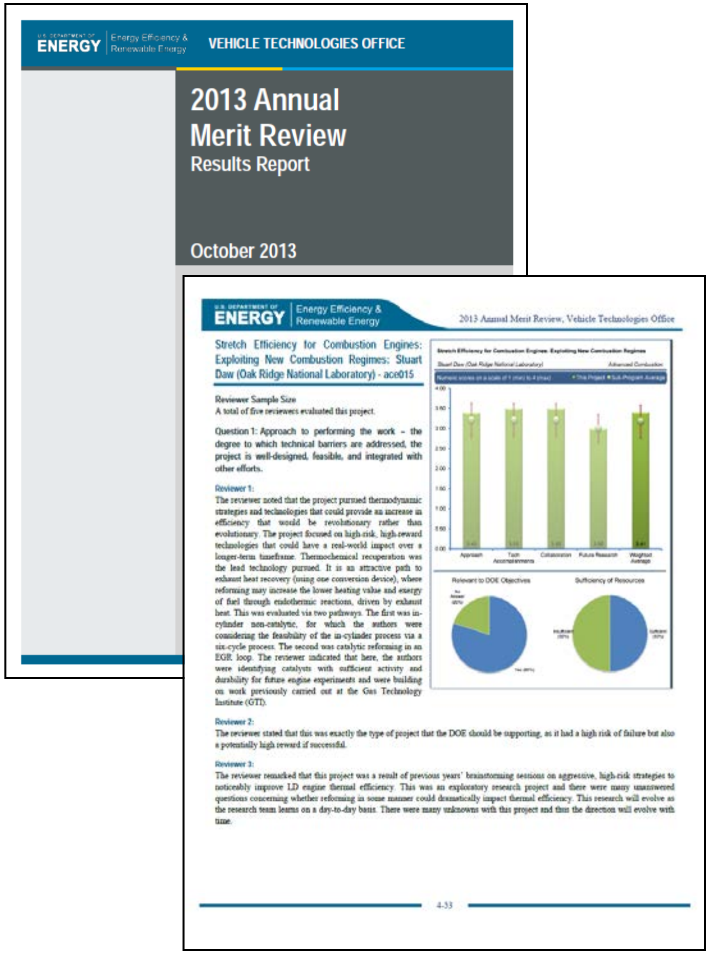
Five Reviewers Evaluated This Project (ACE015) at the 2013 AMR – Comments Overall were Very Positive

Positive Comments (paraphrasing)

- Exactly the type of project that DOE should be supporting, as it had a high risk of failure but also a potentially high reward if successful
- The project leverages a good team of National labs, universities, and incorporates industry input
- TCR is of high interest, and that it is beneficial for DOE to have this type of high risk stretch objective project in its portfolio.

Areas for Improvement (paraphrasing)

- Given the range of interesting concepts involved in this project, more work could be done to evaluate them. ***The flexible engine platform that is operational as of 2014 will serve as a common basis of comparison for evaluating many of the concepts being pursued.***
- Further work is needed to determine whether TCR is being achieved. ***We agree. Improving the speciation and quantification of reformate species to close the energy balance is an ongoing focus of this work.***
- Results presented at the 2013 merit review show that in-cylinder reforming is possible, but much work remains to show the pros and cons of this approach. ***We agree. There are many unknowns, and our intent is to use the flexibility of our experimental engine platform to investigate the parameter space to provide answers.***



http://energy.gov/sites/prod/files/2014/04/f14/2013_amr_04.pdf

COLLABORATIONS

- 2010 USCAR Colloquium (overall direction)
  - 29 invited experts from industry, universities, labs and government to identify long-term research priorities regarding the theoretical and practical efficiency limits of internal combustion engines
  - Full report available at http://feerc.ornl.gov/pdfs/Stretch_Report_ORNL-TM2010-265_final.pdf
- Collaboration with Dick Steeper at SNL on in-cylinder chemistry in low oxygen environments
  - Co-authored 2014 SAE paper containing results from both organizations
  - Plans for collaborative research to continue with Isaac Ekoto (ACE006)

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Negative Valve Overlap Reforming Chemistry in Low-Oxygen Environments

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Szybist, J., Steeper, R., Splitter, D., Kalaskar, V. et al., *SAE Int. J. Engines* 7(1):2014, doi:10.4271/2014-01-1188.

- Collaboration with Gas Technology Institute (GTI) and Cummins
  - New 2014 NDA with GTI on relevant recuperative technologies for syngas production
  - Sharing experimental data and catalyst samples
- University of Michigan
  - Galen Fisher advising on catalyst formulation and operating conditions through subcontract
- Penn State University
  - Graduate student as visiting researcher at ORNL for 9 months (Vickey Kalaskar, advised by André Boehman)

There are Challenges and Barriers to Achieving TCR through Steam Reforming on Engines

Pathway 1. In-cylinder reforming in low oxygen environments

- Determining conditions under which in-cylinder reforming is most thermodynamically favorable
  - Includes need to speciate reformate and close energy balance
- Determine how best to utilize reformate to maximize efficiency
  - Overall dilution level, ignition system, and mix of internal vs. external EGR as a function of engine speed and load

Pathway 2. EGR loop catalytic reforming

- Demonstrating that a catalyst composition can provide good reforming activity while being durable to sulfur and coking
  - Operating space is highly constrained due to engine exhaust conditions (temperature, steam, oxygen availability)
  - Resistance to sulfur poisoning is also highly dependent on operating conditions
- Integration of a catalyst onto an engine system
  - Need to avoid coking and other deactivation during startup and transient conditions
- We believe we're on the right track with a Rh-based catalyst, but much work remains

Pursuing Efficiency through Thermodynamically Inexpensive Reforming and Dilute SI Combustion

Future Work (2/2)

- Two-year path was presented at 2013 AMR – one year completed
- Two strategies of thermodynamically inexpensive reforming, including TCR, are being pursued in this project
  - Reformate enables highly dilute SI combustion to allow efficiency to be increased through well-established pathways (higher compression ratio, higher ratio of specific heat, lower heat transfer)

Pathway 1. In-cylinder reforming in low-oxygen environments

- Exhaust heat drives endothermic reforming reactions to produce H_2, CO, and HC
- Design and installation of flexible multi-cylinder engine platform has been completed
- Parametric investigations on reforming and operating conditions continuing through FY15

Pathway 2. EGR loop catalytic reforming

- Bench reactor characterization with Rh catalyst at engine-relevant conditions
  - Provides feedback to engine for required temperature and oxygen for good performance
  - Sulfur tolerance also characterized – appears to be highly dependent on temperature and steam
- Isolated intake and exhaust for HVA cylinder on multi-cylinder platform to be used to alter to engine exhaust for catalyst performance (temperature, oxygen availability)

Summary

Relevance

Investigate high risk revolutionary combustion strategies with potential for large efficiency increases

Approach: Two Pathways to Achieve Fuel Reforming

- In-cylinder non-catalytic reforming
- EGR loop catalytic reforming (catalyst evaluation and characterization)

Accomplishments

- Identified the importance of long timescales for in-cylinder reforming in collaborative investigation with SNL (kinetically-limited process)
- Completed hardware modifications and installation of flexible multi-cylinder HVA engine platform
- Modeling being used to guide experimental efforts with catalysts in constrained operating space
- Bench flow reactor studies to map performance and durability with Rh-based catalyst

Collaborations

- Collaborative investigation with SNL, subcontract to University of Michigan, graduate student at Penn State, and new non-disclosure agreement with GTI

Future Work

- Experimental parametric studies on in-cylinder reforming with a flexible multi-cylinder engine platform using unique ORNL analytical capabilities to analyze thermodynamics, quantify TCR
- Continue to investigate experimental space of catalyst for performance and durability under constrained operating conditions

TECHNICAL BACKUP SLIDES

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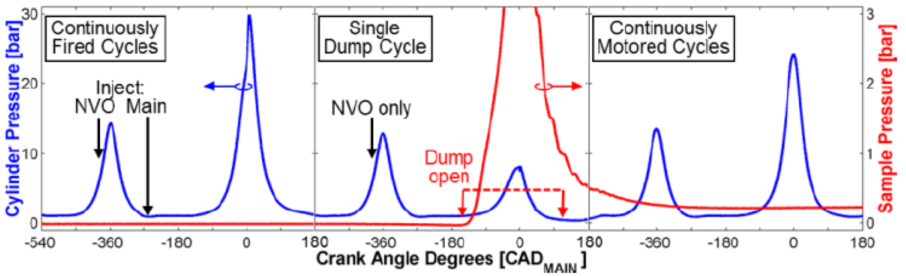
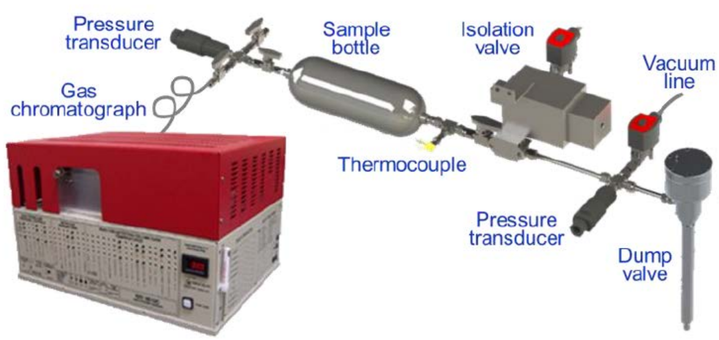
Complementary Measurements at SNL to assess Similar NVO Conditions on Significantly Different Engine Experiment

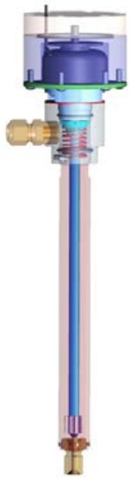
Backup 1

- Gasoline LTC engine at SNL reproduced ORNL condition 3 with iso-octane using techniques discussed ACE006

	ORNL	SNL
Engine cycle	6-stroke	4-stroke
Valvetrain	Variable (HVA)	Fixed (cam)
Engine speed	2000 rpm	1200 rpm
Engine displacement	0.5 L	0.633 L
DI injector	Side-mount	Center-mount
Sampling	Continuous	Dump cycle
HC/CO gas analysis	FTIR	GC FID
H_2 analysis	Magnetic Sector Mass Spectrometer	GC TCD
Peak NVO temperature	1120-1200K	1120-1200K

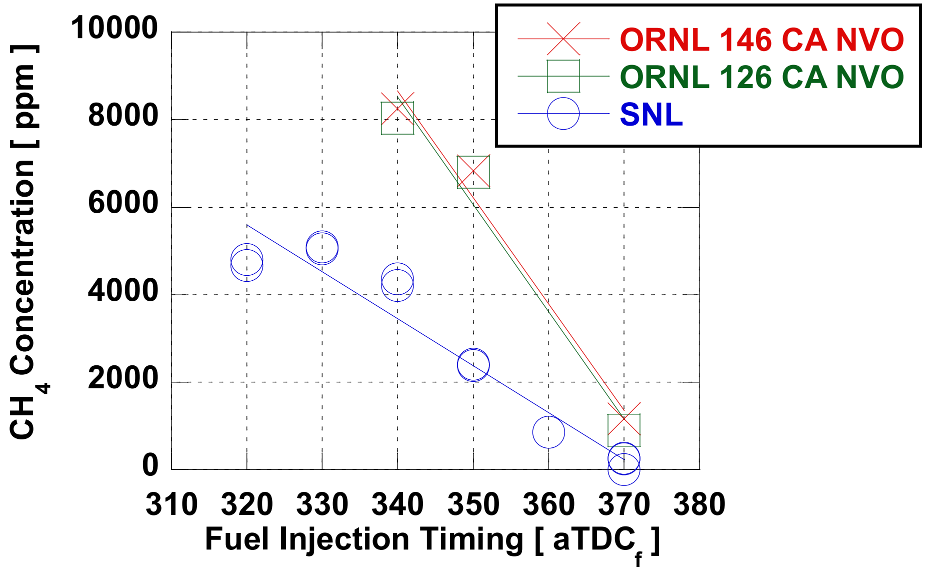


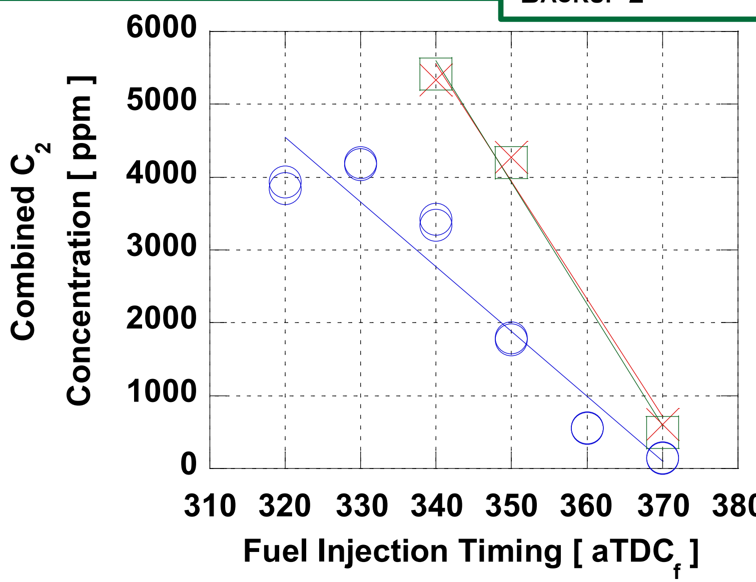




Measurements of Minor HC Species from SNL and ORNL are in Excellent Trend-wise Agreement

Backup 2





- Methane emissions monotonically increase with advancing fuel injection timing
  - Similar to H_2 and CO
- There is a maximum in propylene emissions observed in both the ORNL and SNL data at a fuel injection timing of 340-350 CA
  - Likely intermediate that forms PM