Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes

Project ID: ace015_daw

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Overview

- **Timeline**
  - Start
    - FY05
  - Finish
    - Ongoing
- **Budget**
  - FY11 Funding
    - $250K
  - FY12 Funding
    - $250K

- **Barriers**
  - Max fuel efficiencies of existing IC engines are well below theoretical potential
  - Overcoming these limits involves complex optimization of materials, controls, thermodynamics, and engine architecture
- **Collaborators**
  - Reaction Design
  - Gas Technology Institute
  - Cummins
  - Sturman Industries
  - Borla Industries
  - Universities
    - Texas A&M University
    - University of Wisconsin
    - Illinois Institute of Technology
    - University of Alabama
    - University of Michigan

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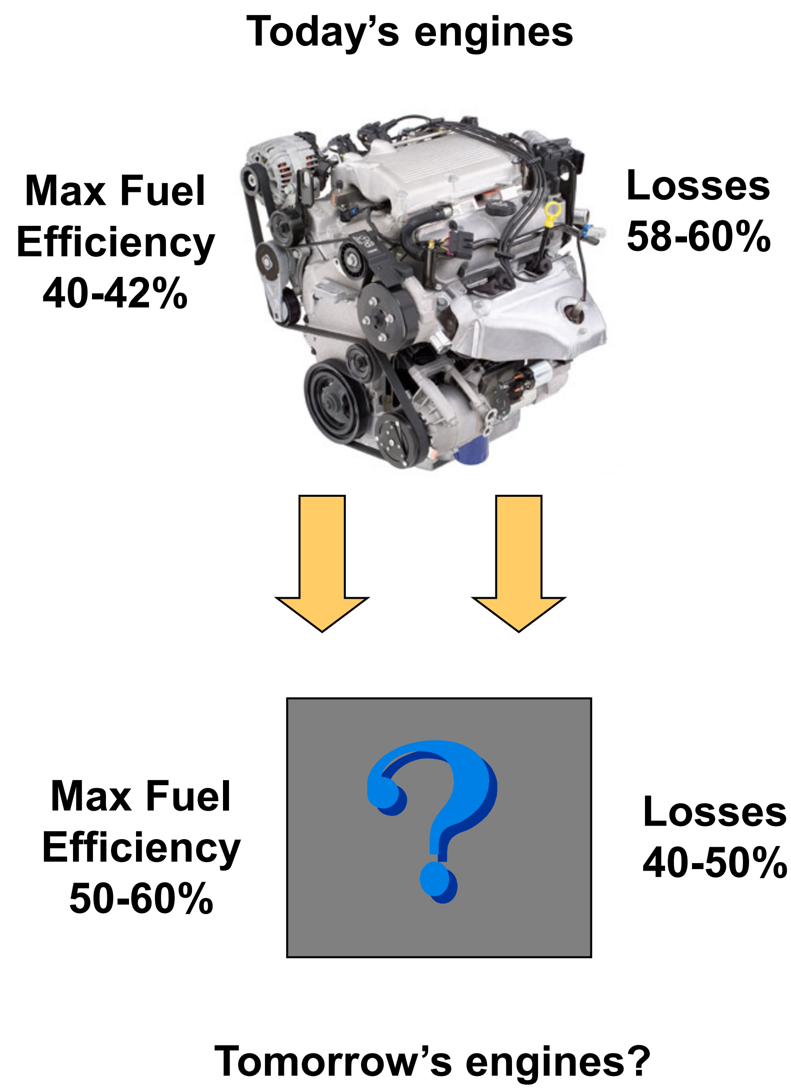
Objective: Increase ICE fuel efficiency via major combustion and architecture changes

- Summarize and update basic understanding of efficiency limits
- Identify promising strategies to reduce losses
- Implement measurements & proof-of-principle demos of selected concepts
- Unique OVT activity:
  - Long term, high risk
  - Basic R&D vs. direct path to commercialization



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Relevance (1): This activity addresses specific goals in OVT-ACE Multi-Year Program Plan*

Primary R&D directions include:

- Improve efficiency of light-duty engines for passenger vehicles and heavy-duty engines for commercial vehicles through advanced combustion research and minimization of thermal and parasitic losses;
- Explore waste energy recovery with mechanical and advanced thermoelectric devices to improve overall engine efficiency and vehicle fuel economy.

Goals include:

- Through simulation and experimentation, conduct R&D on advanced thermodynamic strategies that may enable engines to approach 60 percent thermal efficiency.

*Vehicle Technologies Multi-Year Program Plan 2011-2015:

http://www1.eere.energy.gov/vehiclesandfuels/pdfs/program/vt_mypp_2011-2015.pdf

This is also consistent with the findings of the National Research Council**:

"There seems to be little doubt that, regardless of the success of any pathways discussed, the internal combustion engine (ICE) will be the dominant prime mover for light-duty vehicles for many years, probably decades. Thus it is clearly important to perform R&D to provide a better understanding of the fundamental processes affecting engine efficiency and the production of undesirable emissions. …"

** "Assessment of Fuel Economy Technologies for Light-Duty Vehicles," National Research Council, 2011, ISBN 978-0-309-15607-3.

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Relevance (2): Project addresses long-term priority from March 2010 USCAR Colloquium*

- 29 invited experts from industry, universities, labs, and govt.
- Topics:
  - Theoretical and practical limits of current transportation engines
  - Current engine technology barriers
  - Near and long-term R&D priorities
- One major conclusion: **Work needs to begin now on advanced engine architectures in order to reach 60% peak efficiency goal**
- Promising advanced architectures include:
  - Variable valve actuation
  - Modified combustion chamber geometry
  - Cycle compounding
  - Fully expanded cycles

*ORNL/TM-2010/265, October 2010.

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Milestones

- **FY11 Milestone (completed and published)**
  - **Determine potential theoretical efficiency benefits of implementing thermochemical recuperation (TCR) in a reciprocating engine (September 30, 2011).**
- **FY12 Milestone (on track)**
  - **Demonstrate that in-cylinder TCR has the theoretical potential to significantly increase the maximum thermodynamic efficiency limit of current internal combustion engines (September 30, 2012).**

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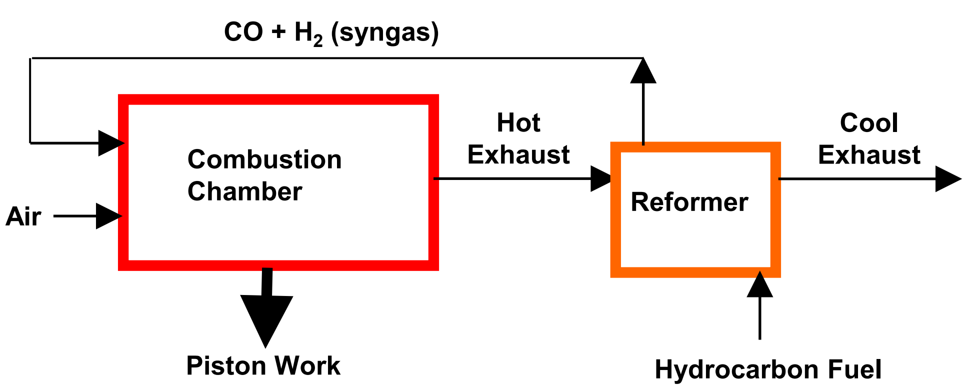
Approach/Strategy: Expert collaborations + analysis & modeling + experiments

- Collaborations
  - Universities, industries, labs
  - Technical meetings, colloquia
- Analysis & Modeling
  - Physics & chemistry (transport & kinetics)
  - Thermodynamics (1st & 2nd Law)



Example: Thermochemical Recuperation of Exhaust Heat for Potential Reuse

- Experiments
  - Measurements to answer basic questions (not define design)
  - Proof-of-principle
  - Lab heat exchangers, reactors
  - Specially modified engines

Ecotec Engine with Sturman HVA

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Approach/Strategy (2): Emphasis this FY has been on fuel chemistry and TCR

- TCR was identified in brainstorming sessions with collaborators as potentially a unique path to effectively implement cycle compounding that could also improve combustion thermodynamics
- Thermodynamic analysis revealed that TCR has theoretical efficiency benefits if:
  - Fuel-specific molar expansion is exploited
  - Fuel-specific reforming reactions are sufficiently fast
  - Syngas is used to improve combustion (e.g., improve dilute combustion stability, allowing higher EGR or leaner operation)

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Technical Accomplishments/Progress

- **Experimental**
  - In-cylinder reforming experiments in HVA engine
    - Measured reaction products for 3 fuels over range of recompression conditions
    - Demonstrated in-cylinder reforming reactions occur at relevant time scales
  - Post-mortem investigations of GTI catalyst
    - Conducted initial TEM and bench reactor studies to understand deactivation
  - Regenerative Air Preheating and TCR (RAPTR) experiment
    - Continued resolving hardware and control system issues at reduced level of effort
- **Analysis and Modeling**
  - Chemical looping study- 2011 Energy & Fuels
    - Demonstrated TCR has important feature in common with chemical looping
    - Implies TCR may be more practical way to boost engine efficiency
  - Thermodynamic fuel effects analysis- Submitted to Energy & Fuels
    - Quantified key thermodynamic effects of fuel chemistry on efficiency
    - Demonstrated no single fuel has ‘silver bullet’ thermodynamic properties
  - Review of GTI-Cummins EGR-TCR experimental data
    - Reviewed conditions under which catalyst deactivation was observed
  - Analysis and modeling of in-cylinder TCR experiments
    - Initiated comparisons of chemical equilibrium and kinetics with observations

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Collaboration and Coordination

- USCAR Colloquium (overall direction)
- Reaction Design (kinetics, Forte, CHEMKIN software)
- Gas Technology Institute, Cummins (EGR -TCR concept, experimental data, catalyst samples)
- Sturman Industries (HVA engine)
- Borla Industries (exhaust water extraction, water injection)
- Universities
  - Texas A&M University & University of Wisconsin (Jerry Caton and Dave Foster- analysis of engine thermodynamics)
  - Illinois Institute of Technology (Francisco Ruiz- concepts for thermal exhaust heat recovery)
  - University of Alabama (Ajay Agarwal- materials for thermal exhaust heat recovery)
  - University of Michigan (Galen Fisher- reforming catalysts)

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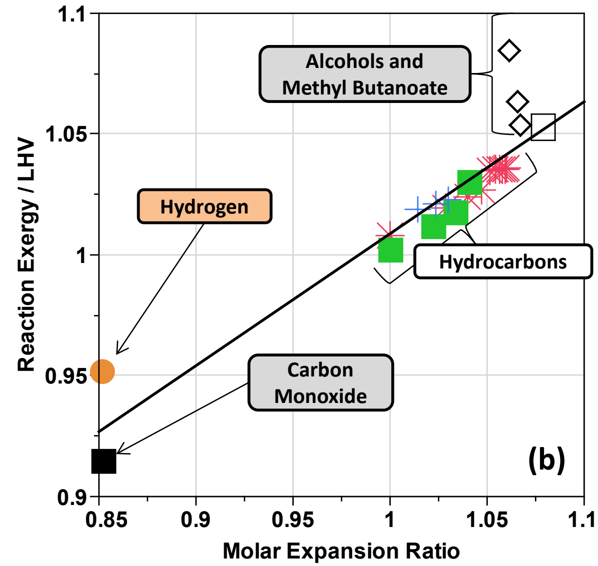
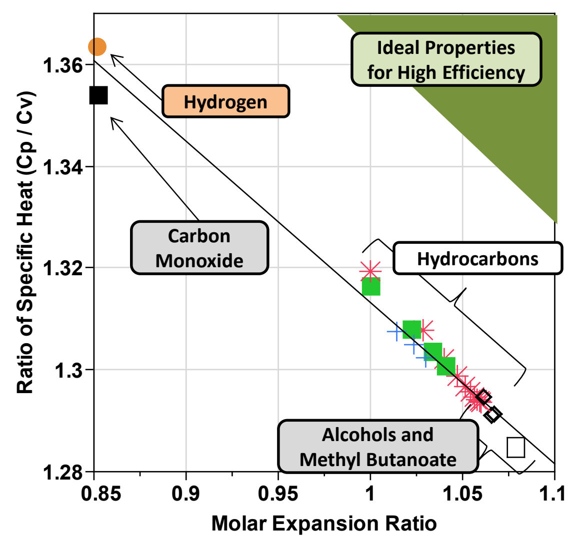
Technical Highlights

Thermodynamic modeling study identified and quantified fuel-specific efficiency potential

- **Molar expansion ratio (MER) found to be primary physical difference between LHV and the work potential of the fuel (exergy)**
  - MER is defined as the ratio of the moles of combustion products to reactants
  - Fuels with high MER (alcohols) have a higher work potential than fuels with low MER (H_2, CO) per unit LHV
- **Work potential increase related to additional moles to perform work even though combustion irreversibility also increases**
- **Other thermodynamic properties make it difficult to translate higher MER into a higher efficiency**
  - **Cannot change one fuel property in isolation**
  - **Ratio of specific heat decreases as MER increases, largely countering MER effect**





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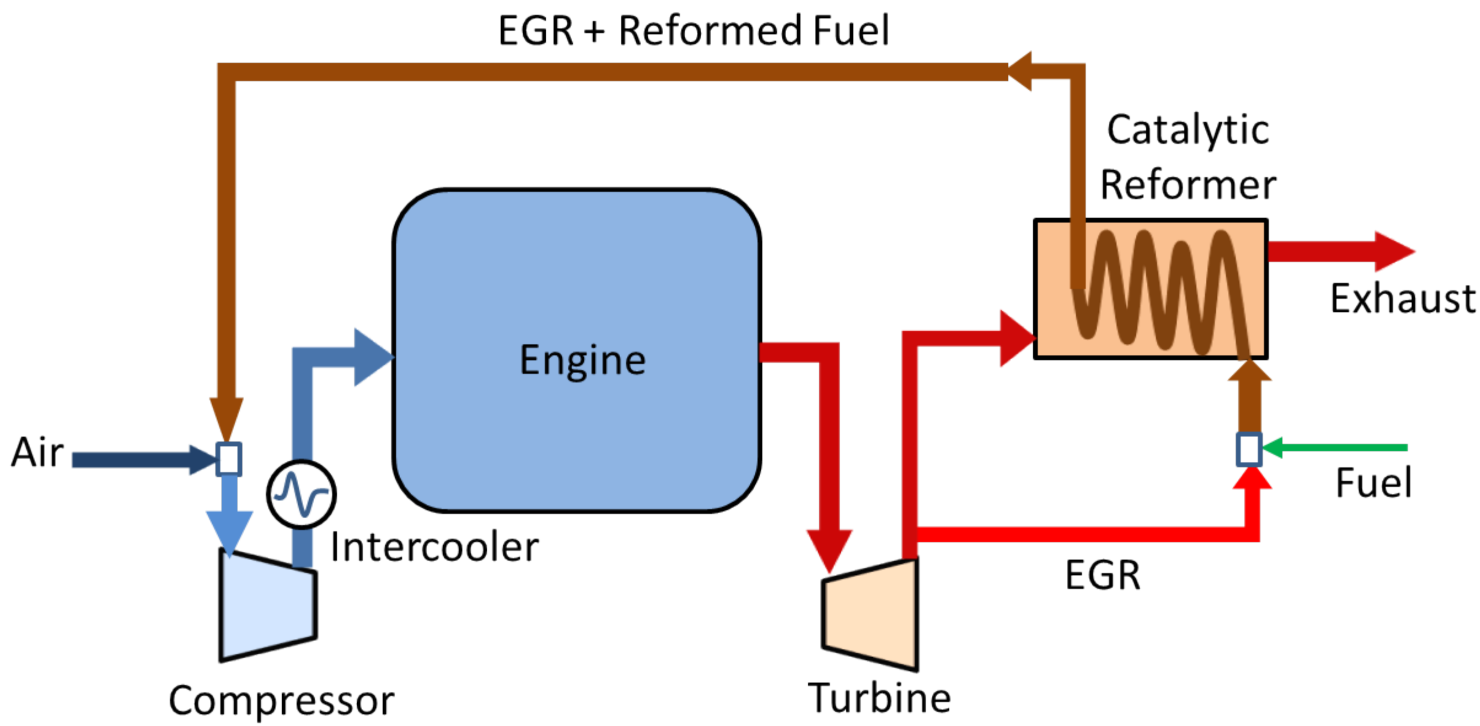
One TCR approach we are investigating integrates catalytic fuel reforming with EGR



- **Endothermic reactions (HC fuel→ CO/H_2) convert exhaust heat to chemical energy.**
- **HC fuel supplemented with syngas (in place of some or all original HC).**
- **H_2 makes higher EGR and CR possible, reduces NOx, potentially extends lean limit.**
- **Thermodynamic analysis indicates circa 5% potential efficiency gain (GTI).**

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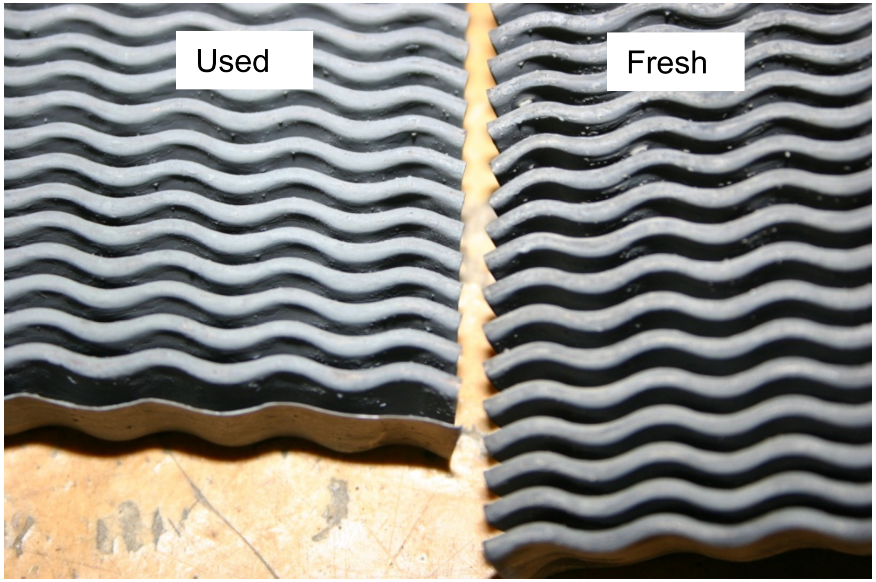
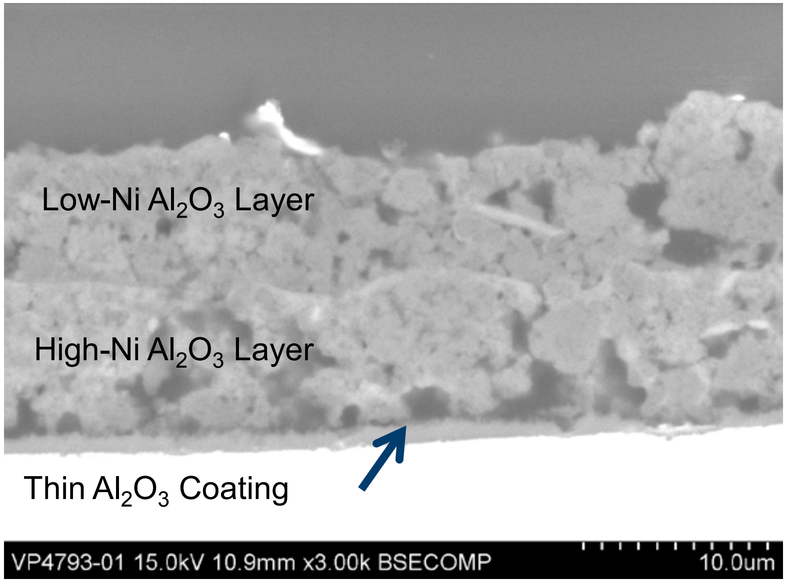
GTI and Cummins implemented catalytic EGR-TCR on a natural gas engine*





- **The reforming catalyst utilized a proprietary washcoat on metal foil.**
- **TCR was achieved initially but shut down as the catalyst quickly deactivated.**
- **Samples of the fresh and used catalyst have been supplied to ORNL for analysis.**
- **Post-mortem analyses are underway at HTML and NTRC.**

* **Pier Final Project Report, January 2011, CEC-500-2009-011.**

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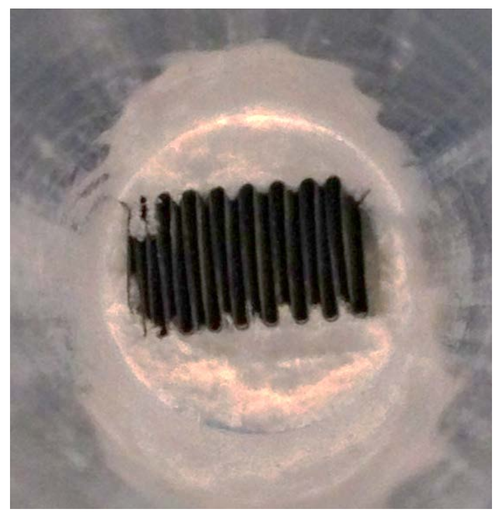
We are evaluating the GTI catalyst function and deactivation in a laboratory bench-flow reactor

Samples are exposed to simulated EGR and fuel in the reactor and reforming reaction rates measured

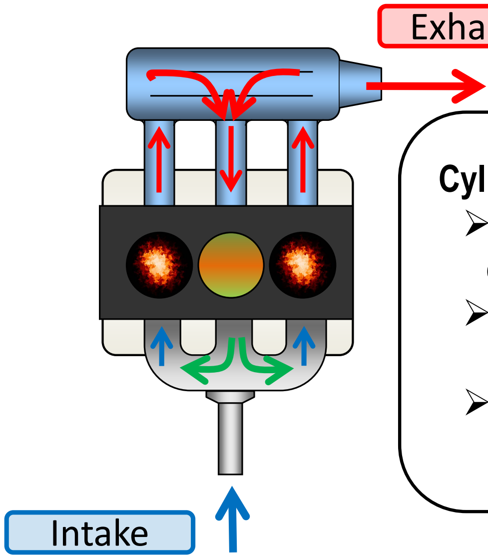
Sample of GTI catalyst inserted in reactor tube



End view of GTI catalyst sample illustrating the 'waffle' cross-section which contacts the gas

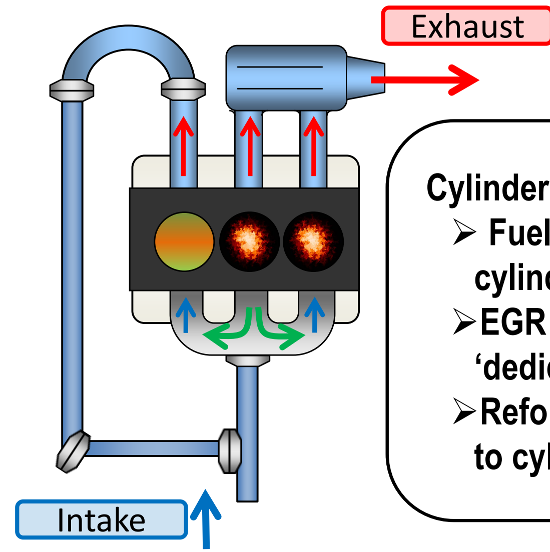
Non-catalytic TCR can also be implemented in-cylinder

Modified VVA Cycle



Cylinder 2 runs in reverse
- Breathes in from exhaust manifold
- Fuel for reforming injected into hot exhaust
- Reformate expelled to intake manifold

Dedicated EGR*



Cylinder 1 runs rich
- Fuel is reformed in cylinder 1
- EGR comes from 'dedicated' cylinder 1
- Reformate is distributed to cylinders via EGR

*Terry Alger and Barrett Mangold, 2009-01-0694

- **Exhaust heat drives endothermic reforming reactions (can be mix of POx and steam)**
- **Volume change from cooling can be exploited to reduce pumping losses**
- **Reformate stabilizes combustion, reduces knock, allows higher compression ratio**
- **With VVA can switch to standard combustion mode as needed**

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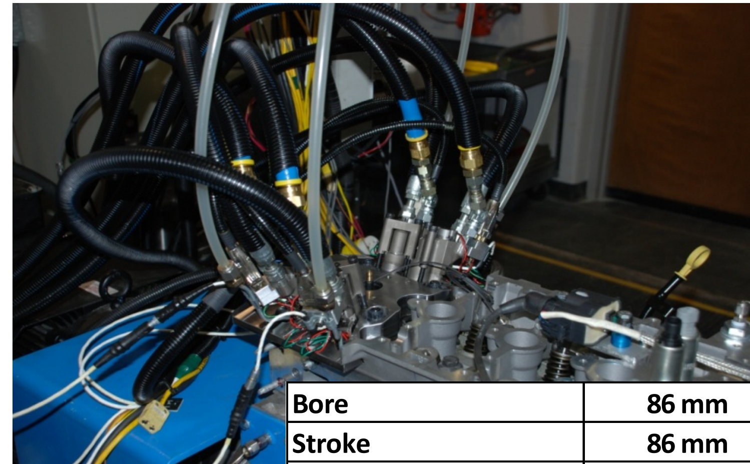
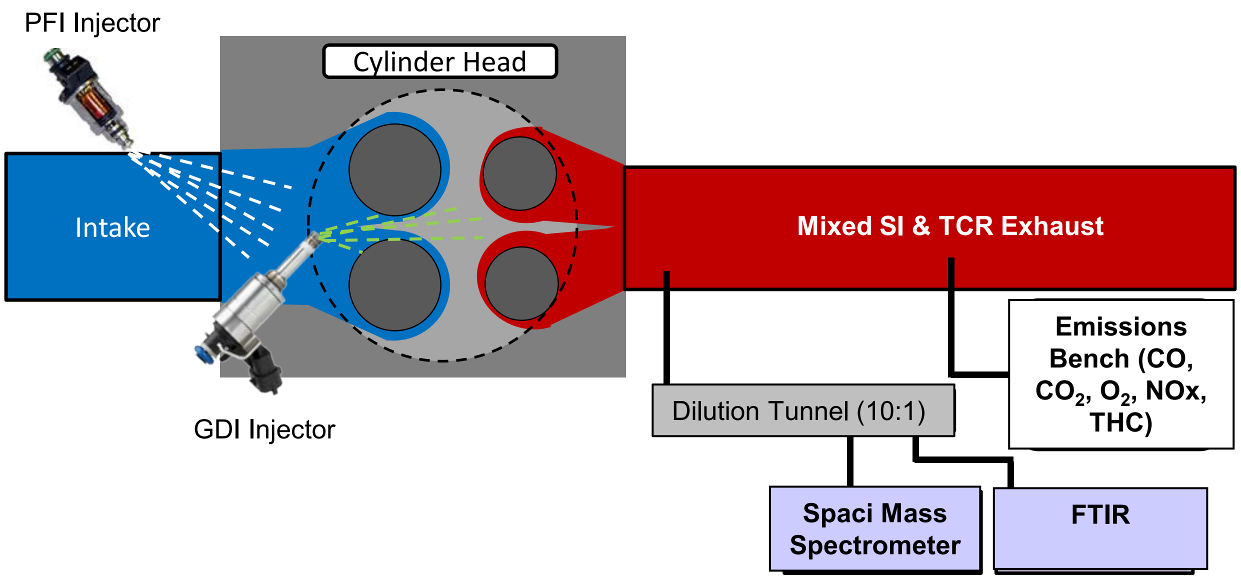
We study TCR in a 6-stroke, single-cylinder research engine with hydraulic valve actuation (HVA)

- **Modified 2.0L GM Ecotec engine with direct injection**
- **Cylinders 1-3 are disabled, cylinder 4 modified for Sturman HVA system**
- **Engine management performed with Drivven engine controller**
- **Custom pistons to increase compression ratio**



Bore	86 mm
Stroke	86 mm
Connecting Rod	145.5 mm
Fueling	Direct Injection
Compression Ratio	11.85
Valves per Cylinder	4



Emission characterization

- Standard emissions bench (CO, CO_2, O_2, NO_X, THC)
- Filter smoke number
- FTIR (CH_4, CH_2O, CH_3OH, CH_3CHO, C_2H_5OH, C_2H_2, C_2H_6, C_3H_8, C_3H_6)
- Mass spectrometer (H_2)

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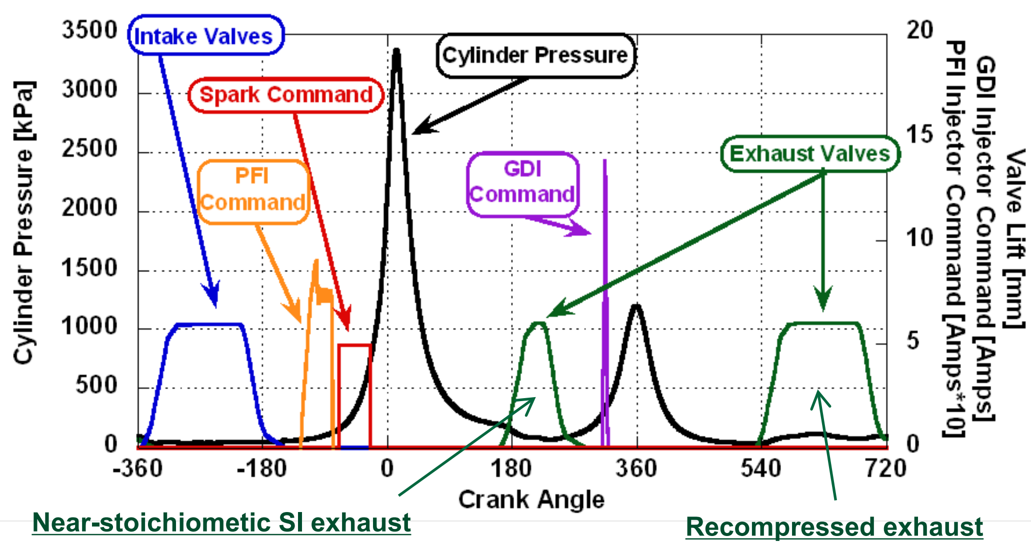
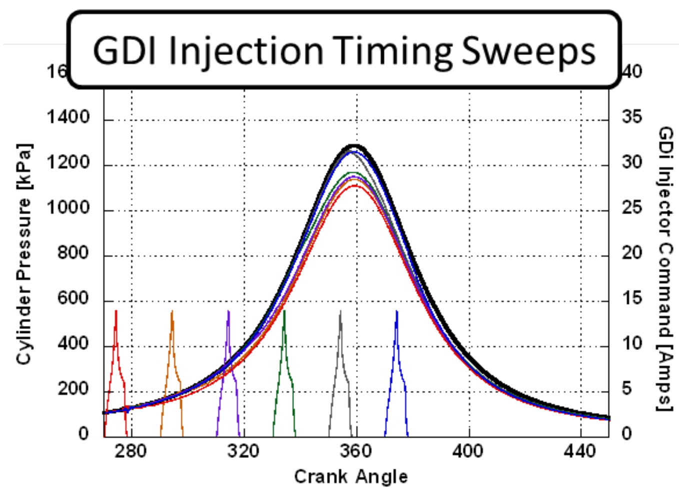
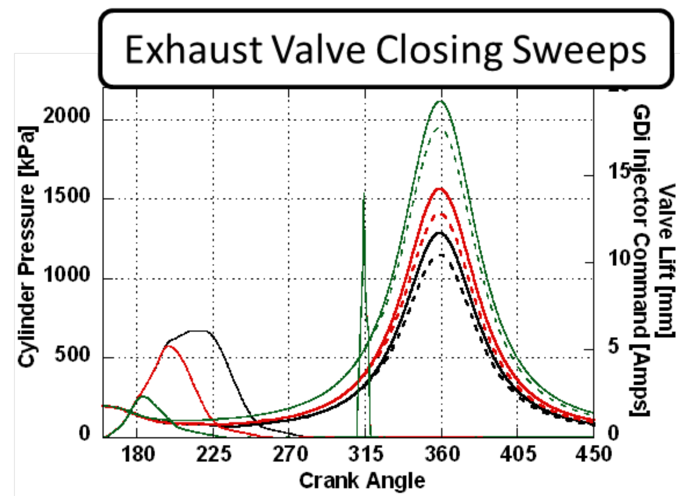
We use a modified 6-stroke cycle to study the chemistry of in-cylinder reforming with hot exhaust

- Hot exhaust residual from SI combustion trapped in-cylinder
- Selected fuel injected into hot exhaust, mixture recompressed
- Measured exhaust T and species*
- 3 fuels investigated so far
  - Isooctane, Ethanol, Methanol
  - Constant inj. duration (≈ constant inj. mass)
  - Gasoline supplied for SI combustion via PFI fueling system







*Currently constrained to measure only mixed SI+TCR exhaust

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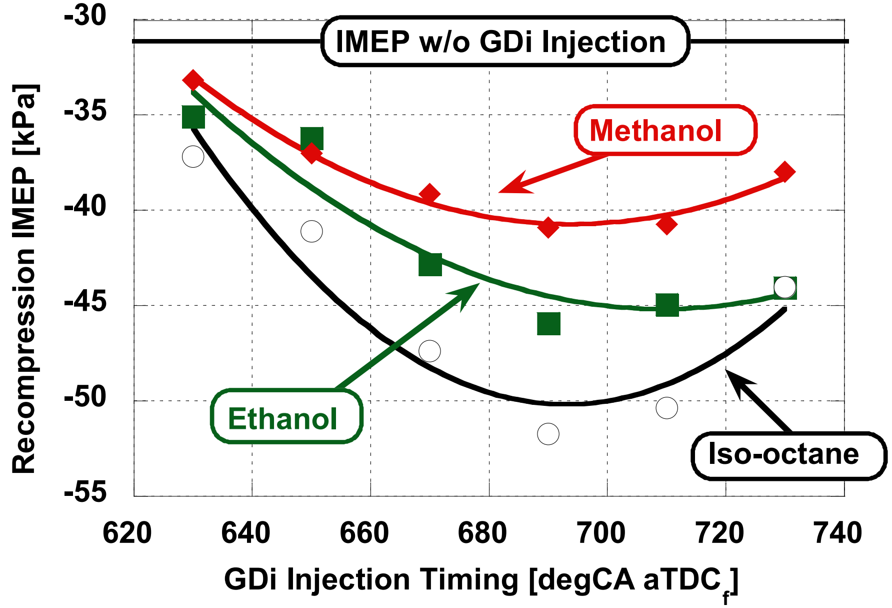
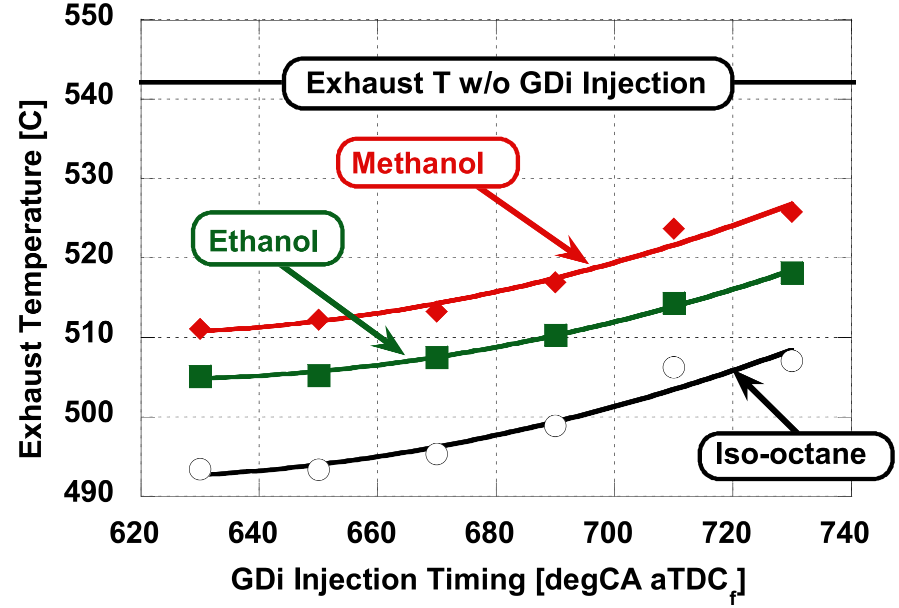
Pressure and temperature changes reveal fuel-specific endothermic reactions at engine timescales





- Significant cooling in all cases
  - Early injection results in greatest cooling
  - Pressure effects confounded by gamma, molar expansion, latent heat, reaction differences
- Exhaust temperature lowest for isooctane despite lowest latent heat of vaporization
  - Lower temperature at earlier injection timing is direct evidence of endothermic reactions
  - Temperature change attenuated because of mixed exhaust
- Reaction times appear to be similar to those reported by Vourliotakis, et al, Int. J. of H_2 Energy, 34 (2009) for non-catalytic ethanol reforming.

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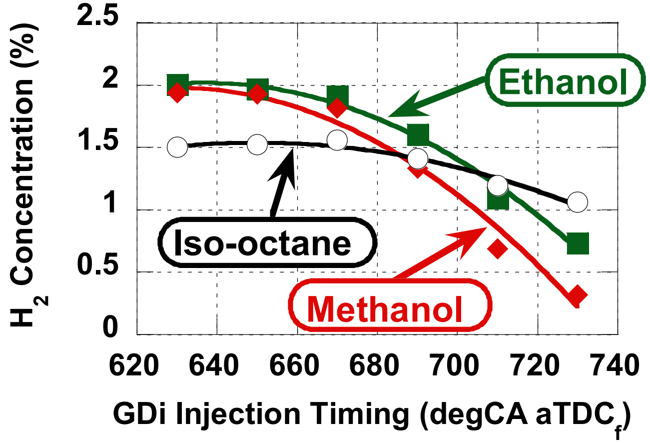
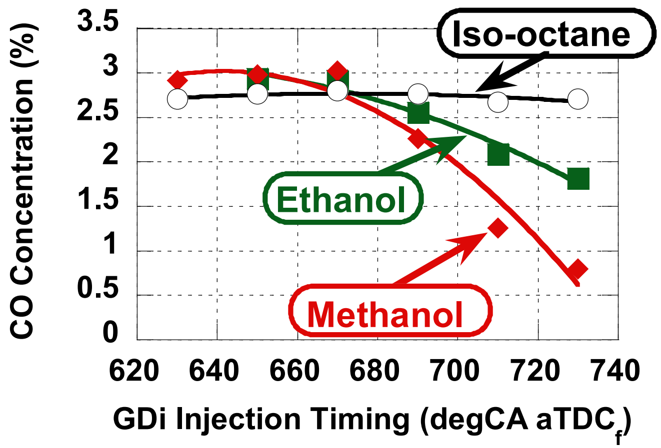
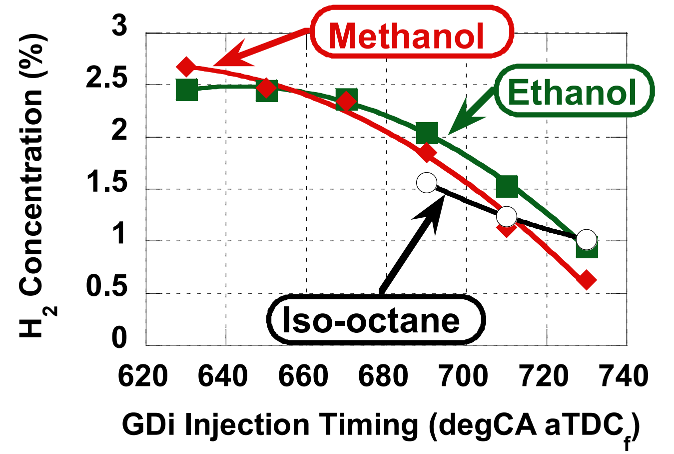
H_2 and CO are generated in significant quantities

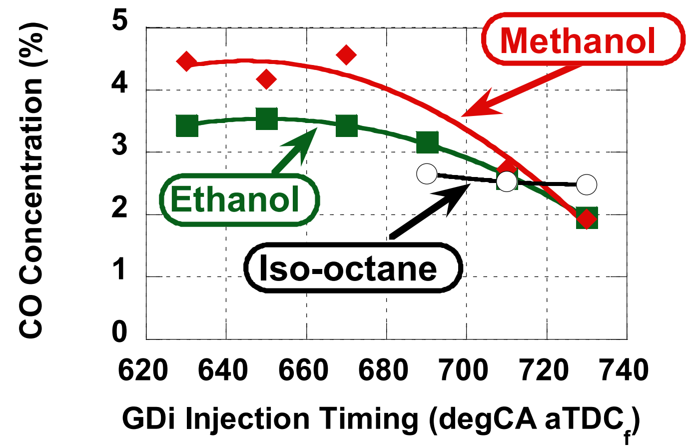
Exhaust Valve Closing: 250 CA





Exhaust Valve Closing: 225 CA





- Concentrations shown are in mixed exhaust
- Operating conditions limited by soot formation for ethanol and iso-octane
- CO comes from both SI combustion and reformation
  - SI combustion goes fuel-rich while injecting GDI fuel because of exhaust residuals

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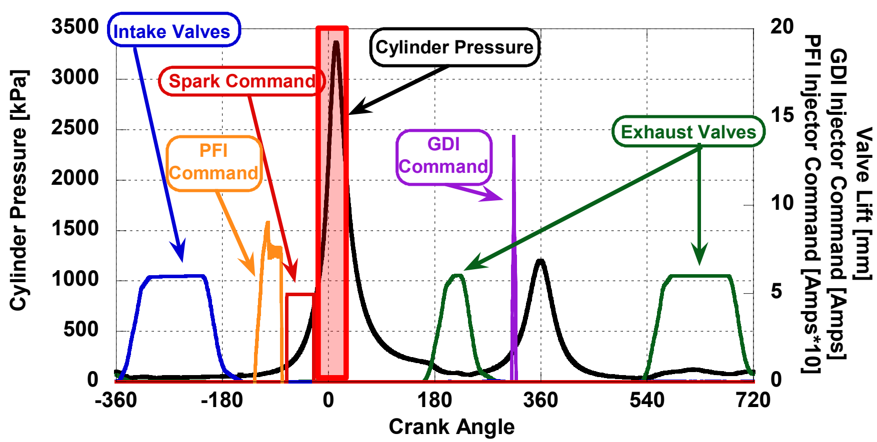
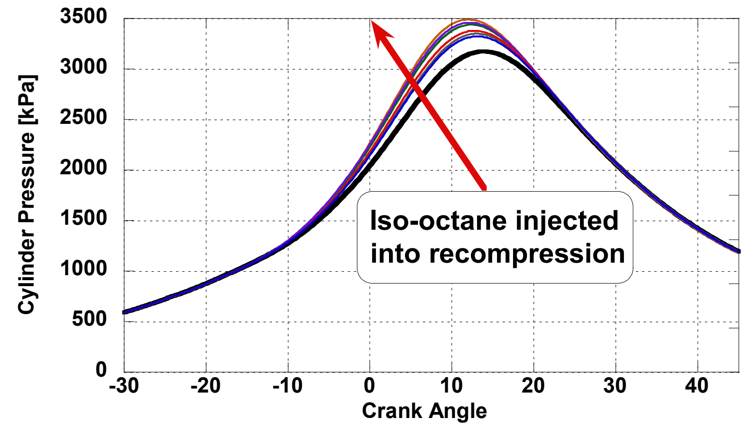
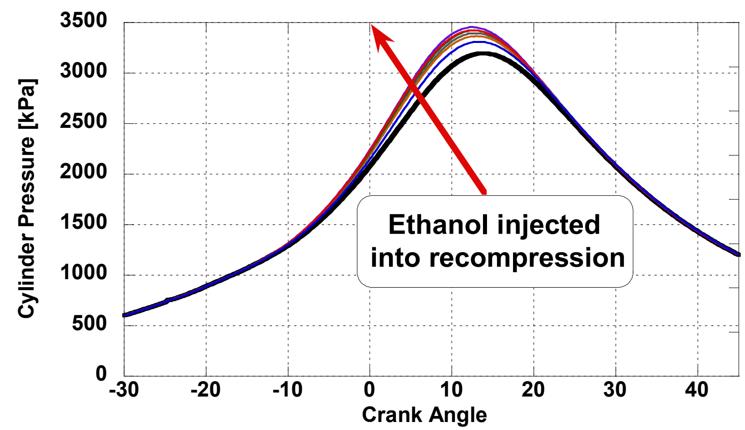
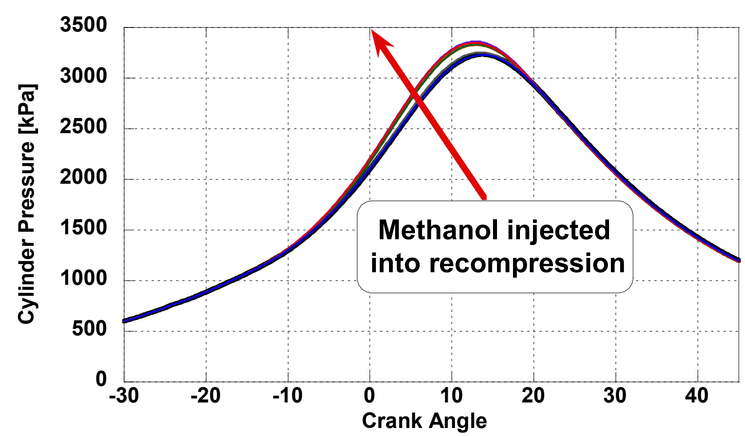
Injecting fuel into recompressed exhaust also affects SI combustion

- Exhaust residuals contain H_2, CO and other hydrocarbon species
- In current setup, residuals cause SI combustion to be fuel-rich
- Largest effect for isooctane, smallest effect for methanol
  - Constant mass injection for all fuels
  - Highest LHV for isooctane
- Results to date convoluted by exhaust mixing









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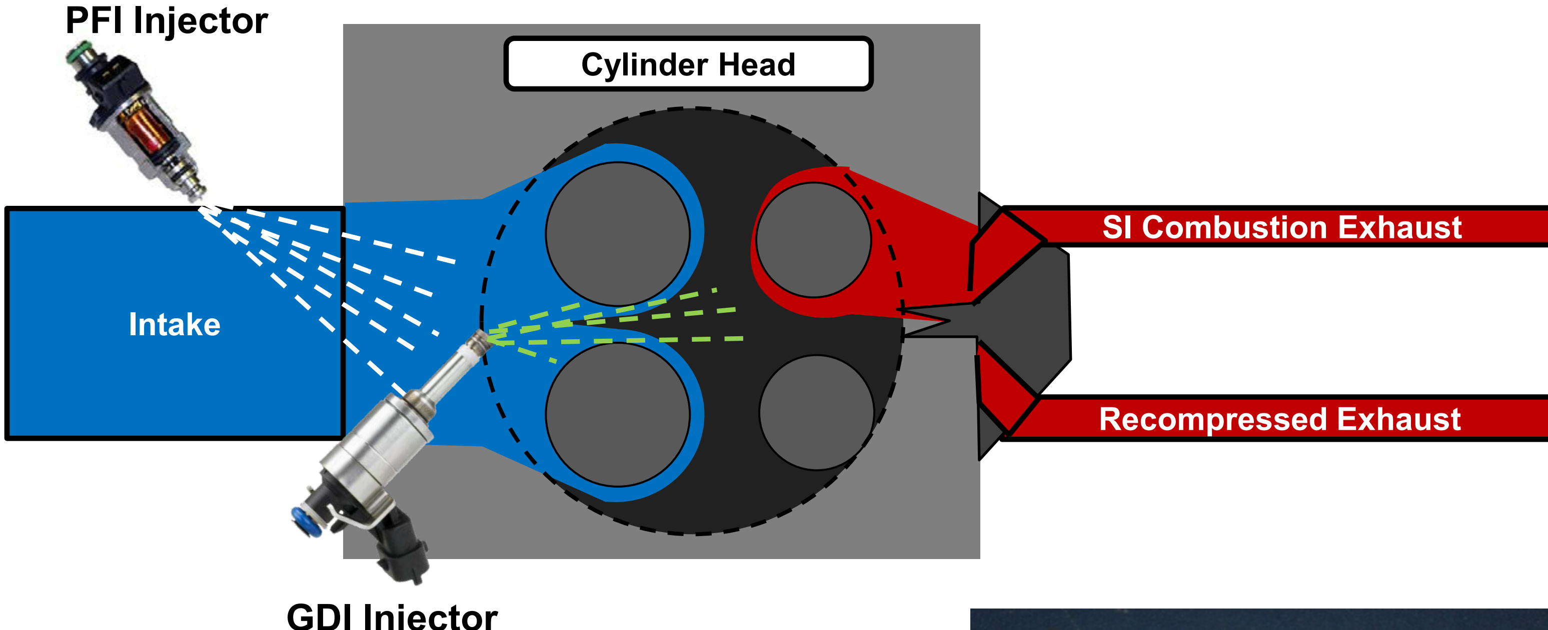
We are modifying the HVA engine to separate SI and reformate exhaust



- Allows for better control of SI combustion stoichiometry
- Permits speciation of recompression products, exergy quantification
  - Are we getting significant TCR and what is the product mix?
- Experimental technique will also be used to investigate NVO chemistry (see project FT08)

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Planned Activities

- **Near term**
  - Modification of HVA engine to segregate exhaust streams
  - Inclusion of other fuels/water in HVA experiments (possibly DME)
  - Thermodynamic and kinetic modeling of observed in-cylinder reactions (chemical equilibrium, Chemkin, Forte)
  - Continued analysis of thermodynamics of in-cylinder and EGR-based TCR
  - Lab replication of GTI-reformer catalyst deactivation and identification of mechanism
- **Longer term**
  - Thermodynamic analysis of other advanced architectures

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Summary

- In-cylinder fuel injection/recompression with hot exhaust in HVA engine appears to promote fuel-specific, non-catalytic, endothermic formation of H_2 and CO at relevant engine timescales (general trends appear consistent with equilibrium limits and ethanol reforming kinetics in literature).
- Once exhaust modifications to the experimental HVA engine are made, it should be possible to better assess extent and nature of the reactions.
  - Modified experiment will also be used for NVO chemistry measurements (see project FT08)
- The potential efficiency benefits of in-cylinder TCR (what is net work generated?) will depend on the reaction details.
- Practical utilization of EGR-based TCR will depend on identifying a reforming catalyst that does not deactivate (or is easily re-activated) under EGR conditions.
- Several other advanced approaches for implementing TCR and exhaust heat recuperation/in-cylinder utilization still need to be thermodynamically analyzed .

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