Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes

Project ID: ace015

C. Stuart Daw (PI), Josh A. Pihl, V. Kalyana Chakravarthy, James P. Szybist, Jim Conklin, Bruce Bunting, Robert Wagner

Oak Ridge National Laboratory

2011 U.S. DOE Hydrogen and Vehicle Technologies Program Annual Merit Review and Peer Evaluation

May 9-13, 2011

Gurpreet Singh and Ken Howden
Vehicle Technologies Program
U.S. Department of Energy

Overview

- **Timeline**
  - **Start**
    - **FY05**
  - **Finish**
    - **Ongoing**
- **Budget**
  - **FY10 Funding**
    - **$250K**
  - **FY11 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**
  - **Owen Bailey (Umicore)**
  - **Galen Fisher (University of Michigan)**
  - **Reaction Design**
  - **Gas Technology Institute**
  - **Sturman Industries**
  - **Universities**
    - **Texas A&M University**
    - **University of Wisconsin**
    - **Illinois Institute of Technology**
    - **University of Alabama**
    - **University of Michigan, Dearborn**

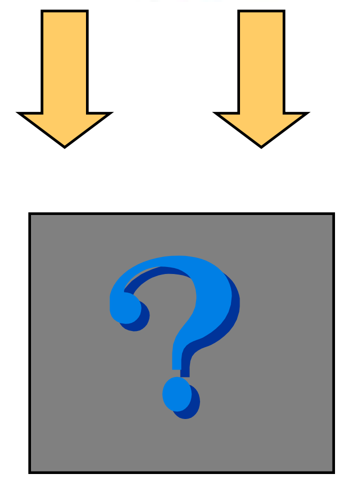
Objective: Reduce ICE petroleum consumption through higher fuel efficiency

- **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**

Today's engines

Max Fuel Efficiency 40-42%

Losses 58-60%



Max Fuel Efficiency 50-60%

Losses 40-50%

Tomorrow's engines?

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

"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. …"

National Research Council 2010 report

ACE MYPP primary R&D directions include:

- **Improve the efficiency of light-duty engines for passenger vehicles (cars and light trucks) and heavy-duty engines for commercial vehicles (heavy trucks) 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.**

ACE MYPP Goals state: "Through simulation and experimentation, this activity will also conduct R&D on advanced thermodynamic strategies that may enable engines to approach 60 percent thermal efficiency."

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

- **29 invited experts from industry, universities, labs, and govt.**
- **Discussion themes:**
  - **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**

***Report published as ORNL/TM-2010/265, October 2010.**

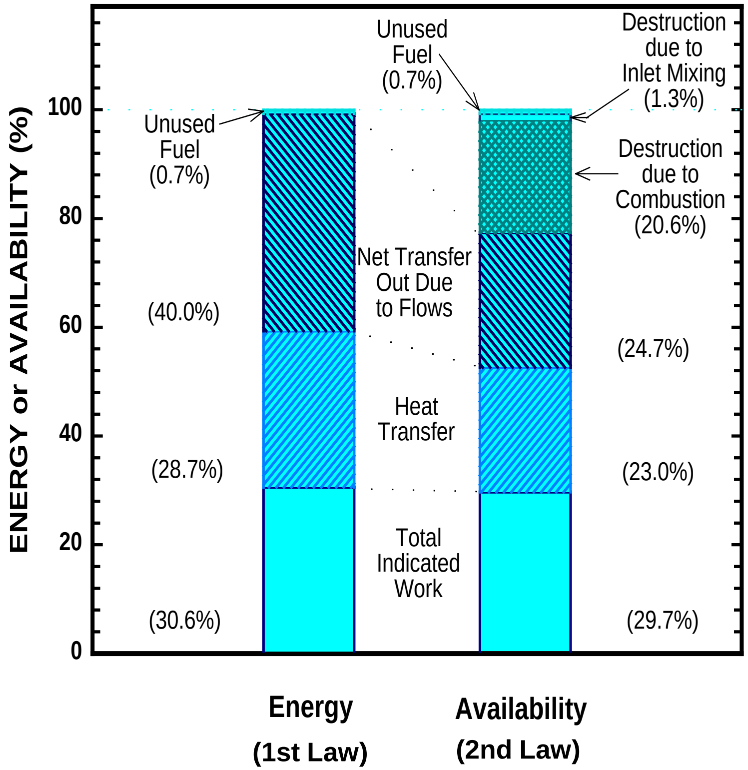
Milestones

- **FY10 Milestone (completed)**
  - **Journal paper on chemical looping combustion (alternative thermodynamic cycle) as a means for increasing combustion engine efficiency - *Energy and Fuels 2011, 25 (2), pp 656–669.***
- **FY11 Milestone (on track)**
  - **Determine feasibility and potential efficiency benefits of implementing thermochemical recuperation in a reciprocating engine. (September 30, 2011).**

Approach: Expert consultations + analysis & modeling + experiments

- **Consultations with Experts**
  - **Individual universities, industries, labs**
  - **Technical meetings, colloquia**
- **Analysis & Modeling**
  - **Thermodynamics of leading concepts (both 1st and 2nd Law effects)**
  - **Physics and chemistry (heat & mass transport and kinetics)**
- **Experiments**
  - **Measurements answer basic questions (not define final design)**
  - **Proof-of-principle**
  - **Special lab heat exchangers, reactors**
  - **Special modified engines**

Octane-fueled spark-ignition engine (J. Caton, 1999)

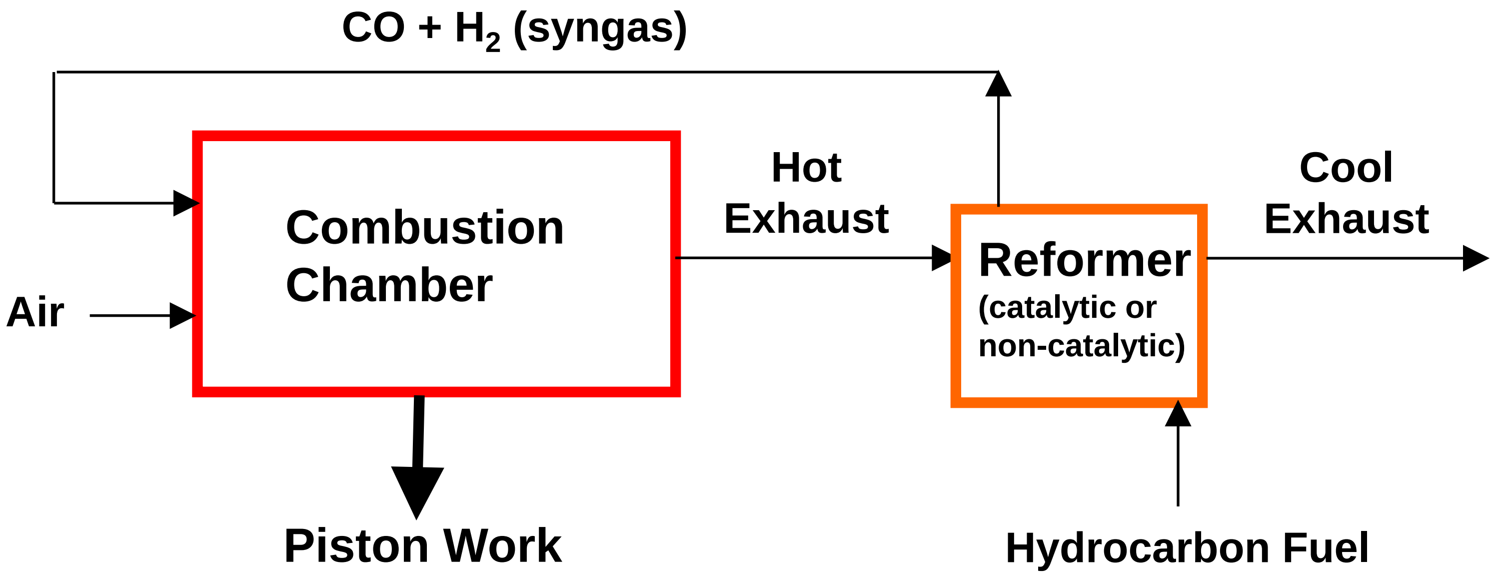


1st Law (energy) vs. 2nd Law (exergy)

Accomplishments/Progress

- **Expert Consultations**
  - **Continued in-depth discussions with Dave Foster, Jerry Caton**
  - **Completed summary report for March 2010 USCAR Colloquium**
- **Analysis and Modeling**
  - **Published thermochemical recuperation study- 2010 Energy and Fuels**
  - **Published chemical looping study- 2011 Energy and Fuels**
  - **Completed thermodynamic fuel effects study**
  - **Initiated CFD modeling of in-cylinder water/fuel injection for exhaust heat recuperation**
- **Experimental**
  - **Continued RAPTR experiment development**
  - **Continued VVA engine experiments**

Thermochemical recuperation (TCR) uses exhaust heat to stage combustion



- **Exhaust heat drives endothermic reforming: HC fuel→ CO/H_2 (syngas).**
- **HC fuel supplemented with syngas (in place of some or all original HC).**
- **Fuel heating value increases, recuperating energy.**
- **If reforming pressure boost captured, significant usable exergy is also recuperated.**
- **H_2 extends lean limit, improves γ, lowers cylinder heat loss, assists cold start, lowers combustion irreversibility, potentially useful for NOx reduction.**

Our analysis* indicates TCR has theoretical potential for significantly boosting efficiency

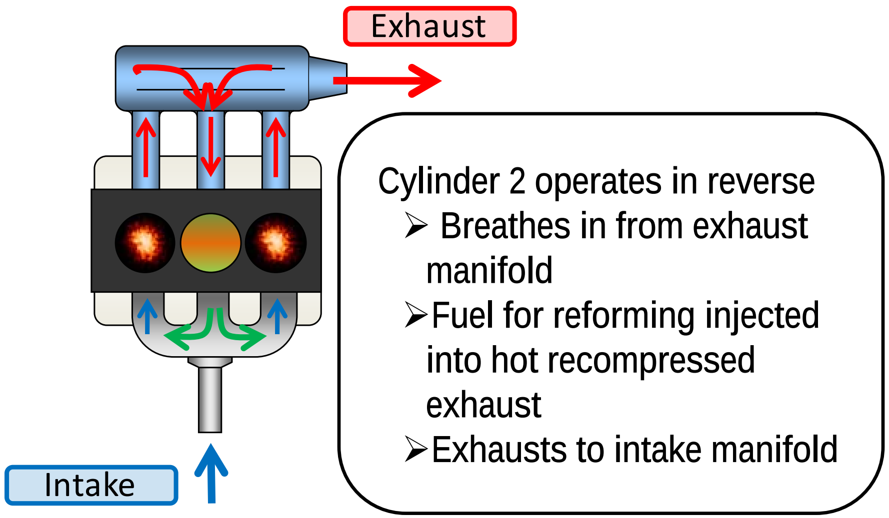
- **For ideal stoichiometric engine fueled with MeOH**
  - **2nd law efficiency increases 3% for constant P reforming**
  - **2nd law efficiency increases >5% for constant V reforming**
- **With lean combustion (e.g., ϕ = 0.4)**
  - **2nd law efficiency for MeOH increases 2% more**
- **2nd law efficiency for constant volume TCR in stoich. engine**
  - **With EtOH increases 9%**
  - **With isooctane increases 11%**
- **Additional efficiency gains possible with added bottoming cycle**

***Energy & Fuels, 2010, 24 (3), pp 1529-1537**

Analysis and Modeling

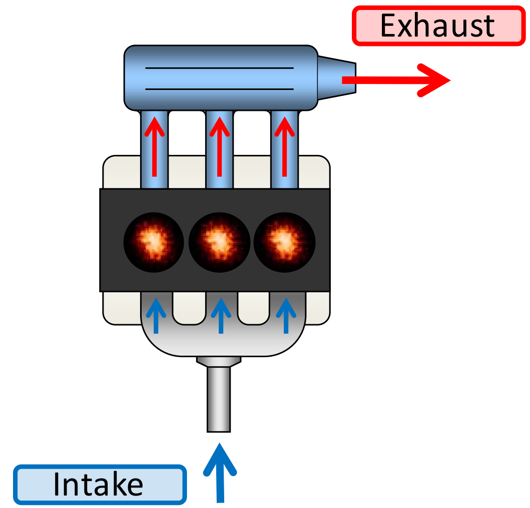
TCR could be implemented on multi-cylinder VVA engines with modified cycles

In-cylinder reforming cycle



- **Captures work from volume expansion to reformate products**
  - **Captured exhaust heat drives endothermic reactions**
- **Reformate burned in combustion cylinders**

Conventional 4-stroke cycle

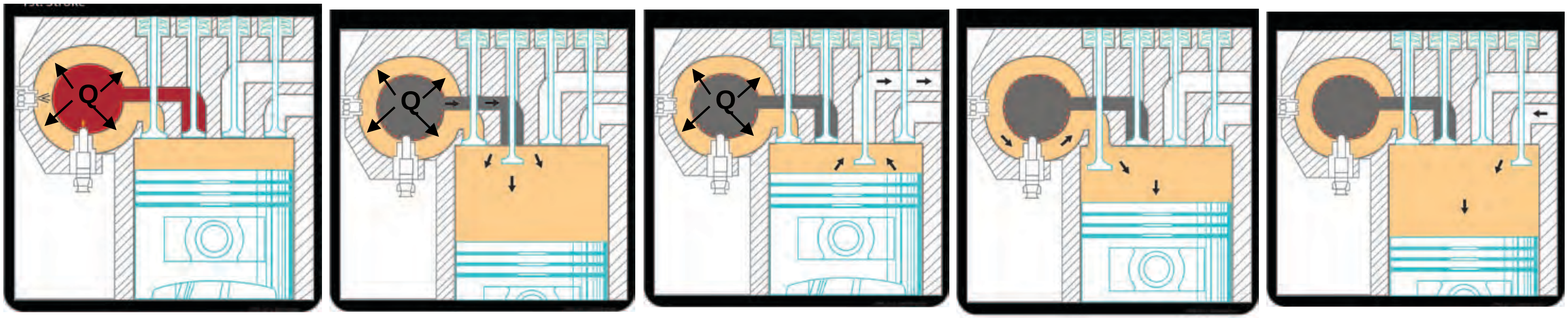


- **Conventional operation can be maintained for high load operation**
  - **Maintains power density when necessary**
- **Requires advanced valve train**

Analysis and Modeling

TCR could also be implemented with modified piston-engine architectures

Modified Bajulasz 2-Chamber Architecture (SAE 860534)



1st stage

- Air & reformate compressed in inner chamber
- Ignition occurs
- Fuel injection & reforming begins in outer chamber

2nd stage

- Combustion gas expands
- Reforming continues in outer chamber

3rd stage

- Combustion gas exhausted
- Reforming continues in outer chamber

Start 4th stage

- Reformate gases expand

End 4th stage

- Fresh intake air mixes with reformate

Close-coupled combustion and reforming chambers allow recuperation of combustion chamber wall heat

Analysis and Modeling

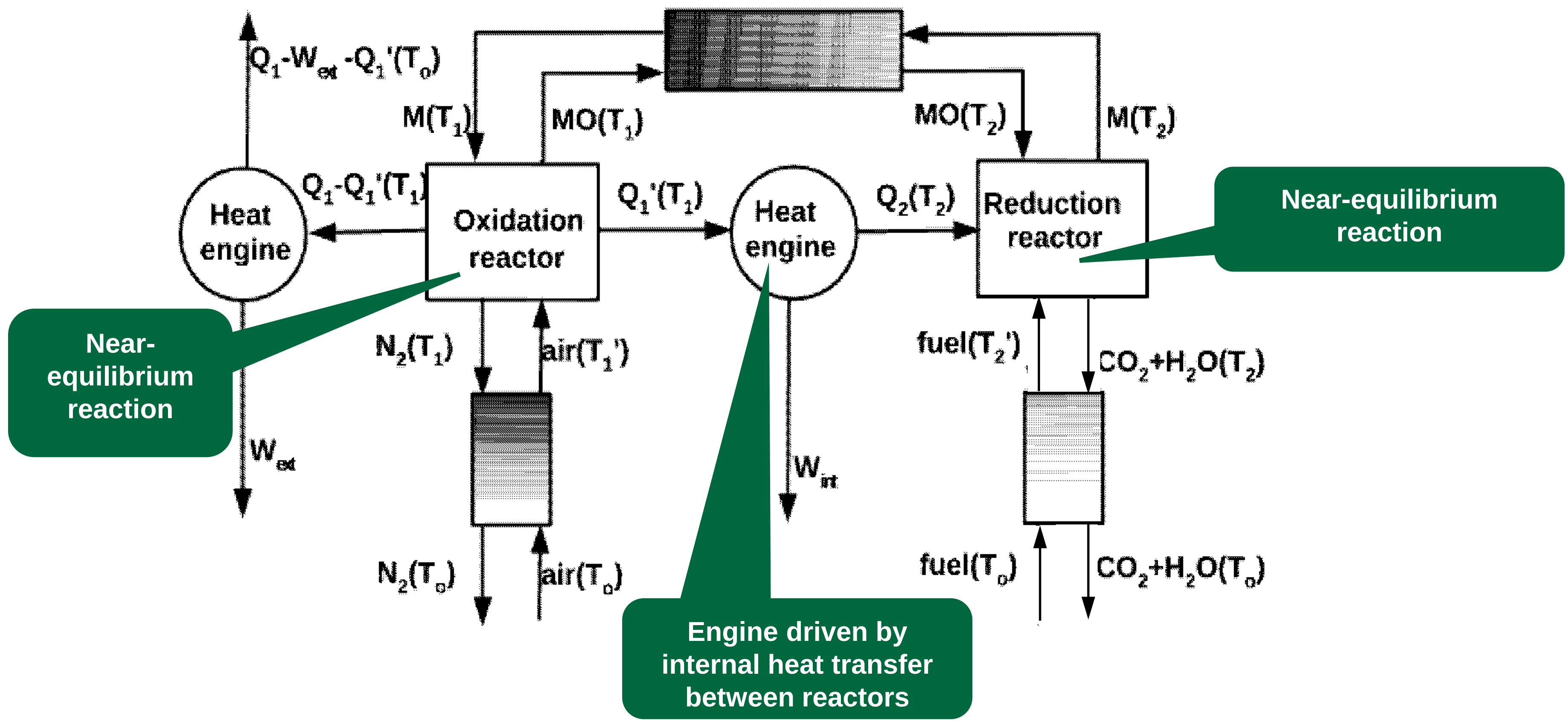
All versions of TCR have some common engineering challenges

- **Time scales for vaporization (fuel and water), and reforming**
- **Highly transient gas-liquid and solid-liquid heat and mass transfer**
- **Liquid injection spray development and droplet formation**
- **Catalytic (heterogeneous) and non-catalytic reforming reaction kinetics**
- **Variable valve actuation**
- **Potential power density reduction**

Thus our experiments are being designed to address key questions about these issues.

Analysis and Modeling

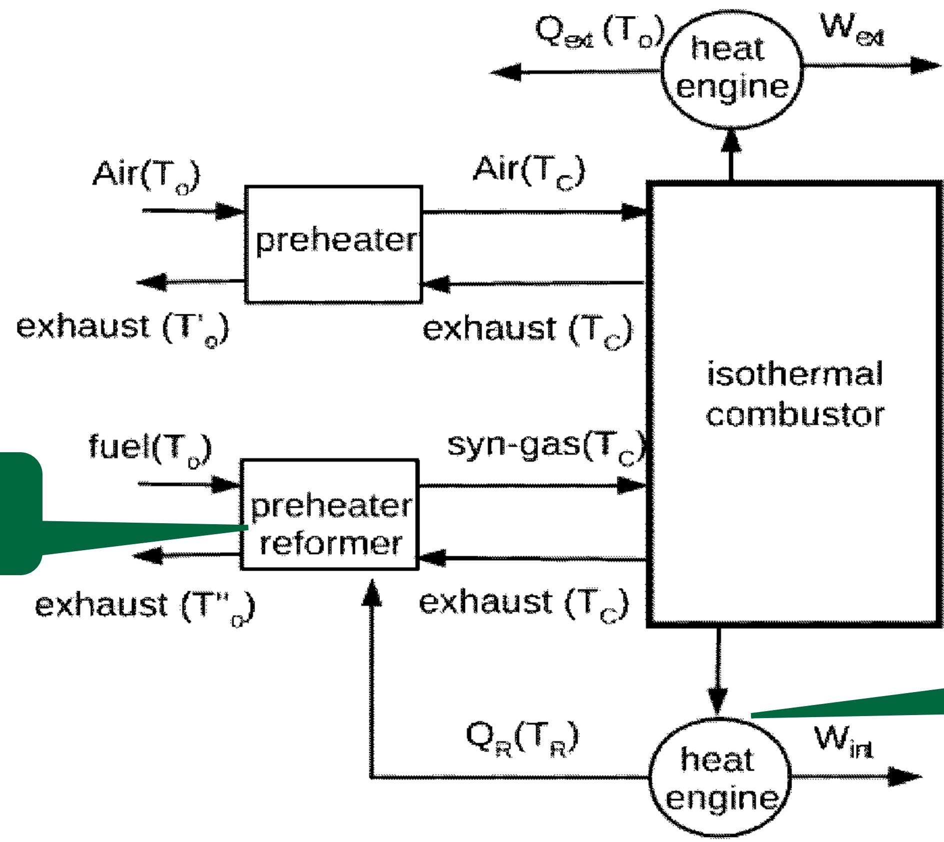
Chemical looping combustion (CLC)*is another approach for staging combustion



- **Irreversibility is reduced by carrying out reactions near equilibrium**
- **Properties of oxygen storage medium and its circulation present major challenges**

***See details in Energy & Fuels 2011, 25, pp 656–669**

TCR + isothermal combustion can imitate some aspects of CLC without a solid O carrier



Near-equilibrium reaction

Engine driven by internal heat transfer

However, this version of TCR would require a very different kind of engine architecture

Analysis and Modeling

We also completed a basic thermodynamic analysis of fuel effects this FY

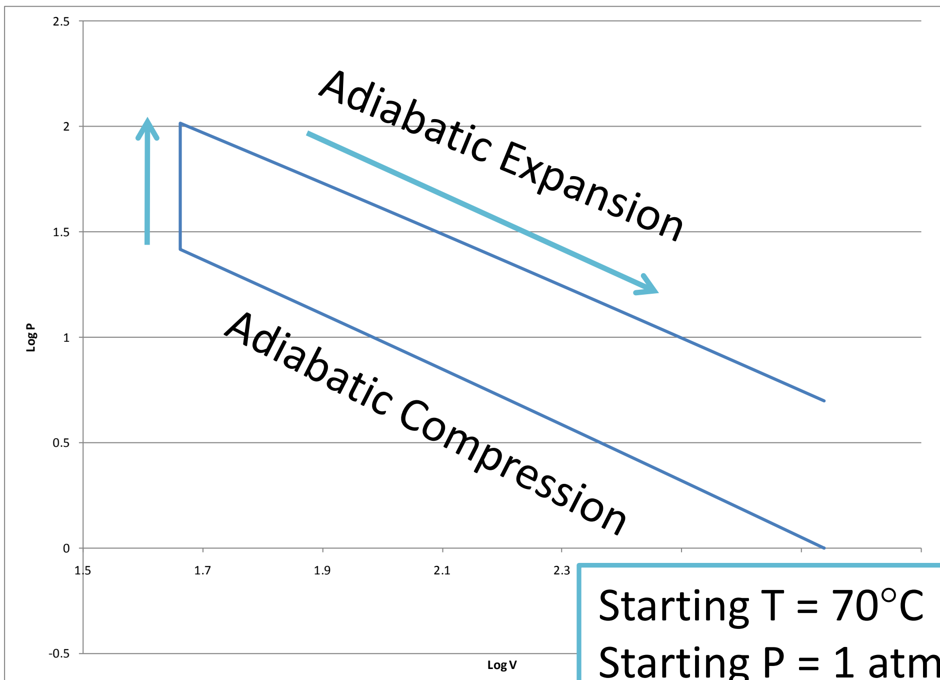
Objectives:

- **Evaluate effects of molar expansion and gamma in 1st and 2nd law efficiencies**
- **Identify any potential advantages for oxygenates vs. pure hydrocarbons**

23 fuels:

- 10 alkanes
- 4 alkenes
- 3 aromatics
- 3 alcohols
- 1 methyl ester
- CO and H_2

Alkanes	
methane	(g)
ethane	(g)
n-propane	(g)
n-butane	(l)
n-pentane	(l)
n-hexane	(l)
n-heptane	(l)
n-octane	(l)
n-nonane	(l)
n-decane	(l)
Olefins	
ethene	(l)
propene	(l)
1-butene	(l)
1-pentene	(l)
Aromatics	
benzene	(l)
toluene	(l)
ethylbenzene	(l)
Alcohols	
methanol	(l)
ethanol	(l)
propanol	(l)
Esters	
methyl butanoate	(l)
Other	
carbon monoxide	(g)
hydrogen	(g)



Starting T = 70°C
Starting P = 1 atm

Ideal Otto cycle:

- Adiabatic compression and expansion
- Equilibrium products during expansion
- Stoichiometric A/F
- **Compression ratio: 9.2**
- **Variable gas properties**

Analysis and Modeling

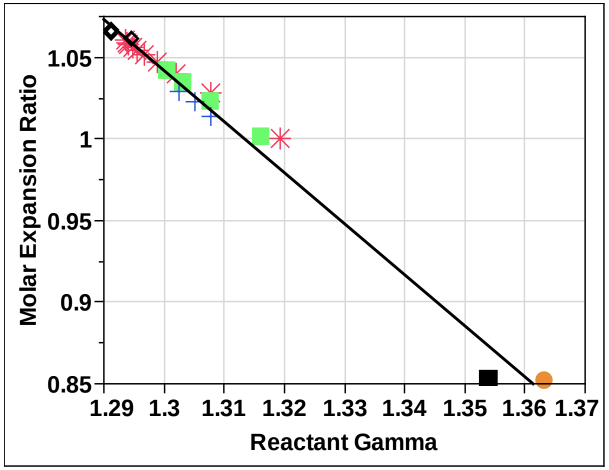
Opposite trends in molar expansion and gamma tend to reduce fuel impact on efficiency

Observations:

- **Large variation in molar expansion pressure rise (23% overall difference, 3% if CO and H_2 excluded)**
- **Efficiency increases with γ of products but variation over fuels is small ($1.231 < \gamma_P < 1.241$)**
- **Efficiency also increases with γ of reactants and variation over fuels is larger ($1.284 < \gamma_R < 1.386$)**
- **Would like a fuel with a high molar expansion and high γs, but the actual trend is opposite**
- **Fuel exergy/enthalpy ratio seems to be useful correlating tool**

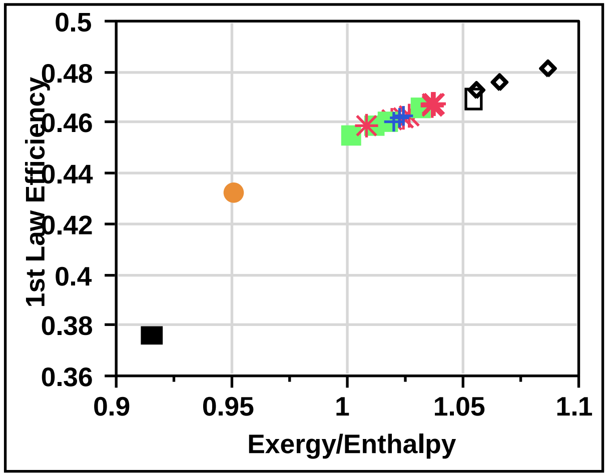
Mole expansion vs. γ

(*) n-paraffins, (■) alkenes, (+) aromatics, (◇) alcohols, (□) methyl-esters, (■) CO, and (●) H_2



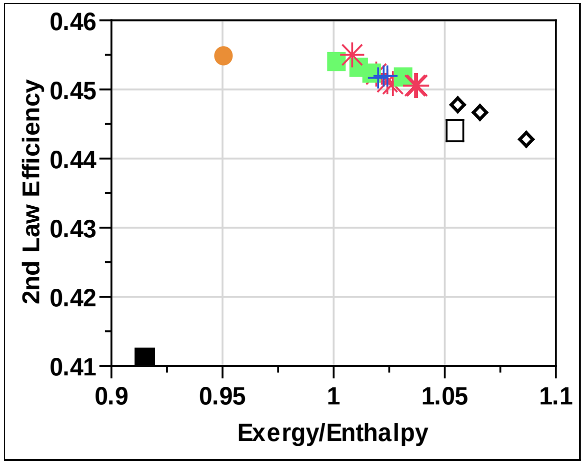
1st law efficiency (based on LHV)

- Max = 48.1% (methanol)
- Min = 37.6% (CO)
- Min excluding CO/H_2 = 45.4% (ethene)



2nd law efficiency (based on exergy)

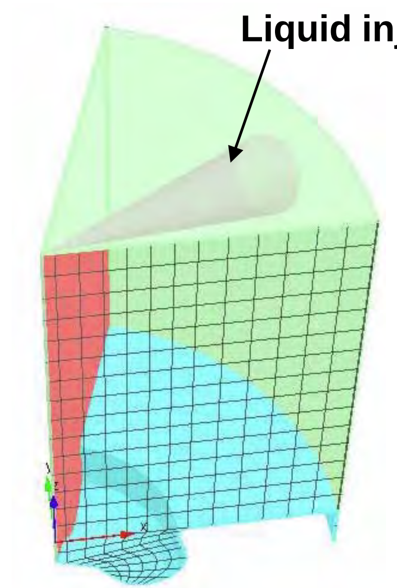
- Max = 45.5% (H_2, methane)
- Min = 41.1% (CO)
- Min excluding CO = 44.3% (methanol)



Analysis and Modeling

We are using CFD simulations to better understand in-cylinder water and fuel injection for TCR and 6-stroke cycle heat recovery

- **Utilizing Reaction Design Forte® CFD model and MFC master mechanisms through CRADA with Reaction Design.**
- **Initially focusing on in-cylinder evaporation of water.**
- **Expand to fuel injection studies later.**
- **Vary cylinder conditions at intake valve closing, wall temperatures, injection profile, and nozzle characteristics.**
- **Determine rates of heat transfer, liquid vaporization in gas and on wall.**
- **Use results to predict generation of positive work and guide experiments.**
- **Begin simulations April-May.**



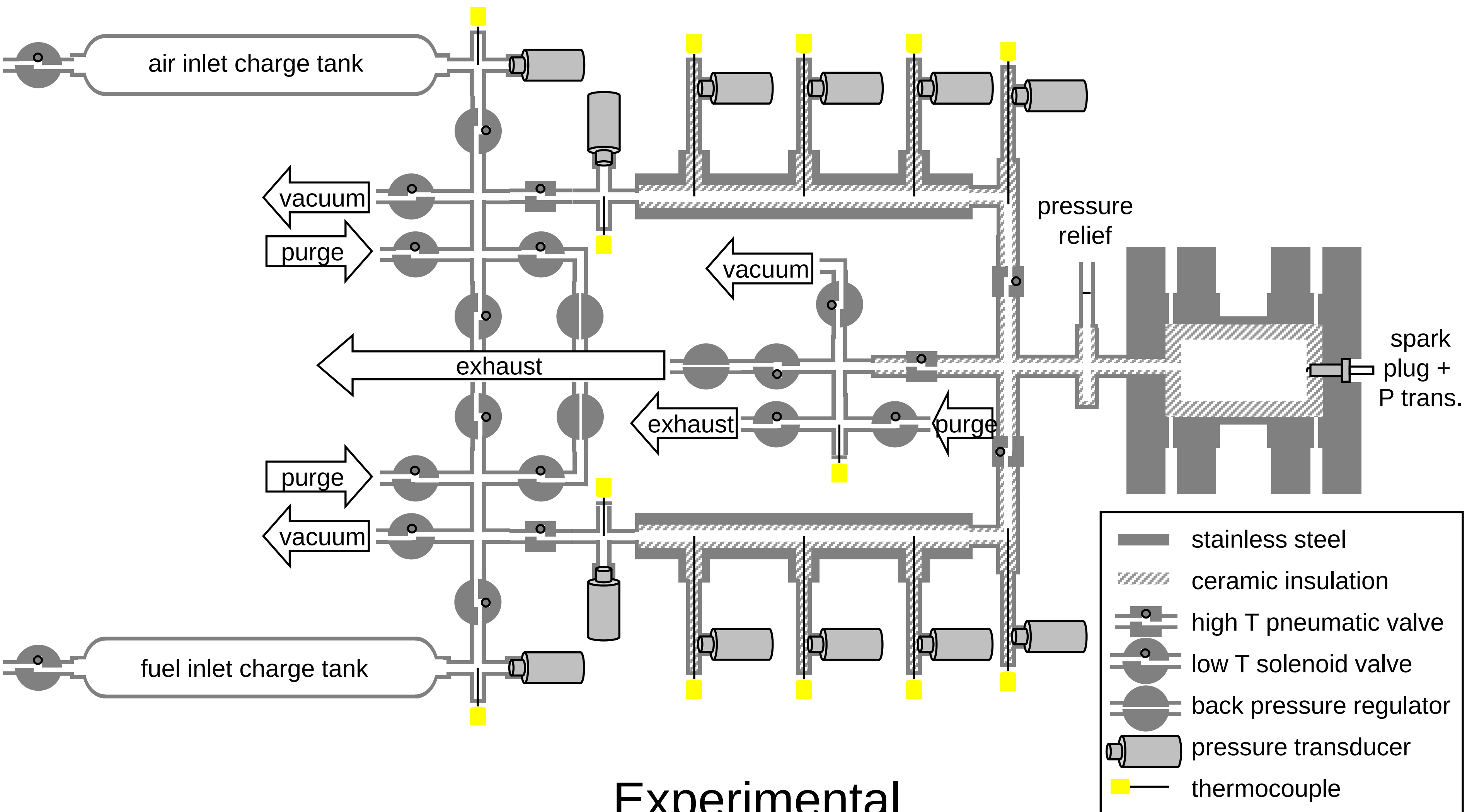
72° sector mesh

- **Start with 5-hole injector, 0.165mm ID**
- **Variable injection profile**
- **Variable cylinder conditions**

Analysis and Modeling

The RAPTR experiment provides basic information about constant volume TCR under ideal conditions

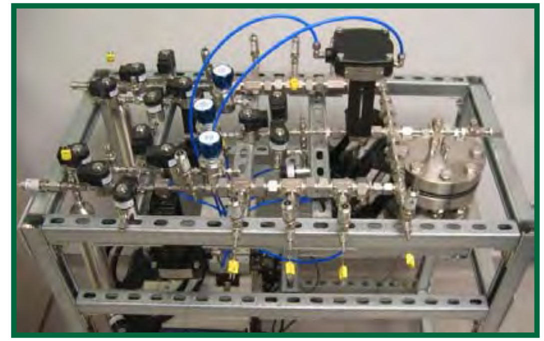
RAPTR (Regenerative Air Preheating and Thermochemical Recuperation)



Experimental

RAPTR is constructed to study key TCR steps

- **Generate hot exhaust for different fuels and A/F ratios**
- **Measure impact of reformate on ignition, heat release rate**
- **High T valves control intake/exhaust with fully adjustable timing**
- **Measure heat transfer and reforming chemistry and kinetics**
- **Screen catalysts, heat transfer materials, injection strategies**



Status

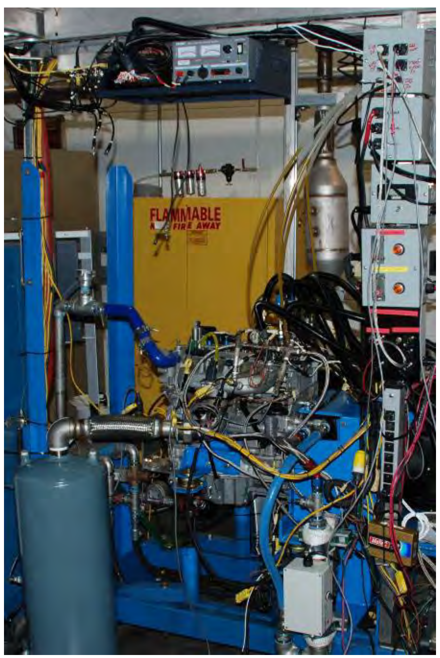
- **System integration complete**
- **Preliminary experiments on gas/solid heat transfer rates in regenerative preheaters under way**

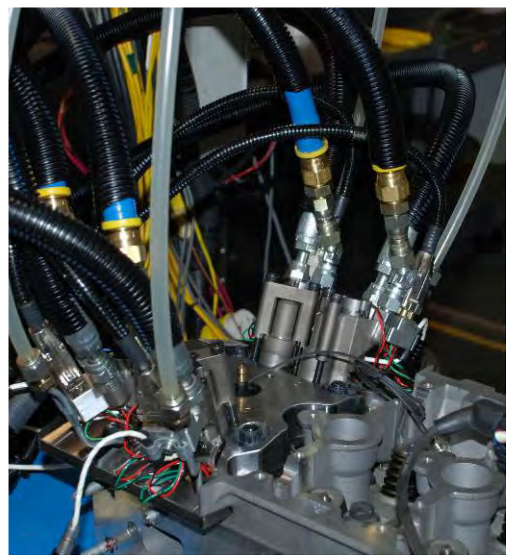
Experimental

We are using a modified single-cylinder VVA engine to study in-cylinder heat transfer and reforming

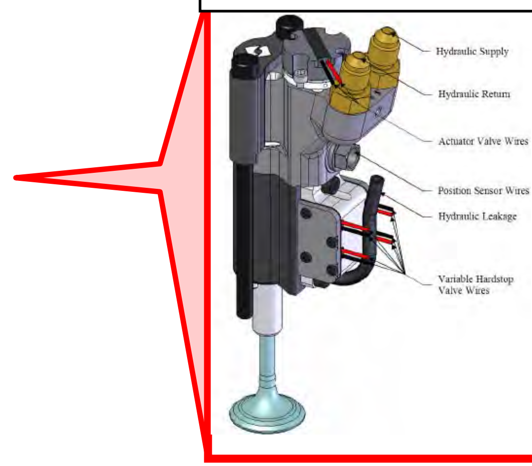
- **Infinitely variable HVA**
- **Water and/or fuel injection into cylinder with hot residual exhaust**
- **Measure cylinder pressure, H_2/CO/selected HCs in exhaust (SpaciMS, FTIR, NDIR)**
- **Validate modeling results for heat & mass transfer, reaction rates**

1 cylinder of Ford 2-L Ecotech Engine





Sturman Hydraulically Actuated Valve

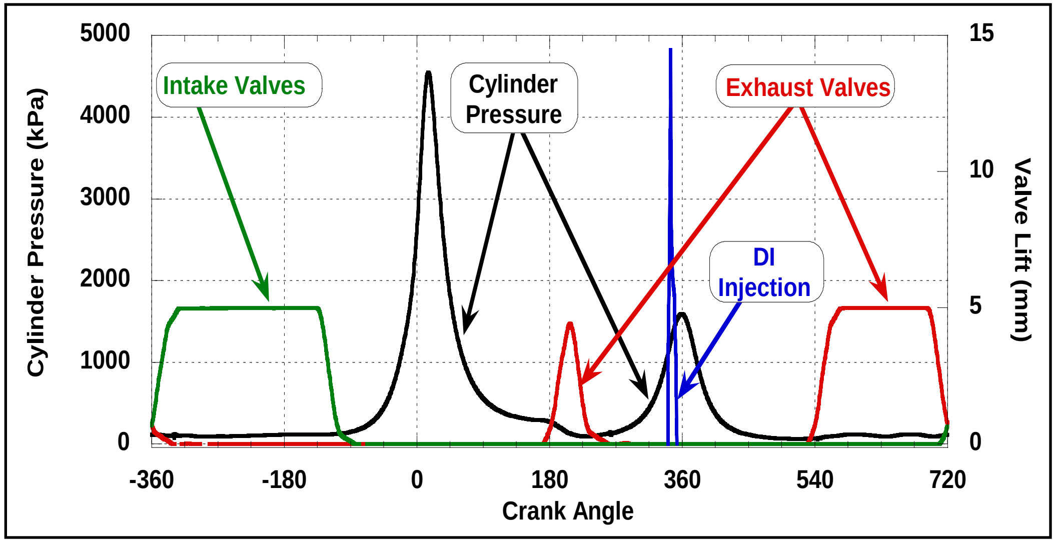


Experimental

VVA engine experiments resume in May

We demonstrated 6-stroke cycle with water injection

- **VVA hardware functioned as intended**
- **But heat transfer and vaporization were slow, revealing need for more detailed modeling, modified design**



Next planned experiments:

- **Investigate in-cylinder reforming with methanol, ethanol, and n-heptane for a range of cylinder pressures and temperatures**
- **Measure pressure profile and reforming products**
  - **Extent of reforming will be quantified by H_2 in exhaust as measured by the SPACI MS**
  - **Additional indications with FTIR measurements of methanol, ethanol and CO**
  - **Vaporization rates, reforming reaction timescales, and potential expansion work indicated by pressure data in conjunction with modeling**

Experimental

Planned Activities

- **Near term**
  - **Analysis of TCR in 6-stroke cycle**
  - **Analysis of modified engine architectures with TCR close-coupled to combustion chamber**
  - **RAPTR experiments with reforming**
  - **Acquisition of additional reformer catalysts**
  - **Water and fuel injection measurements with VVA engine**
- **Longer term**
  - **Extended RAPTR and VVA engine experiments**
  - **More detailed cycle simulations with non-ideal engine components**
  - **Thermodynamic analysis of other advanced architectures**

Summary

- **Thermochemical exhaust heat recuperation (TCR) has the theoretical potential for increasing peak IC engine efficiency by more than 10%.**
- **TCR can theoretically be used to capture some of the efficiency benefits of chemical looping without an oxygen carrier.**
- **TCR can be implemented via both modified cycles in multi-cylinder engines and by modified engine architectures where reforming and combustion are close coupled.**
- **Opposite trends in gamma and molar expansion tend to reduce the thermodynamic effects of fuel type on efficiency.**
- **Analyses are being synchronized with experiments to determine if the expected thermodynamic benefits of concepts can actually be achieved with realistic rates for transport and kinetics.**

Stuart Daw
865-946-1341
dawcs@ornl.gov