Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes

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U.S. DEPARTMENT OF ENERGY

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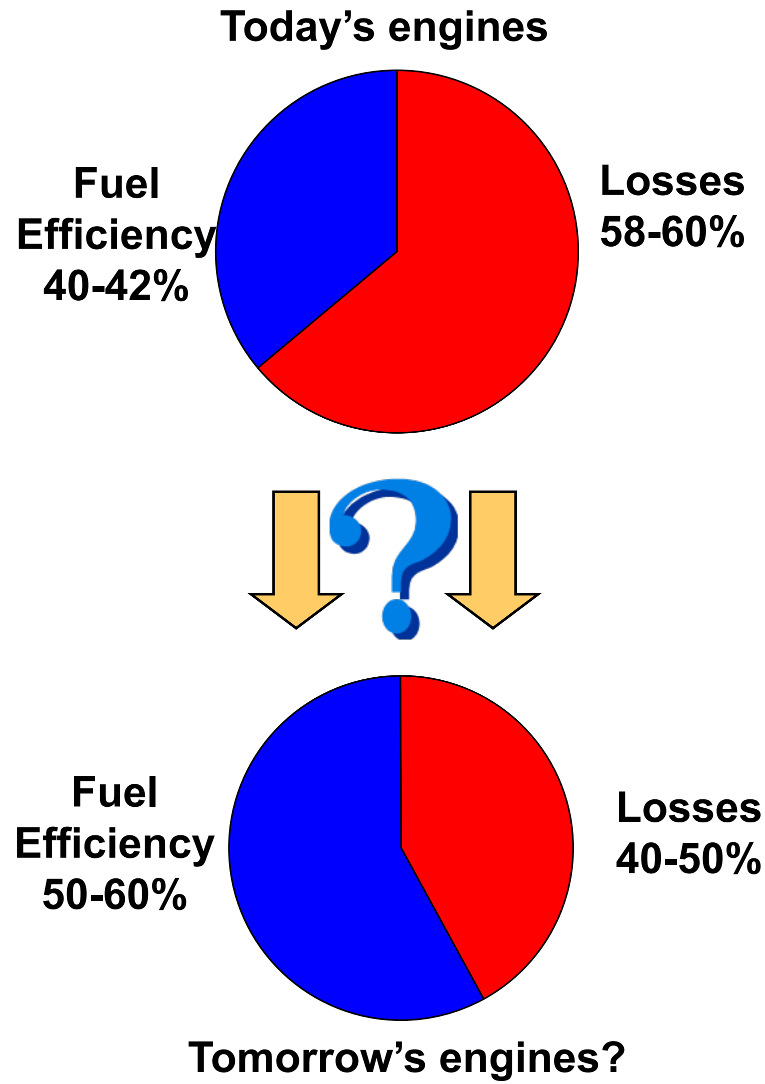
Overview

- **Timeline**
  - Start
    - FY05
  - Finish
    - Ongoing
- **Budget**
  - FY08 Funding
    - $250K
  - FY09 Funding
    - $250K
  - FY10 Requests
    - $250K

- **Barriers**
  - Energy efficiency limits of existing IC engines (including HECC and HCCI modes) are well below theoretical potential
  - Overcoming these limits involves complex optimization of materials, controls, and thermodynamics
- **Partners**
  - Major catalyst supplier
  - Not for profit R&D institution
  - Universities
    - Texas A&M University
    - University of Wisconsin
    - Illinois Institute of Technology
    - University of Alabama
    - University of Michigan, Dearborn

Objective: Reduce ICE petroleum consumption thru higher fuel efficiency

- **Summarize and update understanding of efficiency losses**
- **Identify promising strategies to reduce losses**
- **Implement proof-of-principle demonstrations of selected concepts**
- **Novel aspect within OVT portfolio:**
  – **long term, high risk approaches for reducing thermodynamic losses in combustion**



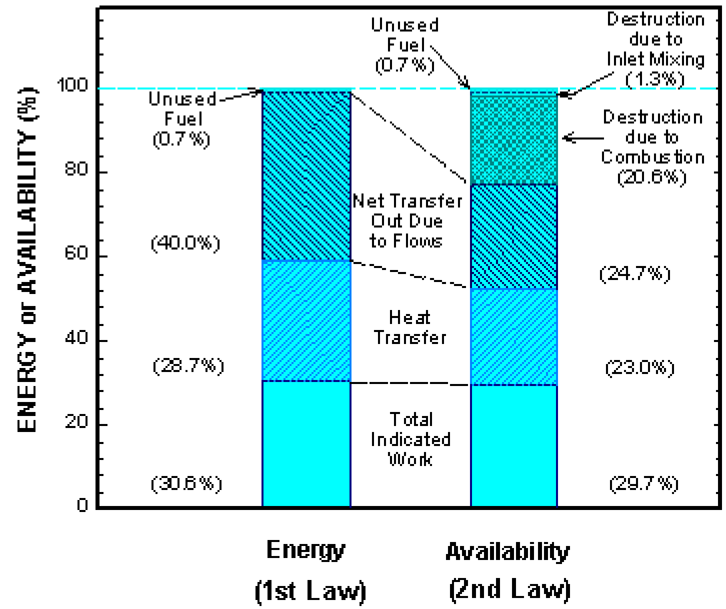
Milestones

- **FY08 Milestone (completed):**
  - Conduct detailed measurements of the function and performance of the reforming catalyst used in the CPER (RAPTR) combustor
- **FY09 Milestone (on schedule for completion):**
  - Journal paper on preheating and thermochemical recuperation (CPER/TCR) as a means for increasing combustion engine efficiency

General Approach: Combine thermodynamic analysis and experiments to identify potential paths for efficiency breakthrough

- **Phase I: Team of experts clarified theoretical ICE efficiency limits based on literature and selected case studies**
  - Identified most promising paths forward
  - Recommended specific topics for more study
  - Most under-investigated issue is combustion irreversibility (20-25% loss off the top!)
- **Phase II (Current): Develop and demonstrate more thermodynamically efficient combustion**
  - Target: Reduce the 20-25% combustion irreversibility loss by half
  - Specific Approach: Proof-of-principle benchtop experimental demo with high flexibility
- **Phase III: Define and demonstrate ICE implementation**

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

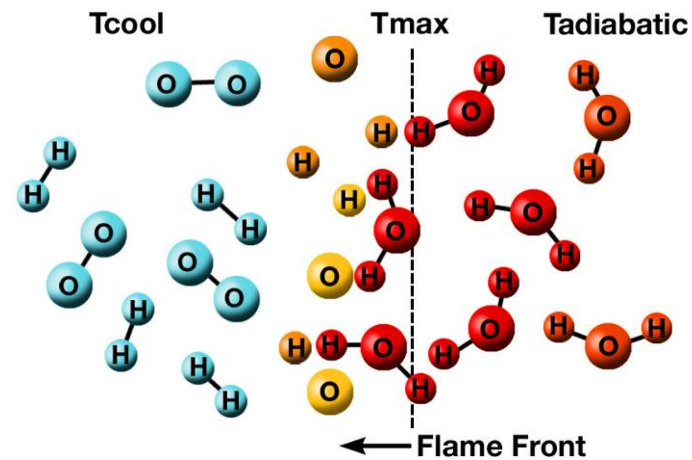


Impact of combustion irreversibility revealed by 2nd Law (exergy) analysis

Phase II experiments address the main irreversibilities in unrestrained combustion

- 'Internal' heat transfer
  - Products to reactants heat transfer over large ΔTs
  - $dS_Q = \delta Q(1/T_C - 1/T_H)$
- Non-equilibrium chemical reactions
  - Large gradients in chemical potential
  - $dS_i = R_i (\mu_p - \mu_r)/T$
- Note: Above entropy sources are not significantly reduced in HCCI

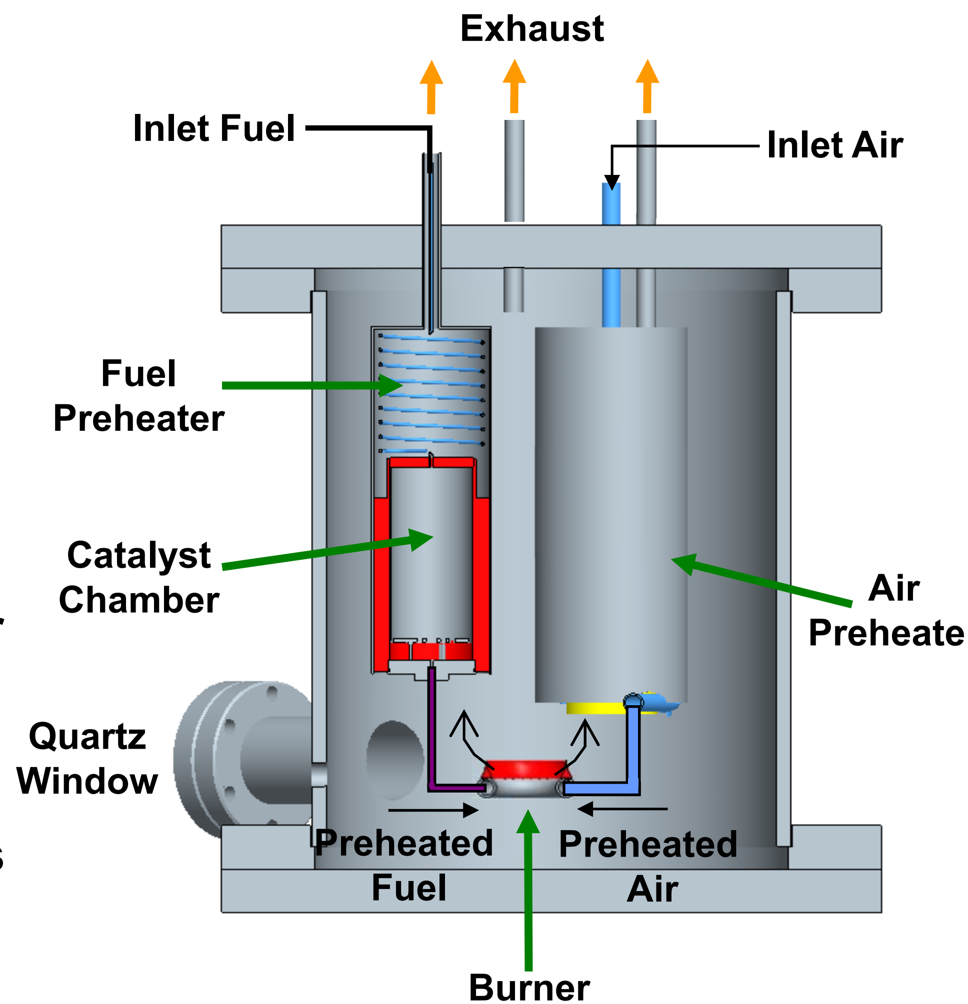
C.S. Daw, V.K. Chakravarthy, J. Conklin, and R.L. Graves, Intl. J. of H_2 Energy 31 (2006) 728-736



Entropy generation is the source of combustion irreversibility

In FY08 an experiment was constructed to study restrained heat transfer and reaction

- **Steady atmospheric pressure combustion with thermal and chemical heat recuperation**
- **Thermal recuperation**
  - **Counterflow heat exchange between reactants and products with reduced ΔT**
- **Chemical recuperation**
  - **Catalytic reforming of fuel near chemical equilibrium (eliminates some non-equilibrium reactions)**
  - **CO/H_2 (syngas) burns with less entropy generation**
- **Objective to demonstrate proof-of-principle for each effect separately and together**



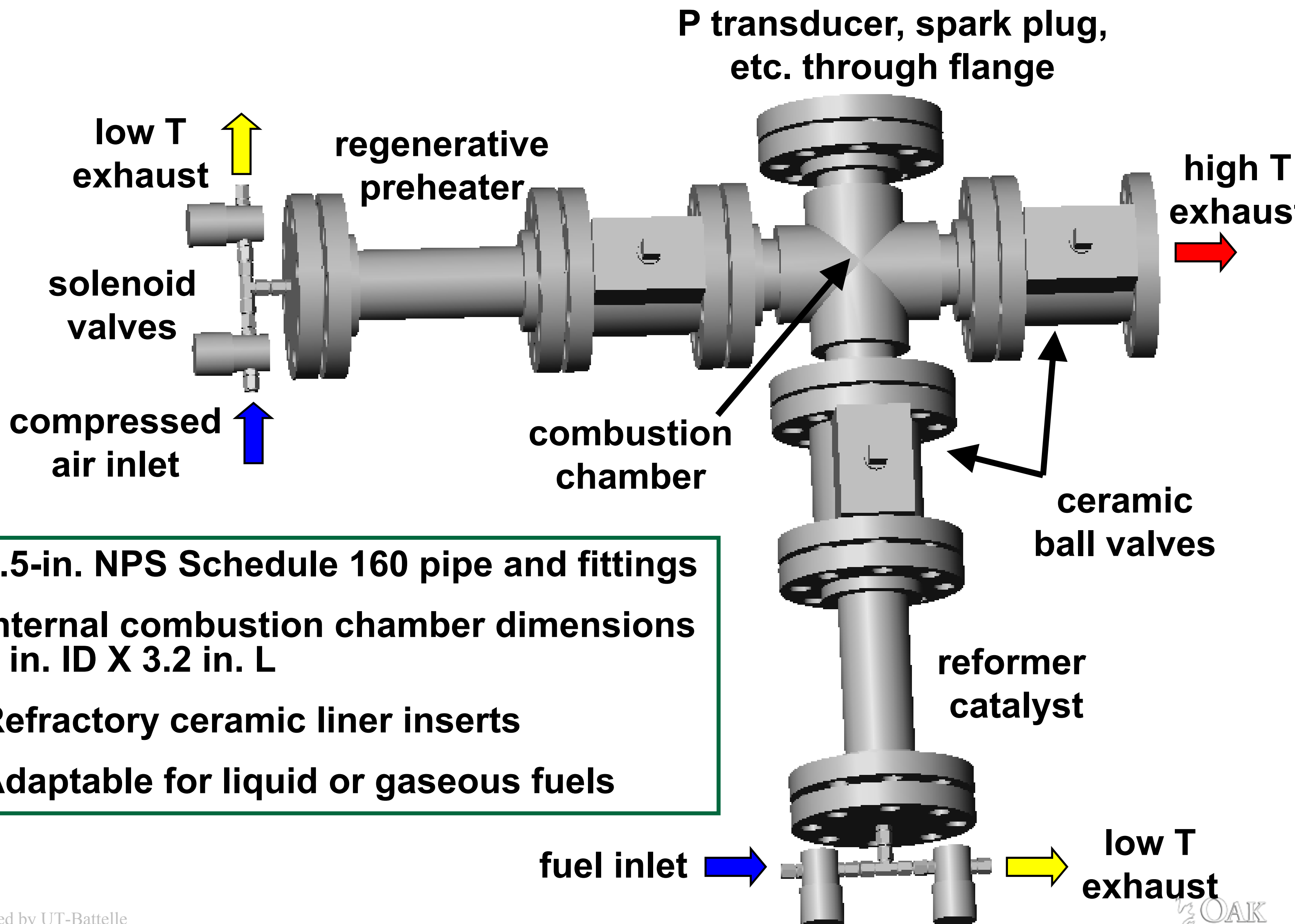
The Phase II experimental plan has been revised based on 2008 Review comments

- "… wondered how the low pressure combustion will add to knowledge (we know about combustion availability but it is a fundamental limitation that low pressure combustion studies will not allow us to break)."
- "… the thermodynamic analysis failed to show the benefits of constant-volume combustion over constant-pressure combustion. Since other programs within DOE are dedicated the study of constant pressure combustion … the value of the proposed experiments to OVT is not clear…."
- "… the second law analysis of IC engines is a very important topic and it could lead to improvements in engine cycles…"; "concerned that the current experiment use constant pressure, steady combustion"
- "… the program should focus on using availability analysis to improve the efficiency of IC engines through constant volume combustion."
- "The technology transfer path for IC engines is not clear. This program will provide much more value to the community if it addresses reducing irreversibility in the context of cyclic, unsteady, constant volume combustion processes."

The revised Phase II experiment targets cyclic, constant volume combustion

- Objective: Demonstrate combustion irreversibility reduction (by up to half of present 20-25% loss) in bench-top, cyclic, constant volume combustor
- Modified approach:
  - Regenerative Air Preheating (RAP)
    - Counterflow heat exchange between exhaust and inlet air via solid media (e.g., as in Stirling engines)
    - Constant volume operation with high pressure generation
      - increased expansion work w/o bottoming cycle
      - more relevant to ICEs
  - TCR (Thermo-chemical Recuperation)
    - Recovered exhaust heat drives endothermic reforming reactions
    - Reforming catalyst included with thermal regenerator solids
- Acronym: RAPTR

The RAPTR experiment is under construction



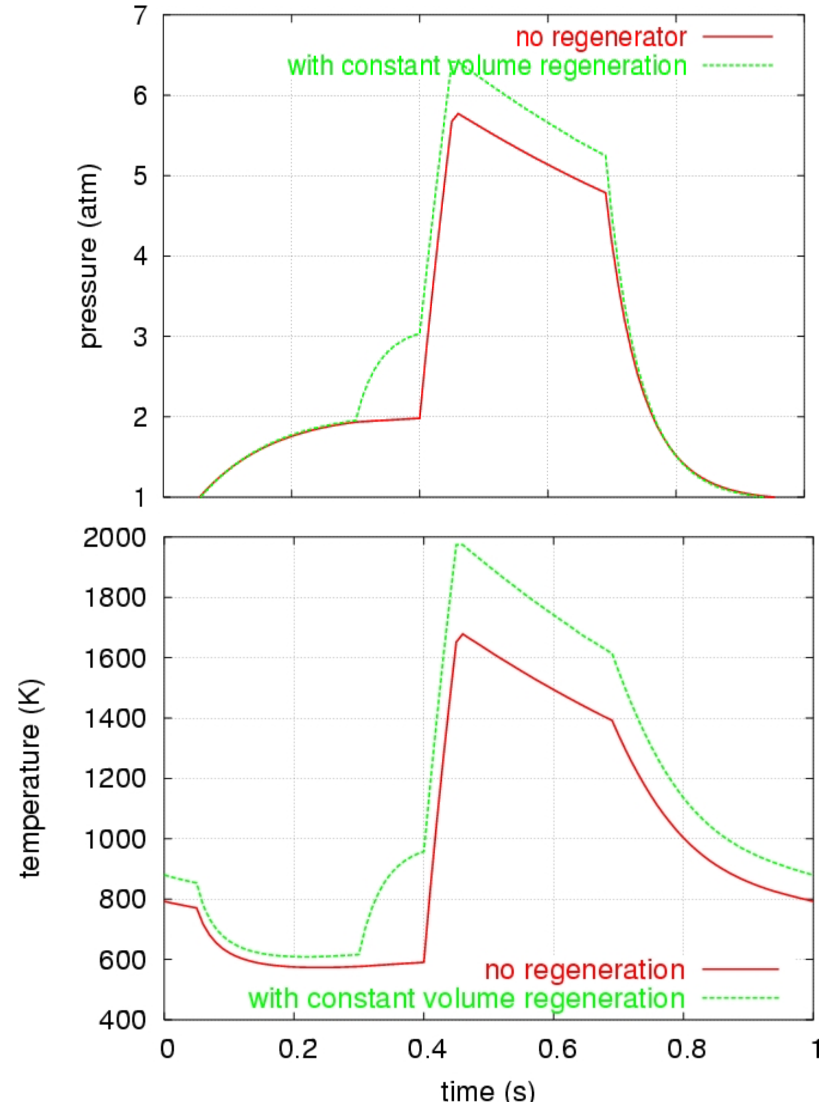
- 2.5-in. NPS Schedule 160 pipe and fittings
- Internal combustion chamber dimensions 2 in. ID X 3.2 in. L
- Refractory ceramic liner inserts
- Adaptable for liquid or gaseous fuels

Revised Phase II experimental plan includes flexibility for studying multiple issues

- Adjustable configuration (tinker-toy design) allows separate and combined assessment of many factors without complexity of full engine mechanism
  - Different regenerator materials (including special features like non-isotropic, water adsorbing, highly porous)
  - Ability to maintain large axial regenerator temperature gradients
  - Air vs. fuel preheating
  - Location of fuel injection and reformer catalyst
  - Fuel effects
- Key measurements
  - Transient temperatures and pressures in combustor, inlet/exhaust, regenerator, catalyst
  - Inlet and outlet flows
  - Comparisons with baseline operation (without preheating or reforming)
  - Partitioning of preserved exergy between work potential, hot exhaust

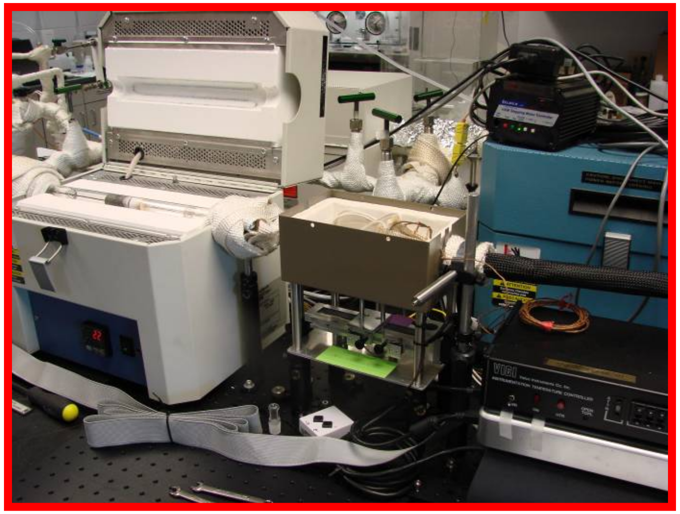
We are modeling RAPTR to predict expected effects of reduced irreversibility

- **Repeated cycling for tens of minutes to reach steady-state**
  - cycling frequency: 1 Hz
  - fuel: CH_3OH
  - equivalence ratio: 0.6
  - initial cylinder pressure: 2 atm
- **Combustion chamber pressure and exhaust temperatures (main and cooled) most direct indicators of irreversibility shifts**
  - Higher peak pressure
  - Divergence in temperatures of main and cooled exhaust



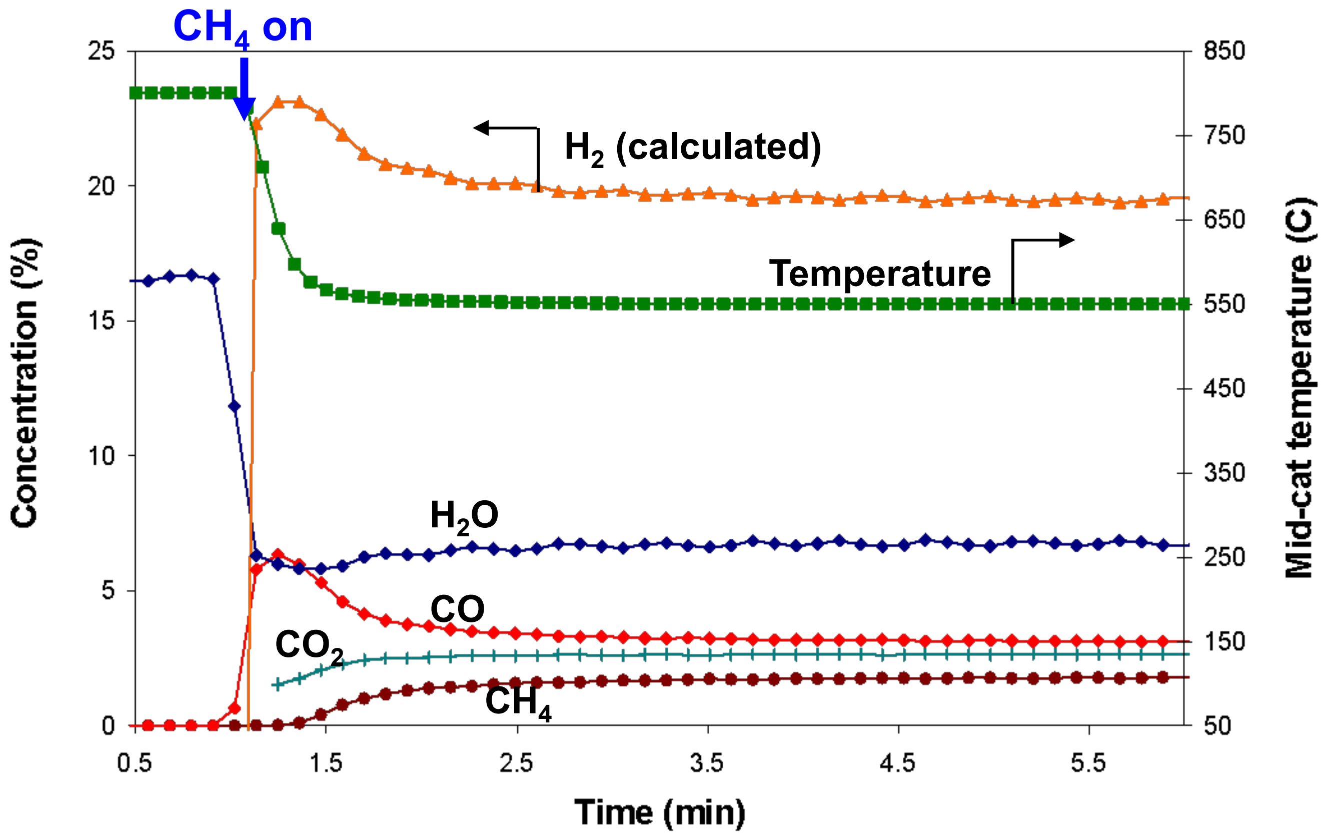
We are also using the ORNL bench flow reactor to screen reforming catalysts

- One is a commercial reforming catalyst from an industrial partner
  - Developed for onboard HC reforming (aftertreatment and fuel cells)
  - Used primarily for partial oxidation reforming
- Characterization includes steam reforming activity, TCR operating envelope
  - Provides global kinetics
  - Methane and ethanol fuels so far
  - Other fuels planned
- Provides important information for experiments
  - Product selectivity
  - Catalyst activity versus temperature
  - Cycling time scales
  - Potential fouling or poisoning



Bench flow studies confirm heat 'recuperation' with endothermic reaction

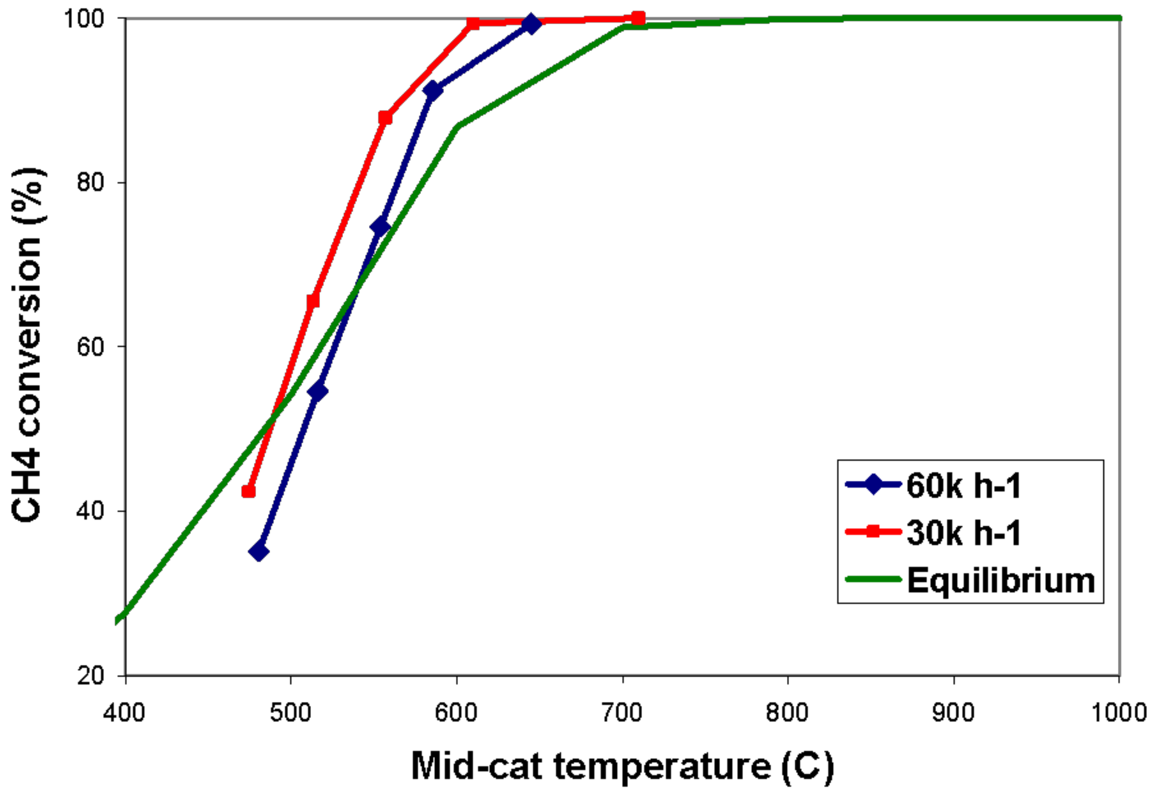
- Step CH_4 input
- Initially 100% CH_4 conversion, drops with decreasing catalyst T
- CO and CO_2 only C products
- Stable performance up to 1000C
  - no apparent coking
  - no thermal aging



8.3% CH_4, 16.7% H_2O, N_2 balance
SV = 60k h^{-1}; furnace T = 800 C

Bench reactor studies also reveal methane conversion near equilibrium limit

- Catalyst very efficient for CH_4 steam reforming
- Conversion limited by thermodynamics, not kinetics
- 100% CH_4 conversion achieved for catalyst T>650C
- Thermal management will be critical to achieve desired exergy benefit

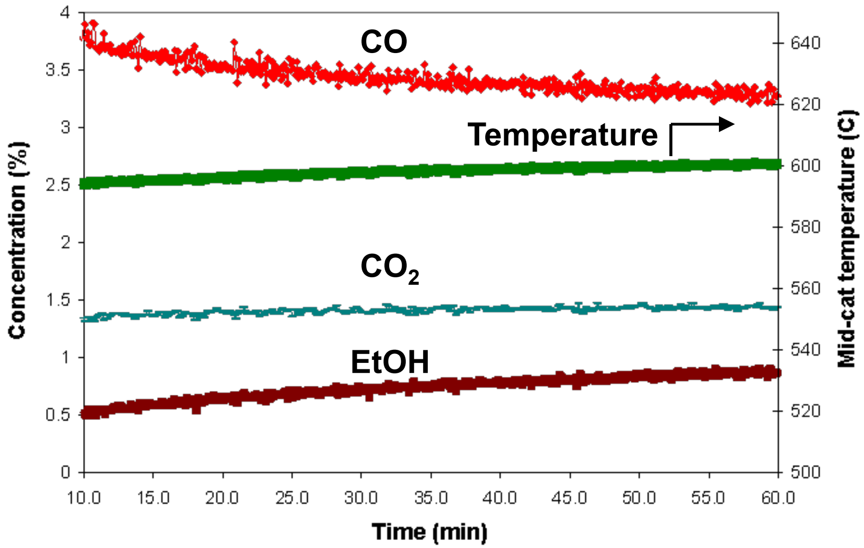


8.3% CH_4, 16.7% H_2O, N_2 balance

The present catalyst is active with ethanol but performance degrades due to coking

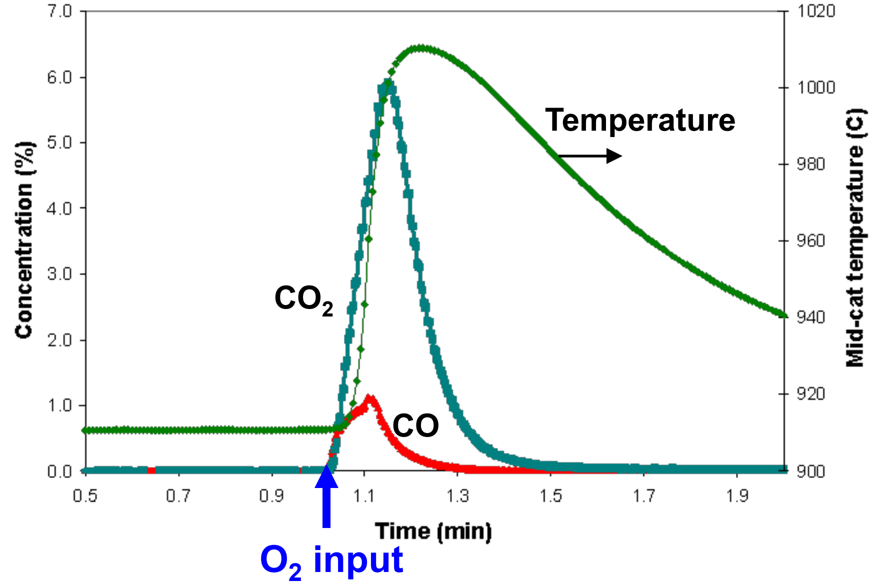
Reforming

4.2% EtOH, 12.5% H_2O, N_2 balance
SV: 60k h^{-1}; furnace T: 700C



Post-O_2 treatment

10% O_2, N_2 balance
SV: 30k h^{-1}; furnace T: 900C

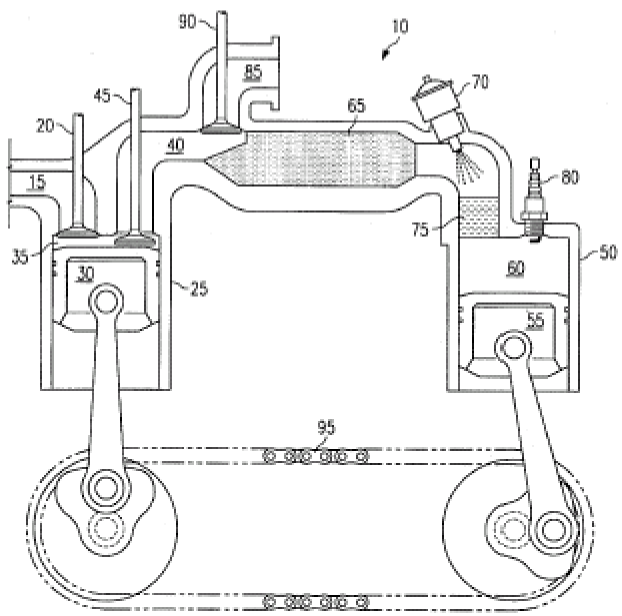


- **Ethanol reactivity comparable to CH_4 across temperature range**
  - 86% conversion at 600C
  - Products: primarily H_2(11%), CO(4%), CO_2(1%); some CH_4, CH_3CHO, C_2H_4(0.9% total)
- **Performance decays slowly due to coking**
  - Recovered after O_2 treatment; mitigated by cyclical operation of RAPTR
  - Catalyst not optimized for ethanol; supplier may have better formulations

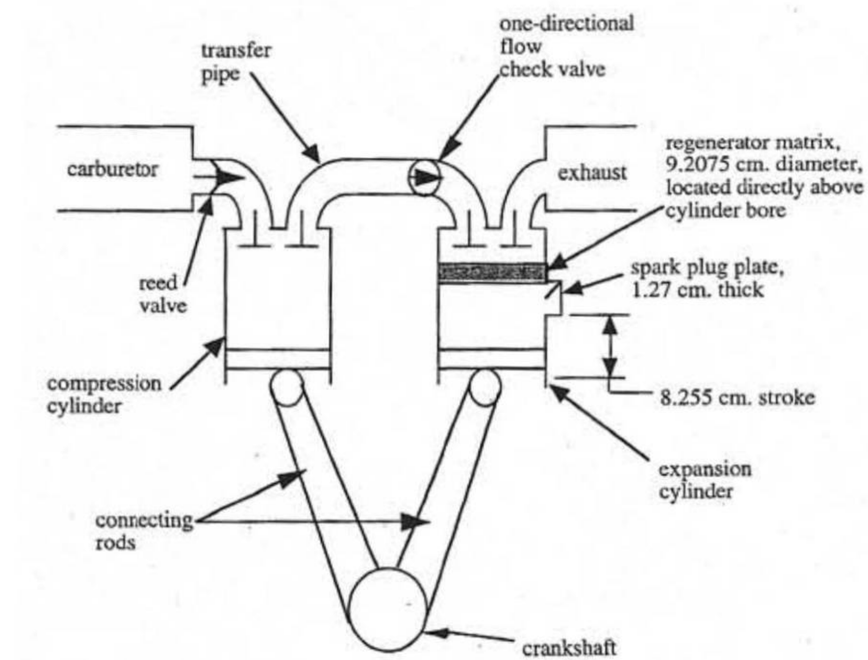
Phase III: Vision for ICE implementation

Engines utilizing thermal and chemical recuperation may include elements of previously discussed concepts

– Complex mechanisms (e.g., duel pistons with flexible phasing)
– But will include new combinations of materials, mechanisms, & controls
– Now developing models to relate bench-top results to ICE concepts



U.S. Pat. No. 5,499,605
March 19. 1996
R.H. Thring



S. Sepka and F. Ruiz, *Journal of Propulsion and Power*, Vol. 13, No. 2, p. 213, 1997

Technology Transfer

- Included several industry representatives during Phase I analysis.
- Published and presented Phase I conclusions.
- Modified Phase II experiment based on 2008 Peer Review input.
- Catalyst supplier provided catalyst samples.
- NDA negotiated with industrial partner interested in TCR.
- Presentation at ACE MOU meeting.
- Publications on basic thermodynamics of TCR in progress.

Planned Activities

- **Near term**
  - Complete RAPTR construction and shakedown with hydrogen, methane
  - Continue characterization of reformer catalyst for other fuels including methanol, ethanol (wet and dry), and iso-octane
  - Conduct experiments & analyses to quantify baseline availability (exergy) balances without thermal and chemical recuperation
  - Confirm significant reduction in combustion irreversibility with addition of thermal and chemical recuperation
- **Longer term**
  - Evaluate fuel effects
  - Evaluate effects of major configuration changes
  - Translate results to proposed ICE concepts

Summary

- Significant reductions in present losses of 20-25% of fuel exergy to combustion irreversibility can theoretically be achieved by thermal and chemical exhaust heat recuperation
- A highly flexible constant volume bench-top combustion experiment is under construction to study and demonstrate such reductions
- Parallel studies of reforming catalysts are underway

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