

Rapid Compression Machine - A Key Experimental Device to Effectively Collaborate With Basic Energy Sciences

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Overview

Timeline

- Project Start Date: Jan 2010
- Project end date: FY2013
- Percent complete: 50%

Budget

- DOE-EERE \rightarrow Argonne Engr.
 - \$250K (FY2010)
 - \$400K (FY2011)
- DOE-BES → Argonne Chemistry
 - \$600K (FY10 & 11)

Barriers

- Inadequate capability to accurately simulate
 - in-cylinder combustion over a range of temperature and pressure conditions
 - Emission formation
 - Effects of multi-component fuels

Partners

- MIT
- Purdue Univ.
- Univ. Akron
- Marquette University
- LLNL

Relevance

<u>Objectives</u>: To help develop a predictive capability of in-cylinder combustion and emissions formation through advances made in chemical kinetics



Milestones for FY10

Month/Year	Milestone
Mar-10 (Completed)	 Improve Argonne's RCM Make hardware changes for improved performance Fix leaky seals Guided by CFD improve combustion chamber geometry for temperature uniformity of the core region
May-10 (Completed)	 Develop computer program for data analysis Run tests using inert gases with similar specific heat ratio as the combustible mixture Through measured profiles deduce correlations for heat transfer losses Develop appropriate code to analyze measured pressure data using CHEMKIN and SENKIN
Nov-10 (Delayed)	 Validation through tests on methane-air mixtures Perform tests on various methane-air mixtures Analyze and validate the model using established chemical kinetic mechanisms

Milestones for FY11

Month/Year	Milestone
March-11 (80% Completed)	 Develop auxiliary systems Liquid fueling system: (low BPT fuels) to ensure accurate fuel metering and also achieve a uniform fuel-air mixture Aerosol fueling: (high BPT fuels) to achieve uniform fuel-air mixtures Rapid sampling apparatus: To track time resolved concentration of species Imaging/ flame speed: To determine fundamental properties of fuel-air mixtures
June-11	 Conduct tests on low-BPT fuels Ethanol and iso-octane Other alcohols and gasoline surrogates (time permitting) Develop data complementary to shock tube studies Validate chemical mechanisms for single component fuels
Nov-11	 Conduct tests on high-BPT fuels N-Heptane Biodiesels and diesel surrogates (time permitting) Develop auto-ignition data complementary to shock tube studies In association with LLNL develop /validate chemical mechanisms

Approach/ Strategy

First let us look at the problem at hand....



The Current Method of Validating Combustion Chemistry

Metrics

- Autoignition delays
- Laminar Flame speed
- Extinction strain rates

Experimental Devices

- Bench scale flames
 - Laminar flames
 - Opposed flow flames
- Jet-stirred reactors
- Shock tubes



Chemical Kinetic Mechanisms

- Detailed
- Reduced



The Current Method of Using Combustion Chemistry



For chemical kinetic studies a quiescent, isothermal, adiabatic combustion zone is desirable



A RCM's operational envelope covers most of the engineering applications



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Argonne's RCM and shock tube will be used to obtain complementary chemical kinetic data





Technical Accomplishments and Progress

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Guided by CFD simulations RCM hardware was modified to ensure isothermal zone ±10 K





Half cross-section

Original

Half cross-section After Modifications



A new piston sealing arrangement was used for leak-free performance and reduced dead volume



Gen-I



Two-part design (Final)



Data analysis model was developed to be able to validate chemical mechanisms using the RCM results



Courtesy : U. Akron

"Effective volume" method used to account for heat transfer to walls $V_{eff} = V_g(t) + V_{add} \qquad t \le 0$ $V_{eff} = V_{eff}(0) \cdot v_p(t) \qquad t \ge 0$ $v_p(t) \text{ determined through tests on inert gas (Argon/ Nitrogen)}$ Mass conservation $\frac{dY_k}{dt} = v\omega_k W_k \qquad k=1,2,...,N$ Energy conservation $C_v \frac{dT}{dt} + v \sum_{k=1}^N e_k \omega_k W_k + p \frac{dv}{dt} = 0$

Progress delayed due to accidental damage to the hydraulic chamber flange

Damaged hydraulic breaking chamber



Further tests delayed by 4 months as a new flange was manufactured

Development of auxiliaries: Liquid fueling system

- Use of liquid fuels (especially bio-diesel) poses new challenges
 - Boiling point as high as 350°C
 - Tendency to separate and pool / condense on the walls
 - Preferential evaporation for multi-component fuels
 - Chemical reactions prior to compression

MIT method (for low BPT fuels)

- Heat the whole RCM to 120°C using heaters (Hardware in place)
- Meter the liquid fuel using a syringe pump

Marquette University/ Stanford/ MSU Method (for high-BPT fuels)

- Nebulize the fuel and rely on increased temperature during compression
- Geometries being optimized to minimize droplet impingement/ separation



Development of auxiliaries: Fast gas sampling device

Courtesy: Toyota R&D.

- The sampling system enables us to collect gas samples directly from the RCM combustion chamber.
- Min. resolution: 55 µsec (= 1° crank angle @3000 rpm)
- Time resolved sampling and subsequent chemical analyses will trace the formation of individual chemical species and nano-particles.



Development of auxiliaries: Flame speed measurement strategy in the opposed-piston RCM



Cylindrical Chambers



Chamber

 \star

RCM Comb.

D~14"

L/D~3-4

L/D~0.44

- Flame speed is a fundamental fuel property that determines burning rate

- Serves as a standard to validate chemical mechanisms



- Optical access through a spark plug port on the combustion chamber wall

Flame radius was measured for various fuels under typical in-cylinder conditions (32.5 bar, 706 K)



50% H_2 / 50% CO; ϕ =0.8; Δ t=0.263ms

Confinement issues dominate and limit flame speed measurements in the RCM



- For given geometry and camera capture rates (~ 4000 fps) various fuels were used to obtain a range of stretch rates.
- Except in the case of (hydrogen rich) fuels with very high S_L values, typical hydrocarbon measurements were confinement limited.
- Currently, evaluating strategies to reduce wall effects, and to use theoretical treatments to correct for such effects.

Collaboration and Coordination with Other Institutions

- MIT (Wai Cheng)
 - Design of the RCM
- Univ. Akron (Gaurav Mittal)
 - Chemkin-pro model
- Purdue University (Li Qiao)
 - Flame speed measurements
- Marquette University (Scott Goldsborough)
 - Aerosol liquid fueling system
- Lawrence Livermore National Laboratory (Bill Pitz)
 - Gasoline surrogate mechanism development

Proposed Future Work : Ignition/ combustion characteristics of alternative fuels and fuel blends

- Ethanol: (BPT: 78.4°C)
 - Energy Density: 19.6 MJ/L
 - Used as 15% to 85% blend in gasoline
 - RCM will be heated to 110°C. Mixture preparation via. MIT method.
- Butanol: (BPT: 117.2°C)
 - Processes exist for commercial production of biobutanol
 - Energy Density: 29.2 MJ/L
 - RCM will be heated to 120°C. Mixture preparation via MIT method.
- Biodiesel: methyl, ethyl or propyl mono esters (Flash Pt: >120°C, BPT= 200-350°C)
 - Higher lubricity, Cetane number > 47
 - At present, most biodiesel in the U S is made from soy oil
 - ASTM D 6751 standards apply
 - Used as blends B0B100
 - RCM will be heated to 350°C?. An aerosol fueling method is being developed in association with Marquette Univ., Michigan State Univ.



OH



Summary

To provide accurate kinetic data to conventional/ alternative and designer fuels under engine like conditions using revived Argonne's Rapid Compression Machine.

- Guided by CFD analysis, piston geometries were altered to obtain a postcompression isothermal zone to within E10 K.
- A zero-dimensional model was developed to assist in validating chemical mechanisms using measured pressure traces.
- Accidental damage to the RCM hardware introduced unforeseen delays; attention was diverted to developing the auxiliary systems while RCM was being repaired
 - Aerosol Liquid fueling system
 - Fast-sampling system
 - Imaging for flame speed calculation
- Very soon tests will be conducted in low-volatile fuels that will be followed by those on bio-diesel surrogates

