

ANNUAL REPORT FOR THE YEAR 2013

OF THE

INTERNATIONAL ENERGY AGENCY IMPLEMENTING AGREEMENT FOR ENERGY CONSERVATION AND EMISSIONS REDUCTION IN COMBUSTION

prepared by the Executive Committee Secretariat

for Dennis Siebers, Agreement Operating Agent Sandia National Laboratories - California

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EXECUTIVE ABSTRACT

The purpose of the IEA Implementing Agreement on Energy Conservation and Emissions Reduction in Combustion program is to improve fundamental and applied combustion technology which is developed to provide predictive design capabilities for internal combustion engines, furnaces, and gas turbines. This document summarizes the progress made in this agreement year.

Since 1978, IEA cooperative research by program participants has focused on developing experimental and computational tools to aid combustion research and on developing advanced laser-optical diagnostic tools that permit time- and space-resolved measurements of combustion phenomena for achieving this end. The Agreement's Annex structure has been planned to improve the modeling and simulation processes as well as the instrumentation required for the supporting experimental activities. In order to to more efficiently organize Agreement Research Activities the Annex structure was revised in the 2013 agreement year.

The new Annex structure adopted by the Executive Committee at its April 23, 2013 Meeting is shown below. In addition to initiating new Collaborative Tasks in Gas Engines and Combustion Chemistry, the HCCI Task was renamed Low Temperature Combustion to more accurately reflect the nature of the research and the Advanced Hydrogen Fueled Internal Combustion Engine Task was incorporated into the newly formed Gas Engines Task. The new Annex Structure is shown below.

Annex 1	Administration and Supportinc Activities
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	Area 1 Advanced Piston Engine Technology
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YEAR 2013 ACTIVITIES OF THE EXECUTIVE COMMITTEE

Chair: Mr. Gurpreet Singh, United States

Vice Chair: Dr. Mario Ditaranto, Norway

The Executive Committee (ExCo) of the International Energy Agency's (IEA) Program of Research, Development and Demonstration on Energy Conservation and Emissions Reduction in Combustion coordinates the cooperative efforts undertaken by participating institutions. The Committee met twice during the business year. The first meeting took place in April at IEA headquarters in Paris. The second took place following the Agreement's Thirty-fifth Task Leaders Meeting in July in San Francisco, Caliornia.

Actions taken by the Executive Committee this year include:

<u>Task Leaders Meeting:</u> The Thirty-fifth Task Leaders Meeting, sponsored by the Executive Committee was held at the St. Francis Hotel in San Francisco, California in July. Principal Investigators, Executive Committee members, and invited guests gathered to hear papers presented on the Agreement's research. Sixty members of the Combustion Research Community attended and forty-three papers were presented on the Agreement's ongoing Collaborative Task activities

<u>Executive Committee Meetings:</u> Minutes of the Executive Committee's meetings of April and July have been published and distributed to IEA Headquarters and to ExCo members. The Proceedings of the Thirty-fifth Task Leaders Meeting were published and distributed to IEA Headquarters and Executive Committee members for distribution to participants. The Agreement's Annual Reports and 30 Year Anniversary Report are available on the public web site.

<u>Future Meetings</u>: The Executive Committee scheduled its next meetings for April 2014 at IEA Headquarters, Paris and June 2014 in Norway The June meeting will be held immediately following the 36th Task Leaders meeting in Norway.

Highlights from Recent ExCo Meetings

Paris France --- April 23, 2013

The Executive Committee:

Welcomed Dr. Mario Ditaranto as the new Principal ExCo Member from Norway.

Approved new Collaborative Tasks in Combustion Chemistry and Gas Engines

Confirmed April 15, 2014 as the date of the Agreement's next ExCo meeting at IEA Headquarters in Paris, subject to meeting room availability

Confirmed February 20, 2014 in Hawaii as the date and location of the Agreement's 2014 Strategy Meeting, reminded members that attendance is voluntary, and added a

morning Strategy Session on April 15, 2014 in Paris prior to meeting of the Executive Committee that afternoon.

Confirmed July 21-25, 2013 at the St. Francis Hotel in San Francisco, California as the dates and location for the 2013 Task Leaders Meeting to be hosted by the United States.

Confirmed the afternoon of July 25, 2013 at the St. Francis Hotel in San Francisco, California as the time and location for the next meeting of the Agreement's Executive Committee

Accepted the proposal from Norway to host the 2014 Task Leaders Meeting in Trondheim with a tentative date of June 2014.

San Francisco, California --- July 25, 2013

Dr. Ditaranto from Norway was unanimously elected as ExCo chair and Prof. Greenhalgh from the United Kingdom was unanimously elected as Vice Chair for the Agreement Year 2013-2014. Their appointment becomes effective at the conclusion of this San Francisco ExCo Meeting

Dr. Ditaranto has agreed to assume leadership of the Nano Particle Diagnostics Collaborative Task

Prof. Xu reports that China is interested in joining the Agreement. If approved by their government, they will be represented on the ExCo by Tsinghua University.

The Annual Strategy meeting will be held in Maui, Hawaii February 20-21 2014. An additional Strategy discussion will take place at IEA Headquarters on the morning of the April 2014 ExCo. Attendance will be limited to ExCo members.

Pending the availability of a meeting room, the date for the next ExCo meeting at IEA Headquarters has been moved to Tuesday, April 29, 2014. The ExCo meeting will begin at 1:30pm. As noted above it will be preceded by a Strategy Meeting in the morning.

June 9-13, 2014 were identified as the dates for the 36th TLM to be hosted by Norway. Trondheim is the likely venue.

Prof. Greenhalgh agreed to host the 2015 TLM on behalf of the United Kingdom, St.Andrews in Scotland is the likely venue. The third week of July is the target date for the meeting

SUMMARY OF RESEARCH ACTIVITIES FOR A PROGRAM OF APPLIED RESEARCH, DEVELOPMENT, AND DEMONSTRATION IN ENERGY CONSERVATION AND EMISSIONS REDUCTION IN COMBUSTION

Introduction

The Implementing Agreement for A Program of Applied Research, Development, and Demonstration in Energy Conservation and Emissions Reduction in Combustion requires that the Executive Committee define and adopt detailed specifications for each research task undertaken within the program.

For most of its existence the Agreement consisted of a single Annex comprised largely of individual/single investigator tasks. Although this model worked well, the Executive Committee recognized that more attention should be paid to multi-nation/multi-investigator collaborative tasks. As the result of a series of strategic planning meetings six broad areas were identified for collaborative task development. In the spring of 2011 this culminated in an expansion of the number of Annexes within the Agreement such that each of these collaborative research areas were designated as a separate Annex. At the same time the original concept of single contributor tasks was retained for those investigators who preferred to contribute in that manner.

Moving forward, the Agreement will be comprised of multiple Annexes with Annex 1 being reserved for Administration and Supporting Activities, Annex 2 being Individual Contributor Tasks, and Annexes 3 and beyond being Multi Nation Collaborative Tasks

Briefly the focus of the individual Annexes is summarized below:

Annex 1 --- Administration and Supporting Activities

The objective of the work in this area is to provide administrative support services and information dissemination as called for by the work in Annexes 2 - 10.

In addition from time to time the Executive Committee may request that a Special Session of invited speakers focused on a Research Area or Policy Matter of current interest be added to the Program for an upcoming Task Leaders Meeting

Annex 2 --- Individual Contributor Tasks

This Annex has been planned to improve fundamental and applied combustion technology which is developed to provide predictive design capabilities for internal combustion engines, furnaces, and gas turbines. The Annex is divided into the following Areas:

Area 1: Advanced Piston Engine Technology

The objective of the cooperative work in this Area is the development of combustion

technology, both analytical and experimental, that will provide improved models for advanced internal-combustion piston engines, namely lean homogeneous-charge, stratified-charge, and diesel engines. The research will contribute primarily to technology common to these engine concepts and will provide data bases and descriptive and predictive system codes, in addition to practical demonstrations

Area 2: Advanced Furnace Technology

The objective of the cooperative work in this Area is the development of combustion technology, both analytical and experimental, that will provide models for furnaces and boilers. The research will provide a data base and descriptive and predictive system codes, as well as practical demonstrations.

Area 3: Fundamentals

The objective of the cooperative work in this Area is to conduct theoretical investigations of the fundamental physical phenomena relevant to the combustion process as is called for in Areas 1, 2 and 4, and to support the development of new diagnostic techniques for application in the future.

Area 4: Advanced Gas Turbine Technology

This Area covers work related to the development of combustor and gas turbine modeling and verification, to the study of emissions formation and control mechanisms, and to practical studies in fuel injection and fuel/air mixing.

Annex 3: Sprays in Combustion

Spray investigations aim at a deeper understanding of the complex interrelated aerodynamic and thermodynamic mechanisms involved in transient & steady spray combustion, which are responsible for the tradeoffs among energy conversion efficiency, nitrogen oxides and soot emissions in advanced engines and combustors. Tasks in the context of spray propagation involve a wide set of investigations on atomization, fuel-air mixing and combustion under high temperature and high pressure, as encountered in advanced diesel engines, gas turbines – and to some extent also boilers

Annex 4: Low Temperature Combustion (formerly HCCI)

The combustion process in the HCCI (Homogeneous Charge Compression Ignition) engine is mainly driven by the chemical kinetics. Thus the chemical properties of the fuel are of outmost importance. Many small molecule fuels like methane and methanol have relatively simple and well controllable combustion process but it has been shown that many fuels experience a two-stage ignition process with a time period between the two stages without significant heat release.

The intent of this Annex is to look into the interaction between HCCI and fuels. It will include activities for both the gasoline and diesel type of fuels and HCCI with fully premixed charge and direct injection.

Annex 5: Advanced Hydrogen Fueled Internal Combustion Engines (No longer active – related work can be found in Annex 9)

Annex 6 Alternative Fuels

The present day engine combustion technology has been fully developed for crude oil based traditional liquid fuels: gasoline and diesel fuel.

The aim of the Annex is develop optimum combustion of future fuels and thereby significantly reduce engine out emissions together with noticeable increase in engine efficiency. The development of combustion techniques focuses especially on synthetic and renewable fuels. This Annex concentrates mainly on road transportation. There is a potential of engine out emission reduction by 70% to 90 % or even more. Dedicated fuels need new combustion technology to meet optimal emission reduction.

Annex 7 Nanoparticle Diagnostics

This Annex focuses on research concerning the measurement of nanoparticles produced by combustion. The development of diagnostics to characterize the physical or chemical characteristics of the nanoparticles, and demonstration of the application of these diagnostics, are within the scope of this Annex. The development may include experimental, numerical, or both approaches to the research. Demonstration may be inflame studies of nanoparticle formation and oxidation, or post-flame measurements of nanoparticle emissions.

Annex 8: Hydrogen Enriched Lean Premixed Combustion for Ultra Low Emission Gas Turbine Combustors

In response to national policies gas turbine manufacturers have set the goal to adapt their large gas turbines for CO2-mitigated power generation, whereby up to 90% of the carbon contained in the fired fossil fuel is captured and stored as CO2. In order to mitigate CO2 emissions Zero Emission Power Plant concepts are being explored on a global scale. Gas turbine based configurations are playing a significant role in these scenarios. Following up on the previously conducted collaborative effort on "Hydrogen enriched Lean Premixed Combustion for Ultra-Low Emission Gas Turbine Combustors" it is proposed to widen the future collaborative task activities to gas turbine combustion issues linked to respective Zero Emission Power Plant concepts.

Annex 9: Gas Engines

This task seeks to establish collaborations among IEA membership countries in the field of gas engines.

The following topics were identified as of particular interest/suitable for collaboration:

Ignition systems

Diesel micro pilot injection Extension of lean limit for LPG fuel Optimization of injector and spark plug location Fuels/kinetics

Self-ignition and knock Tailored combustion systems and kinetics for various gaseous fuels with different physical and chemical properties Operation to even leaner and/or more dilute mixtures Effect of injector configuration and fuel on spray characteristics and mixing process

Novel Concept and Modelling Approaches

LIF experiments of various gas jets Full scale experiments in optical engines; combustion verification in single-/multi-

cylinder Engines

Annex 10: Combustion Chemistry

The aim of this work is to build reaction mechanisms taking into account the formation and the consumption of species detected in combustion processes. Thanks to these models, precious information on the degrees and the rates of reactants conversion, the formation of pollutants, the effects of additives can be obtained. These mechanisms will then be used in the numerical simulation of combustion devices (engines, furnaces, boilers...) to define their best operating conditions.

The Combustion Chemistry (CC) task has to be envisioned as a supporting task to the other IEA tasks (HCCI, Alternative Fuels, Spray...). It will aim at a tighter coordination and enhanced communication between research groups in kinetics. The main focus of this collaborative task is to extend and to improve the understanding kinetics to reduce pollutants formation. The combustion of hydrocarbons, oxygenated species and surrogate fuels needs to be well understood through more elaborate mechanisms ; such knowledge could be exploited to optimize the combustion processes or devices.

Additional information on any of the work areas of the Agreement may be obtained by contacting:

Dr. Robert J. Gallagher Secretary, Executive Committee IEA Combustion Agreement 5380 Mallard Drive Pleasanton, CA 94566 USA email: <u>bobgall@aol.com</u>

How to Join the Agreement

Participation in IEA Combustion is based on mutual benefit to the Implementing Agreement and the interested newcomer.

If there is interest in joining the Implementing Agreement please contact the IEA Combustion ExCo Secretary, Dr. Robert Gallagher (Bobgall@aol.com). The Secretary will provide you with details on the Implementing Agreement and invite you to attend an ExCo Meeting as an Observer. By attending you will become familiar with the Implementing Agreement's current and future research areas. Assuming mutual interest, the next step would be to make a formal presentation to the ExCo at its next regularly scheduled meeting identifying the research areas in which you would propose to contribute. Prior to this ExCo presentation you would also be welcome to attend the next Task Leaders meeting as an Observer and, if you wished to, make a presentation related to a combustion related research topic in which you were currently engaged.

Contracting Parties to IEA Combustion Agreement are usually governments. Therefore, for interested parties it is necessary to seek support from their government to join the Implementing Agreement. The government will later appoint a Delegate and an Alternate to represent the Contracting Party in the ExCo.

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Summary of Accomplishments for the 2013 Agreement Year

Introduction

In the summary which follows the reader will find highlights from the Research conducted by Agreement Participants during the past year. If further detail is of interest the leaders identified for each of the Tasks should be contacted directly.

Annex 1 – Administration and Supporting Activities

In addition to overseeing the Administrative Duties of the Secretariat the Executive Committee requested that the organizers of the 2013 Task Leaders Meeting (TLM) arrange for a Special Session of Invited Speakers to provide overview presentations on the State of the Art and Future Trends in Engine Combustion Modelling and Diagnostics. The following presentations were made at the TLM.

Paul Miles, Sandia: Quantitative Measurements of Flow and Scalar Fields Supporting Predictive Simulation for Engine Design

Lyle Pickett, Sandia: Spray Combustion Research for the Engine Combustion Network

<u>Christopher Rutland, University of Wisconsin:</u> Sub-Model Needs for Accurate Prediction of IC Engine Combustion

Joe Oefelein, Rainer Dahms, Guilhem Lacaze, Anthony Ruiz, Sandia: Advances in the Simulation of Direct Injection Processes in Diesel Engines

Chitralkumar V. Naik, Karthik Puduppakkam, and Ellen Meeks, Reaction Design: Simulation and Data Comparisons for In-Cylinder Soot Formation in a LTC Engine using a Detailed Reaction Mechanism

Highlights from the Special Session included the following:

Paul Miles, Sandia: Quantitative Measurements of Flow and Scalar Fields Supporting Predictive Simulation for Engine Design

Initial discrepancies between experimental results and predictive simulations resulted in the modification of reduced chemical kinetic mechanisms which significantly improved the prediction of UHC to CO oxidation of moderately rich mixtures and <u>considerable improvement in emissions predictions</u>

Ignition timing depends strongly on temperature, equivalence ratio, and dilution. On-going heat and mass transfer impact ignition processes involving hundreds or thousands of species and reactions. Faithfully capturing all of these processes is required to calculate even something as simple as whether or not ignition even occurs.

Engine combustion processes are complex. However:

Quantitative measurements can be acquired in complex, realistic engine modelling. These measurements have impacted and will continue to impact engine modelling

A hierarchy of models is required, High-cost, high accuracy simulations must be coupled with low-cost model development to impact engine design

Lyle Pickett, Sandia: Spray Combustion Research for the Engine Combustion Network

There is much we **Don't Understand** (even conceptually) about diesel spray combustion.

In addition, **<u>Quantitative</u>** data is lacking at high-temperature engine conditions (>900 K)

The Engine Combistion Networlk (ECN) has defined a program collaborative research at specific target conditions

Opportunity for the greatest exchange and deepest collaboration.

- Understanding facilities/boundary conditions.
- Understanding diagnostics and quantification.
- Standardize methodologies for post-processing.

Leverages the development of quantitative, complete datasets.

- Unique diagnostics to build upon past understanding.
- Moves from "qualitative" to "quantitative".
- Sharing results/meshes/code/methods saves time and effort.

A website has been established (<u>www.sandia.gov/ECN</u>) to facilitate information exchange

Workshops have been organized with voluntary participation



<u>Christopher Rutland, University of Wisconsin:</u> Sub-Model Needs for Accurate Prediction of IC Engine Combustion

Topics

- Multi-component fuel modeling
- Spray modeling
- Wall heat transfer modeling
- Mixing and combustion modeling
- Soot modeling

Outline

- Advanced engine combustion strategies -> high fuel economy and low emissions
 - Often these exploit new physical phenomena:
 - Mixed mode combustion
 - Volumetric flame propagation
 - Controlled stratification
- Many processes not fully understood
 - Cavitation phase change, non-ideal vaporization (azeotropic effects, supercritical phenomena), fuel composition effects
 - Wall heat transfer, wall film vaporization/combustion, effect of knock
 - Fuel preparation (atomization, drop breakup/collision-coalescence)
 - Turbulent mixing (at large and small scales), cyclic variability
 - Combustion chemistry, flame kernel development, flame propagation, combustion mode transitions
 - Emissions (UHC, CO, NOx, PM)
- Need to understand physics
 - Optimize
 - Potential to find new concepts
 - Integrated approach: modeling and experiments
 - CFD codes are invaluable
 - Rely on accurate, validated, physics based sub-models

<u>Summary</u>

- Demonstration of several important modeling areas for engine CFD
 - Fuel properties and spray characteristics
 - Wall heat transfer
 - Combustion modeling
 - Particulate emissions and wall films
- Future Needs
 - Address fundamental aspects of:
 - Turbulent mixing and combustion
 - Fuel spray characteristics
 - Particulate matter emissions
 - Coordinated effort: basic experiments and advanced CFD
 - Optimize advanced engine technologies
 - Platform to explore and find new concepts

Joe Oefelein, Rainer Dahms, Guilhem Lacaze, Anthony Ruiz, Sandia: Advances in the Simulation of Direct Injection Processes in Diesel Engines

Objective and Approach

- Study effects of high-pressure phenomena on fuel injection processes (here at conditions relevant to Diesel engines)
 - Focus on typical conditions when cylinder pressures exceed the thermodynamic critical pressure of the fuel
 - Understand major differences compared to classical spray theory
- Use LES with detailed model framework designed to account for real-fluid multicomponent thermodynamics and transport
 - Compare results with experimental data from the Sandia high-pressure combustion vessel (Pickett et al.)
 - Perform detailed thermodynamic analysis of resultant multicomponent mixtures to understand interfacial dynamics

Summary and Conclusions

- Performed detailed analysis of high-pressure injection processes using LES and real-fluid model
 - Focused on detailed thermodynamics of resultant multicomponent mixtures to understand interfacial dynamics
 - Model captures behavior of multicomponent hydrocarbon mixtures at highpressure supercritical conditions
 - Revealed that envelope of mixture conditions varies from compressed liquid to supercritical state (i.e., never saturated)
- At these conditions, the classical view of jet atomization and spray as an appropriate model is questionable
 - Distinct gas-liquid interface does not necessarily exist
 - Lack of inter-molecular forces promote diffusion over atomization
 - Theoretical analysis describes when and why for given conditions

Chitralkumar V. Naik, Karthik Puduppakkam, and Ellen Meeks, <u>Reaction Design</u>: Simulation and Data Comparisons for In-Cylinder Soot Formation in a LTC Engine using a Detailed Reaction Mechanism

Outline

- Motivation and approach
- Fuel surrogate and its detailed reaction mechanism
- New soot model
- Engine CFD simulation using FORTÉ
- Results and analysis
- Summary

3



Systematic approach



Model Fuel Library contains detailed mechanisms for 56+ components





- Self-consistent
- Validated (400 fundamental experiments) *
- Range of C# for natural gas, gasoline, diesel, jet, and biofuels *
- Master mechanism: 2000-8000+ species

* Naik et al., SAE Int. J. (2010) 3, 241-259.6 * Puduppakkam et al., SAE 2010-01-0545.



Summary

LTC diesel engine simulation using FORTÉ CFD

- 4-Component surrogate for the European diesel
- Detailed fuel combustion mechanism
- New pseudo-gas soot model developed and validated
- Simulation captured combustion phasing
- Trends and magnitude of in-cylinder soot levels captured
 - No adjustment between cases

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Annex 2 – Individual Contributor Tasks

The following invididual Contributor Task was undertaken during the past year:

Joakim Bood, Andreas Ehn, Billy Kaldvee, Olof Johansson, and Sven-Inge Möller: New laser-based Techniques for Challenges in Combustion Diagnostics

Challenge #1: Quantitative concentration measurements with LIF



Motivation for studies of fluorescence lifetimes

- Allow determination of quenching rates
- Quenching correction of fluorescence signals \to quantitative species concentrations if the temperature is known
- Temperatures may be determined if the chemical composition and the pressure is known
- Concentrations of quencher molecules can in certain cases be measured if temperature and pressure is known



IEA 35th TLM Combustion, San Francisco, CA, USA / July 25 2013

Challenge #2: Large probe volumes and limited optical access









IEA 35th TLM Combustion, San Francisco, CA, USA / July 25 2013

LIDAR concept



Potential ps-LIDAR applications

Large scale industrial burners & power plants

-Thermometry -Soot mapping -Spray mapping -Fuel visualization

Fire applications

-Thermometry -Soot mapping







IEA 35th TLM Combustion, San Francisco, CA, USA / July 25 2013

Challenge #3: Detection of "new" species





IEA 35th TLM Combustion, San Francisco, CA, USA / July 25 2013

Summary

- Lifetime imaging based on two ICCD cameras makes an important step towards quantitative LIF measurements.
- ps-LIDAR is a promising technique able to probe large measurement volumes with only one optical access.
- Photofragmentation-LIF allows 2-D detection of species that have previously not been possible to measure (H₂O₂/HO₂).



IEA 35th TLM Combustion, San Francisco, CA, USA / July 25 2013

Annex 3 - Sprays

The following activities were undertaken within the Sprays Task during the past year

<u>Martti Larmi, Aalto University</u>: Experinmental and Computational Spray and Jet Studies at Aalto Universiy

<u>S. Lee¹, L. Allocca², A. Zhang¹, A. Montanaro², J. Naber¹</u>: Visualization of Diesel Spray Characteristics under Various Conditions Using a Hybrid Schlieren/Mie Scattering Imaging System. 1 – Michigan Technological University, 2 – Instituto Motori

<u>H. Kawanabe</u>: LES Analysis of Mixture Formation and Combustion Processes in a Diesel Spray

Christopher Powell, Daniel Duke, Nicholas Sovis, Andrew Swantek, Zak Tilocco (CTR) Alan Kastengren, Yuan Gao, Su Han Park, Jin Wang (APS), Argonne National Laboratory: X-Ray Diagnostics of Fuel Injection and Sprays

<u>Keiya Nishida University of Hiroshima:</u> Effect of Temporally-Splitting of Fuel Injection on Mixture Formation and Combustion of Diesel Spray

Highlights from the work included the following:

Martti Larmi, Aalto University: Experinmental and Computational Spray and Jet Studies at Aalto Universiy

Recent Publications

 Yu J., Vuorinen V., Kaario O., Sarjovaara T., and Larmi M., Visualization and analysis of the characteristics of transitional underexpanded jets, to appear in Int. J. Heat and Fluid Flow.
 Yu J., Vuorinen V., Kaario O., Sarjovaara T., and Larmi M., Characteristics of High Pressure Jets for Direct Injection Gas Engine, SAE International Journal of Fuels and Lubricants, 6, 1, 149-156, (2013).

[3] Kaario O., Vuorinen V., Hulkkonen T., Keskinen K., Nuutinen M., Larmi M., Tanner F.X., Large-Eddy Simulation of High Gas Density Effects in Fuel Sprays, to appear in Atomization and Sprays, (2013).

[4] Wehrfritz A., Vuorinen V., Kaario O., and Larmi M., Large-Eddy Simulation of High Velocity Fuel Sprays: Studying Mesh Resolution and Breakup Model Effects for Spray A, to appear in Atomization and Sprays, (2013).

[5] Nuutinen M., Vuorinen V., Kaario O., and Larmi M., Imbalance Wall Functions with Density and Material Property Variation Effects Applied to Engine Heat Transfer CFD Simulations, to appear in International Journal of Engine Research (2013).

[6] Vuorinen V., Duwig C., Yu J., Boersma B., Larmi M., Large-Eddy Simulation of Highly Under-Expanded Jets, Physics of Fluids 25, 016101, (2013).

[7] Vuorinen V., Schlatter P., Boersma B., Larmi M., and Fuchs L., A Scale-Selective, Low-Dissipative Discretization Scheme for the Navier-Stokes Equation, Computers & Fluids, 30, 70, 195-205, (2012).
[8] Yu J., Vuorinen V., Hillamo H., Kaario O. and Larmi M., An experimental investigation on the flow structure and mixture formation of low pressure ratio wall-impinging jets by a natural gas injector, Journal of Natural Gas Science and Engineering, 9, 1-10, (2012).

Conclusions

Current computational methods capable of capturing detailed near-nozzle behavior

High pressure jets mix better than low pressure jets

Power of Proper Orthogonal Decomposition in data analysis.

LES captures contrasts in scalar dissipation rate.

Future Research: cylinder temperature effects, methane and hydrogen jets

<u>S. Lee¹, L. Allocca², A. Zhang¹, A. Montanaro², J. Naber¹</u>: Visualization of Diesel Spray Characteristics under Various Conditions Using a Hybrid Schlieren/Mie Scattering Imaging System. 1 – Michigan Technological University, 2 – Instituto Motori

Objectives

Experimental study of diesel spray combustion at high-pressure and high-temperature using high-speed visualization: ignition delay, lift-off length, and ignition location

Investigation of important parameters to affect spray such as injection pressure, nozzle geometry, fuel properties

Provision of CFD validation data to model spray combustion

Summary and Conclusions

High-speed (40,000 fps) hybrid Schlieren/Mie Scattering imaging system is able to quantitatively characterize diesel spray combustion: Penetration, Ignition Delay & Location, Lift-off

In non-evaporating conditions Mie-scattering and schlieren techniques are equivalent to determine the tip penetrations

In the vaporization, a short plume of liquid stays with relatively constant length. Vaporization of the fuel keeps penetrating into the ambient gases beyond the liquid plume

Higher injection pressure reduces ignition delay and liquid penetration length under diesel combustion environment

Location of ignition is affected by momentum of injected fuel

H. Kawanabe: LES Analysis of Mixture Formation and Combustion Processes in a Diesel Spray

Background and Objectives

Diesel Combustion

Precise in-cylinder combustion control is required. Thermal efficiency Exhaust emissions High Pres. Inj, High EGR, LTC etc.

The basis of combustion control is optimization of mixture formation. Mixture formation by unsteady fluid motion Detailed process of ignition and combustion

Numerical calculation based on LES is applied Mixture formation process and flame structure are investigated

Summary

The ignition and combustion processes, especially heat release processes in the sprays were discussed using the flame index FI.

Heat release in the former part of the combustion occurs by the ignition of premixture. Then, in the latter part of the combustion, heat release from premixture is observed on the boundary of unburnt gas in the upstream region and burnt gas in the downstream region, and diffusion flame is formed in the surrounding region of spray in downstream.

In the latter part of combustion, heat release by combustion of premixture decreases, while that by diffusion flame increases with time. For the 2 MPa ambient pressure case, heat release by combustion of premixture is dominant, and for the 4 MPa ambient pressure, heat release mainly occurs from diffusion flame.
<u>Christopher Powell, Daniel Duke, Nicholas Sovis, Andrew Swantek,</u> <u>Zak Tilocco (CTR)</u> <u>Alan Kastengren, Yuan Gao, Su Han Park, Jin Wang (APS), Argonne</u> National Laboratory: X-Ray Diagnostics of Fuel Injection and Sprays

Spray Diagnostics Developed at Argonne

- Phase Contrast Imaging
 - Penetration through steel
 - High-speed, single-shot images
 - Nozzles, injectors, sprays
- Radiography
 - Absorption of x-rays by the fuel
 - Ensemble averaged
 - Quantitative measure of fuel distribution





Experimental Method - Radiography

- Uses focused beam, raster scan
- Gives a quantitative, timedependent map of the fuel distribution
- Good spatial resolution (5 x 5 μm)
- Good time resolution (4 μs)
- Ensemble averaged, cannot see shot-shot variation
- High pressure, but room temperature



Studies of Spray-Spray Interactions Collaboration with Monash Univ, Australia Measurements of group-hole diesel nozzles

- 3 injectors with different angles between the
- nozzle holesSignificant dynamics, overlap between the sprays
- Monash is using data for CFD validation



Studies of GDI Sprays

Goals is to map the fuel distributions from two different spray patterns, use for validation of spray and engine simulations



Future Work

- Measurements in collaboration with the Engine Combustion Network
 - Diesel injection
 - Gasoline injection
- Cavitation and injector flow
 - Collaboration with Sandia
 - Steel nozzles visualization of cavitation regions
 - Plastic nozzles quantitative measurements of fluid density
 - Combine with high speed imaging and high fidelity simulations of internal flow
- Studies of natural gas injection
 - Measurements of gas jet density
 - Validation of gas mixing, combustion, and engine simulations

<u>Keiya Nishida University of Hiroshima:</u> Effect of Temporally-Splitting of Fuel Injection on Mixture Formation and Combustion of Diesel Spray



Effect of Temporally Splitting



Conclusions

Ambient Gas Entrainment

- 1. In the single injection, as the injection amount is decreased, the ambient gas entrained into the spray (per fuel Ma/Mf) is increased.
- 2. The ambient gas entrained into the spray under the split injection with higher injection pressure is increased compared with the single injection.

Flame Characteristics

3. The split injection with higher injection pressure decreases the flame temperature and soot formation (KL).

The following factors in the split injection supposedely contribute:

- Decrease in the droplet size due to higher Pinj
- Increase in the ambient gas entrainment due to higher Pinj
- Increase in the ambient gas entrainment due to smaller injection amount in each injection stage

Annex 4 – Low Temperature Combustion

The intent of this IEA task is to look into the interaction between HCCI and fuels. It will inckude activities for both the gasoline and diesel type of fuels and HCCI with fully premixed charge and direct injection. In the latter case a gradual stratification will result with later and later fuel injection.

The following activities were undertaken within the Low Temperature Combustion Task during the past year

John Dec, Yi Yang, Chunsheng Ji, and Jeremie Dernotte, Sandia: Progress on Gasoline Compression Ignition Combustion

<u>Y. Moriyoshi, T. Kuboyama, T. Yamada, Chiba University:</u> Possibility of Practical Usage of Gasoline HCCI as an Automotive Powertrain by Using Boosting and Combustion Switching

<u>Scott Curran</u>, <u>Vitaly Prikhodko</u>, <u>Jim Parks and Robert Wagner</u>: Recent Advances in Multi-Cylinder Advanced Combustion on Light-Duty Compression Ignition Engines

<u>Shi-Jin Shuai, Tsinghua University</u>: Multiple Premixed Compression Ignition (MPC!) for Low Octane Gasoline Engines

<u>Martti Larmi, Aalto Uiversity:</u> PPC Diesel Combustion at Low Load Conditions in Marine Engines

Hongming Xu. University of Birmingham: Fuelling Strategy for Dieseline Engines

Bengt Johansson, Lund University: Partially Premixed Combustion, PPC – The Benefit of Ethanol for Close to Stoichiometric Operation

Highlights from the work included the following:

John Dec, Yi Yang, Chunsheng Ji, and Jeremie Dernotte, Sandia: Progress on Gasoline Compression Ignition Combustion

Motivation

- Global demand for transportation fuels is increasing and CO2 emissions from transportation is a major source of GHG.
- Strong motivation to reduce petroleum consumption.
 -- Engine-efficiency improvements are central to achieving this.
- Critical that both gasoline & diesel fractions of crude oil be used efficiently. – Current diesel engines are very efficient, but gasoline engines are not.
- Low-temperature gasoline combustion (LTGC) has the potential to provide high efficiencies with very low NOx and PM emissions at a reasonable cost.
- LTGC includes:
 - HCCI Þ most well-known form of LTGC
 - Stratified and partially stratified variants of HCCI
 - Spark-assisted HCCI
 - Fueled by gasoline or alternative fuels with volatility and autoignition characteristics in the range of gasoline (e.g. ethanol or gasoline/ethanoblends)

Scope and Objectives

- Recent results have shown that boosted LTGC can achieve high loads with acceptable combustion noise and ultra-low NOx and PM.
 - Suggests the potential for engines operating full time with LTGC.
- Further increases the high-load capabilities of LTGC and in thermal efficiency are needed to make LTGC more viable in the marketplace.
- To this end, our recent work has focused on three factors that can impact
 - LTGC-engine performance: 1) fuel reactivity, 2) fueling strategy, and 3) CR.
- Determine how these three factors can improve boosted LTGC-engine performance, in terms of stability, efficiency, and high-load capability.

Fuel reactivity: Increase the anti-knock index (AKI) of gasoline by

- > Varying the ethanol content: E0, E10, E20 Þ also include E100.
- > Increasing the AKI of the base fuel with no ethanol.

Fueling Strategy: Investigate the potential of Partial Fuel Stratification (PFS) using "std. PFS" and "Early-DI PFS" vs. premixed fueling.

Compression Ratio (CR): Increase the CR from 14:1 to 16:1.

Summary and Conclusions

Ethanol content has almost no effect on gasoline autoignition for naturally aspirated operation, but a large effect for boosted operation.

- For boosted operation with Pin ≥ 2.4 bar, blending with ethanol up to 20% has little effect on the T-E. ▷ Efficiencies lower with E100.
- Ethanol blending up to E20 is beneficial for extending the high-load limit.

Increased max. load from 16.3 bar IMEPg for E0 to 20.0 IMEPg bar for E20.

• CF-E0 performance generally similar to E10, despite its higher AKI.

Gives higher T-E for PM fueling Þ more advanced CA50 for same PRR.

• PFS fueling provides increased T-E and load with good stability for E0, E10 and CF-E0. Did not work well for E20 Þ low ITHR and f-sensitivity.

Early-DI PFS combined with reduced Tin provides the highest T-E.

- Increasing the CR from 14:1 to 16:1 increases T-E by ~1 T-E %-unit
- Achieved peak T-E of 50% with CR 16, using Early-DI PFS & new injector.

Fueling with new GDI injector gave good combustion performance at a lower load allowing a more advanced CA50 for higher T-E. Suggests that further gains can be made by optimizing the fuel stratification

Y. Moriyoshi, T. Kuboyama, T. Yamada, Chiba University: Possibility of Practical Usage of Gasoline HCCI as an Automotive Powertrain by Using Boosting and Combustion Switching



Issues for Combustion Switching

- For the acceptable HCCI combustion

Large A/F and G/F are required.

- For the stable SI combustion

Low EGR rate and stoichiometric A/F are required.



G/F: Mass ratio between total incylinder gas (G) to fuel (F) A **large gap** between the mixture condition for the HCCI combustion and that for the SI combustion

One-step cycle transition in mixture condition between HCCI range and SI range is necessary to achieve the combustion mode switching with small torque fluctuation and low exhaust gas emissions.

Objectives

- To find a control strategy for the one-step cycle switching between HCCI combustion and SI combustion with a low torque fluctuation and low exhaust gas emissions.
- To examine the effect of external boosting on the high load limit of HCCI with the BDSC system and HCCI combustion characteristics.

Summary

6

Brake thermal efficiency of blowdown supercharged HCCI achieved 39% at 510 kPa in BEMP with compression ratio of 14 at 1500 rpm using a low friction base engine.

Combustion switching in one-step cycle between HCCI and SI was successfully demonstrated using blowdown supercharged HCCI under a constant engine speed and IMEP.

The maximum load is increased with increasing the intake pressure with a lysholm compressor. The highest load is 935kPa in IMEPg with 200 kPa in intake pressure at 1500 rpm.

The maximum load of the boosted BDSC-HCCI engine can be achieved comparable to the full load of naturally aspirated SI engine. The efficiency of boosted HCCI operation is improved by more than 12% at the same load.

Blowdown supercharged HCCI can cover almost Japanese driving cycle points while an easy combustion switching method between HCCI and SI enables a practical usage. Turbocharged HCCI that can fully cover NA-SI load range is found another choice for a practical usage.

Scott Curran, Vitaly Prikhodko, Jim Parks and Robert Wagner: Recent Advances in Multi-Cylinder Advanced Combustion on Light-Duty Compression Ignition Engines



Study Motivation and Overview

Overview

- Apples to apples comparison of **PPC and RCCI** on the same engine platform with the same hardware
- ORNL Light-Duty Multi-Cylinder Advanced Combustion Cell
 - 1.9 L DI/PFI RCCI engine based on GM ZDTH engine
 - Modified open bowl RCCI pistons
- Efficiency & emissions comparison to RCCI and conventional combustion modes
 - Diesel, Stoich (λ =1) GDI, Dilute GDI (λ =1), Lean GDI (λ >1)
- Detailed HC speciation
 - Volatile and semi-volatiles, aldehydes
 - Unburned fuel, partially oxidized species etc...
- PM size distribution, morphology and composition
 - FSN correlation to PPC PM?
- DOC effectiveness

ica AK

International Energy Agency 35th Task Leaders Meeting on Energy Conservation and







Next Steps

 Apples to Apples comparison with RCCI with same hardware

7

- Detailed HC Speciation and PM analysis
 - Multiple fuels
 - Multiple loads
 - Collaborate with PNNL on SPLAT
- PPC/ GCI Parameter Sweeps
 - Injection timing and number of pulses
 - Swirl
 - Boost
 - Intake Temp

AC

– EGR

International Energy Agency 35th Task Leaders Meeting on Energy Conservation and

- Cyclic Dispersion analysis
- Step changes mode switching



CAK RIDGE NATIONAL LABORATORY





MCE Advanced combustion shows potential for improving efficiency over conventional combustion modes along with reductions in engine out NOx and PM

Stock fueling system and modified pistons show remarkable flexibility in combustion regime operation allowing for direct comparison of LTC modes on similar production viable hardware

Initial results with PPC with explored injections strategies show slightly higher than diesel efficiency at 2000 RPM, 4.0bar BMEP with RCCI like NOx and Soot with elevated comb noise



<u>Shi-Jin Shuai, Tsinghua University</u>: Multiple Premixed Compression Ignition (MPC!) for Low Octane Gasoline Engines





- The proposed <u>Multiple Premixed Compression Ignition (MPCI)</u> combustion mode shows a control flexibility for mixture homogeneity and heat release, and can realize high efficiency and low NO and soot emission simultaneously.
- Low octane gasoline-like fuel has a high volatility and auto-ignition, and is a very good fuel for compression ignition (CI) engines like diesel engines.
- The engine test results show that the RON66 fuel has a higher efficiency (up to 13%) and lower NO (about 80%), soot (about 90%) and CO (about 90%) emissions than that of diesel fuel, but with a penalty of HC increase (about 88%).
- Further researches of MPCI are needed to cover a wide engine speed range.

Martti Larmi, Aalto Uiversity: PPC Diesel Combustion at Low Load Conditions in Marine Engines

Contents

- □ Partially Premixed Combustion (PPC)
- □ The Research Engine EVE
- □ Validation of the computational model
- Current injection system of EVE
- Combustion and Emission Analysis
- Conclusions



Partially Premixed Combustion

 A compression ignited combustion process in which part or all of the fuel is injected early

2

3

- Ignition delay is controlled to enhance better homogeneity or premixing of airfuel mixture.
- PPC intend to endow better combustion with low NOx and Soot emissions.

Problems with PPC

- Spray-Wall impingement
- Lubrication oil dilution resulting to the formation of unburnt HCs
- Ignition timing control

Objective of the study

To Investigate the possible conditions for a marine engine accompanying the PPC mode of combustion.



Conclusions

□ Difficult to maintain the condition accompanying the PPC with the conventional injection system.

□ Piston position and the start of injection is the crucial parameter in determining good fuel-air mixture prior to combustion.

□ Air fuel homogeneity is dependent on sweep of inclusion angle and increased injection pressure.

 $\hfill\square$ 140 Inclusion angle was figured out to be an optimal inclusion angle favoring the PPC mode of combustion in the EVE.

□ Piston bowl plays an essential role in determining good air-fuel mixture prior to combustion thus reducing soot emission.

□9 holes injectors showed the better results as compared to the 10 holes injectors due to the increased momentum of single spray of 9 holes than that of 10 holes.

16

17



Conclusions...



□ Standard piston top: with the injection optimization and implementation of EGR, NOx has been reduced by 44%, CO by 60%, and Soot by 67%.

□ Deeper piston bowl: the piston optimization resulted in more promising result, NOx has been reduced by 58%, CO by 55%, and Soot by 66%.



Hongming Xu. University of Birmingham: Fuelling Strategy for Dieseline Engines





Diesel and gasoline engine technologies are merging!

Source: DEER, Tim Johnson October 4, 2011

What is dieseline and why?



- Gasoline, which has high volatility but low self-ignitability, is generally produced as a high octane number fuel. It is associated with the main problem in the HCCI engine of over-rapid combustion rate at upper loads and misfire at low loads.
- Diesel fuel, on the other hand, has a high cetane number with larger carbon content and heavier molecular weight with low volatility, is better suited to auto-ignition but often requires a lower compression ratio than the conventional Diesel if the HCCI mode is adopted.



A mixture of Diesel and Gasoline (dieseline), mixed either online and off line, avoids any compromise and makes it possible to use the complimentary properties of the 2 different fuels.

Xu, 2006 IEA Task Leader Meeting





- Using stoichiometric mixture ratio (total λ) for the highest gasoline percentage, with diesel used to create multiple-point ignition to suppress knocking of gasoline combustion.
- EGR ratio is for the control of engine load

Advantages:

- > 1) high power density;
- > 2) significant reduction of pumping losses;
- 3) soot emissions will be lower than the diesel combustion over a wide operating window; 4) suitable for TWC aftertreatment irrespective of the strategy of injection or the intake temperature and pressure;
- 5) reduced knocking tendency and increased combustion robustness for higher fuel economy and lower emissions.

Conclusions

- 1. Using EGR instead of the throttle to control engine load allows the development of high power density engines using TWC for after-treatment. SDCI can achieve high indicated thermal efficiencies in a relatively wide load range (IMEP of 4.3 to 8.0 bar)
- 2. The gasoline percentage has an important impact on the combustion phase control. Using more diesel fuel may advance the combustion phase and provide a wider range of ignition timing control by means of adjusting the DI timing.
- 3. The PM emissions of SDCI combustion (accumulation mode) are lower by up to 90% in number than the conventional CI diesel combustion results. Higher gasoline percentages result in smaller particle numbers in the accumulation mode.
- 4. The effect of injection timing on Particulate emissions is more significant than fuelling ratios.

Bengt Johansson, Lund University: Partially Premixed Combustion, PPC –The Benefit of Ethanol for Close to Stoichiometric Operation

Outline

- Background
 - PPC
 - Previous results
- Close to stoichiometric operation of PPC
 - Fuel used
 - Efficiency
 - Combustion efficiency
 - Thermodynamic efficiency
 - Emissions
 - Conclusions





PPC and fuel efficiency

- How to get high efficiency
 - Dilution
 - Fast burn
 - Complete combustion



SAE paper 2010-01-1471



SAE International

2013-01-0277

Conclusions

- It is possible to operate PPC from lean conditions to close to stoichiometric conditions.
- Gross indicated efficiency decreased for all the fuels in close to stoichiometric operation:
 - Ethanol showed higher efficiency and less efficiency reduction than gasoline and diesel fuel.
- Pronounced soot emission increase for diesel and gasoline. Ethanol showed very low soot in all conditions.

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Ethanol - Clean Stoichiometric PPC (with TWC).



Annex 5 - Advanced Hydrogen Fueled Internal Combustion Engines (No longer active – related work can be found in Annex 9)

Annex 6 - Alternative Fuels

Sustainability and the environment are key issues of this Collaborative Task. The research is focused on new and sustainable fuels in combustion, especially on renewable fuels in gas engines, in spark ignition engines, in compression ignition engines and in advanced combustion systems such as HCCI or kinetically controlled combustion.

The improved performance of internal and external combustion devices and emission reduction are goals of the alternative fuel studies. The collaborative task has sub-projects on computational and experimental research. The aim is to increase the understanding of the combustion of alternative fuels and also to promote collaboration between experimental and computational research.

Both simulation and computational methods are essential parts of the collaborative task. In addition to its main focus on engine combustion, the task also links to furnace combustion, gas turbine combustion, general fuel chemistry, combustion properties and emission characteristics of new fuels.

The following activities were undertaken within the Alternative Fuels Task during the past year:

H. Salsing and I, Denbratt ,Volvo GTT/Chalmers: DME Combustion in Heavy Duty Diesel Engines

S. Shua, Tsinghua Universityi: Cleaning and Diversification of Automotive Fuels in China

T, Sarjovaara, J. Alantie and M. Larmi, Aalto University: Ethanol Dual-Fuel Combustion on Heavy Duty Engine

<u>G. Valentino, S. Merola, C. Tornatore, L. Marchitto, S. lannuzzi</u> <u>Istituto Motori CNR:</u> Optical Investigation of Post-injection Strategy Impact on the Fuel Vapor within the Exhaust Line of a Light Duty Diesel Engine Supplied with a Biodiesel Blend

H. Xu, University of Brmingham: Research into Furan Series Bio-fuels

C. <u>Park^{*}, S. Oh, Y. Lee, T. Kim, H. Kim, Choi, and K. Kang:</u> Effect of Inter-Injection Spark Ignition (ISI) Strategy in a Lean-burn LPG Direct Injection Engine

Highlights from the Task included the following:

H. Salsing and I, Denbratt ,Volvo GTT/Chalmers: DME Combustion in Heavy Duty Diesel Engines



Renewable fuels

- Operating range of heavy duty vehicles



Source: Volvo Technology Corporation, 2007

CHALMERS

Objectives

- Acquire understanding of the combustion of DME in Diesel engines
 - What are the challenges?
 - How can combustion be improved?
- Develop a DME combustion system based on this understanding with regard to regulated emissions and fuel consumption



DME and its use in a Diesel engine

- Properties of DME differs from Diesel fuel
 - High vapour pressure
 - O Handled as condensed gas, requires a different fuel system
 - Low viscosity, lubricity, surface tension and heating value
 - O Larger amounts of fuel injected at lower pressure
 - O Breakup length, atomization, spray angle
- Hardware therefore differs
 - Low injection pressure
 - O Penetration, air entrainment
 - Large diameter nozzle
 - O Penetration, air entrainment, spray angle

CHALMERS

The challenges

- Initial studies showed at low engine-out NO_x that the mixing controlled combustion was too slow/poor resulting in:
 - High emissions of CO
 - High fuel consumption
 - High exhaust temperatures
 - High peak cylinder pressures
- These issues need to be solved by optimizing the combustion system

Baseline

DME

adapted

pis to n

•

Updated Improved

Improvements:

F IE

Development Steps

High

pres s ure

CO, reduced by more than 90 %

Fuel consumption, lowered by more than 20 %

nozzle Iniection



Baseline

DME

adapted

pis to n

Updated Improved

FIE

Development Steps

High

pressure

nozzle Iniection

CHALMERS

Summary and Conclusions

- Combustion system design has as expected a major influence on combustion and emissions formation
- Using DME in a combustion system optimized for Diesel fuel is not suitable
- CO is the greatest challenge at low NO_x conditions (high EGR)
- Particles
 - Nucleation mode particles only
 - Can be reduced by:
 - Low ash oil
 - Optimized piston rings/liner system
- With an optimized combustion system NO_X aftertreatment systems and particulate filters should not be needed

S. Shua, Tsinghua Universityi: Cleaning and Diversification of **Automotive Fuels in China**

Challenges by Rapid Growth of Vehicle Production in China



- <u>Air pollution</u>: the air quality in one-fifth of the 333 prefecture level cities didn't reach the target in 2010 due to high PM2.5 in air (2013 "Beijing Cough").
- Energy security: the oil import dependency >58%(2012).
- Traffic accident: the death toll is 62,000 in 2011, occupying 75% of the total deaths. (US:42,000; Japan:4611)
- Traffic jam: two-third of rush hours was in traffic jam among 667 cities.
- No space for parking: Beijing has more than 5 million vehicles, and the parking space shortage is more than 2.35 million.







air pollution

energy security

traffic accident

traffic jam



- Double pressures from fuel supply increase and fuel quality improvement
 - Fast growth of gasoline and diesel fuel consumption, increased by 7.5% on an annual basis (2005-2011).
 - Newly built oil process capacity was over 15 million ton.
 - 20 billion RMB was invested in the production of gasoline fuel complying with Euro 3 standard in 3 years.
- Contradiction between oil deterioration and fuel cleaning
 - According to the BP report, the detected global oil reservation reached 1.383 trillion barrels up to 2010, but the high sulfur oil occupied about 70% with sulfur>1.5%.
- Contradiction of oil supply for fuels and chemical raw materials
 - The light oil (naphtha) demand for ethylene production reached 70 million ton per year with annual average increase of 20%.
 - $\ -$ The reformed gasoline also needed the naphtha to improve the octane number.
- Update of petroleum processing technology
 - Complex devices, extended process chain, large process loss and high cost.





Questionnaires on the fifth stage of gasoline and diesel national standards

Main modifications:

- Reduction of RON from 90/93/97 to 89/92/95
- Reduction of sulfur concentration from 50ppm to 10ppm
- Olefins fraction modified from <28% to <25%
- Reduction of maximum summer RVP
- Reduction of MMT in gasoline from 8mg/L to 2mg/L

Impact of Octane Number on Fuel Efficiency and Emissions of Gasoline Vehicles



- Higher octane fuel helps to achieve better fuel efficiency
 - The extent of improvement varies with adopted engine and vehicle technologies.
 - Higher octane fuel has greater energy saving potential for advanced engine.
 - Increase of 1-2 octane number will result in about 1% fuel economy improvement.





✓	Natural		Gas	
	•	clean	fuel	W

- clean fuel with regional rich supply and competitive price
- conventional NG production: 94.8 billion $\ensuremath{\mathtt{m}}^3\!,\!4\%$ for motor vehicle (2010)
- unconventional coal and shale gas production : 20.0 and 6.5 billion m³ in 2015
 ✓ Ethanol
 - renewable with enough supply (E10 can be available in 6 provinces, and partially available in 27 cities of 4 provinces)
 - bioethanol production: 1.84 million tons (2010)
- ✓ <u>Biodiesel</u>
 - renewable and can be made from waste cooking oil
 - biodiesel production capability: 500k tons (2010)

✓ Methanol

- can be made from coal (rich resource) with rich supply and competitive price
- methanol production capability- 26.27 million tons(2011)



• With the rapid growth of vehicle production in China, the demand for emissions and fuel consumption reduction is becoming stronger and stronger, leading to the cleaning, diversification and high-efficient utilization of automotive fuels.

• Desulfurization of gasoline and diesel fuels is the main requirement for meeting future stringent emissions standards in China but challenging the update of the oil refinery technologies.

• Natural gas, bio-ethanol and biodiesel are the most promising alternative fuels to be applied in China in terms of the technology mature and resource.

• Methanol is a controversial alternative fuel in China, but may be one of the feasible alternative fuels for vehicles due to its abundant coal resource and low cost.

Summary



• With the rapid growth of vehicle production in China, the demand for emissions and fuel consumption reduction is becoming stronger and stronger, leading to the cleaning, diversification and high-efficient utilization of automotive fuels.

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• Natural gas, bio-ethanol and biodiesel are the most promising alternative fuels to be applied in China in terms of the technology mature and resource.

• Methanol is a controversial alternative fuel in China, but may be one of the feasible alternative fuels for vehicles due to its abundant coal resource and low cost. T, Sarjovaara, J. Alantie and M. Larmi, Aalto University: Ethanol Dual-Fuel Combustion on Heavy Duty Engine

Background (1/2)

- Natural gas Dual-Fuel (DF) engines have long history
- · Lately increased intrest on on-road application
- Lean-burn Natural gas DF engines can have very low NO_{x} and Soot
- Diesel mode as a back-up
- Natural gas has drawbacks on energy density, storaging and distribution



Aalto University School of Engineering

Background (2/2)

- Ethanol, as a liquid, could offer benefits on energy density, storaging and distribution
- Existing distribution on some market → existing markets?
- Ethanol fumigation has been studied earlier
 - Max. Ethanol share 30-50%
 - Mostly pre common-rail age engines
- The aim was to study possibilities of common-rail injection system on ethanol DF to achieve high ethanol shares (well above 50%)



Conclusions (1/2)

- Having only one diesel injection/cycle the ethanol share was very limited – like in previous studies
- Multiple diesel injections allowed very high ethanol shares
 - At maximum 80% energy share was achived
- With multiple injections, the timing of diesel main injection seems to have most significant role
- Difference in HRR between 75% and 100% load
- Ethanol DF proved to be viable concept, if possibilities CR injection system are utilized



Conclusions (2/2)

- Lessons learned:
 - CR could have been higher
 - →Smoother cold running, smaller diesel injection << 30 mg/cycle
 - \rightarrow Better efficiency in both modes
 - \rightarrow Most likely will limit the max ethanol share at high loads
 - Tch has clear effect on knocking and misfiring
 - \rightarrow Constant Tch makes everything much easier

25

 \rightarrow Suitable Tch window gets narrower as load increases



Aalto University School of Engineering

Future Work

- A manuscript has been sent to Energy –journal and it is in review process
- Reseach work has been continued by emission study and further ethanol DF concept development and also the potential of E85 blend as DF fuel has been studied
 - Not with the same engine
 - Papers coming...
- <u>2014 aim is to utilize learning of ethanol DF to natural</u> <u>gas DF</u>



Aalto University School of Engineering
<u>G. Valentino, S. Merola, C. Tornatore, L. Marchitto, S. lannuzzi</u> <u>Istituto Motori CNR:</u> Optical Investigation of Post-injection Strategy Impact on the Fuel Vapor within the Exhaust Line of a Light Duty Diesel Engine Supplied with a Biodiesel Blend

Motivation

The current technology has shown the potential to use post injections, applied in conventional high temperature combustion conditions or with innovative combustion regimes, to produce additional unburned HC to increase the exhaust gas temperature and generate exhaust conditions useful for diesel after treatment. After-treatment systems, used to reduce particulate matters from diesel exhaust, are mainly

After-treatment systems, used to reduce particulate matters from diesel exhaust, are mainly based on the principle of filter regeneration with the production of high concentration of hydrocarbons at the exhaust, needed for diesel particulate trap (DPF) regeneration.

The ability to produce periodically exhaust conditions with high hydrocarbons concentration is associated to exhaust gas temperatures of about 600°C, to avoid that the conversion efficiency can dramatically drop as the temperature decreases below a critical value.

Additional required exhaust conditions include low NO*x* and PM levels to reduce the regeneration frequency and thus the additional energy requirements of the after-treatment devices.

Motivation

A major concern when using late post-injections is that the fuel can impinge on the cylinder wall leading to an engine lubrication oil dilution that results in a decrease in oil viscosity with the risk to damage mechanical parts.

When using commercial diesel fuel (B5), it may evaporate out of the engine oil, on the other hand, biodiesel components that show higher boiling temperatures may be absorbed on the oil film resulting in a permanent oil dilution that affects the wear of engine components.

This presentation will give results of an optical technique based on the UV-visible extinction spectroscopy, used to investigate the impact of a late post-injection strategy on the fuel vapor within the exhaust line of a diesel engine.

Tests were carried out supplying the engine with commercial diesel fuel (B5) and a blend of RME (30% by vol) with commercial diesel (B30) at two engine operating conditions:

2000rpm@5bar 2750rpm@12bar of BMEP

CONCLUSIONS

High temporal resolution optical technique based on the UV-visible extinction spectroscopy was applied to investigate the post-injection strategy impact on the fuel vapor within the exhaust of a diesel engine. The engine was fuelled with commercial diesel fuel (B5) and a blend of RME in diesel fuel (B30).

•The fuel vapor emission in the exhaust line, due to the regeneration strategy, was related to the engine working condition by applying an optical methodology that exhibited a high sensitivity to the regeneration injection strategy.

•Results of the optical investigation demonstrated that during the post-injection activation, the occurrence of a transition state induced the emission in the exhaust line of vapor followed by unburned hydrocarbons generation whose concentration is affected by the fuel composition and by the injection strategy.

•Time evolution to a steady condition was more critical for the blend B30 denoting a poorer tendency of biodiesel to interact with DOC. Further, the blend B30 exhibited a slower temperature raise compared to the neat diesel that may cause a delay in the initiation of the oxidation reaction of the trapped soot within DPF.

•The efficiency of late post-injections, in terms of temperature increase downstream DOC, is mainly related to the fast conversion of the fuel vapor to light hydrocarbons and it is strongly affected by the fuel composition.

H. Xu, University of Brmingham: Research into Furan Series Bio-fuels

Why DMF and MF are good?



DMF: Physical properties very close to gasoline, very high octane number (RON=119) and relatively low volatility; energy density higher by 60 per cent in volume and by 40% in mass over ethanol.

MF: Density (913.2 kg/m^3at 20°C) is higher than DMF (889.72 kg/m^3at 20°C) and its flash point (-22°C) is lower than DMF (16°C), which would also overcome the cold engine start problems usually associated with bio-ethanol. Its latent heat of vaporization (358.4kJ/kg) is higher than DMF (330.5kJ/kg).

Stable in storage and not soluble in water and therefore it cannot become contaminated by absorbing water from the atmosphere.

The most attractive advantage is that making DMF/ MF: They consume only one-third of the energy in the evaporation stage of its production, compared with that required to evaporate a solution of ethanol produced by fermentation for biofuel applications. Will not compete with land and food.



Breakthrough - new process of making DMF/MF



Nature 447 (7147): 982. doi:10.1038/nature05923, 2007

Current research topics



- Spray behaviour and combustion characteristics for DMF/MF and DMFgasoline blends by optical/laser-based diagnostic techniques.
- Two-phase flow spray models for DMF/MF-gasoline blends
- Chemical kinetics and develop combustion models for DMF/MF-gasoline blends
- Combustion and engine-out emission characteristics (especially of the nonconventional components) of DMF/MF-gasoline blends using GC-MS and FTIR
- Effect of engine design and operating strategies (including for the new combustion mode HCCI) when DMF and MF are used
- Impact of DMF/MF on engine hardware and environment including users, involving health and safety issues.

http://www.birmingham.ac.uk/research/activity/mechanical-engineering/vehicletechnology/future-power/DMF-engine-performance/index.aspx



Conclusions



- Although MF has a similar chemical structure to DMF, its combustion characteristics are notably different. MF has a much faster burning rate, which makes its CID and combustion duration the shortest among the four studied fuels at equivalent engine conditions.
- Similar to DMF, MF has greater knock suppression ability than gasoline.
- Due to the combined effect of significant knock suppression abilities, fast burning rate and high incylinder peak pressure, MF consistently produces higher net indicated efficiency than gasoline and DMF within the entire tested load range.

C. Park*, S. Oh, Y. Lee, T. Kim, H. Kim, Choi, and K. Kang: Effect







Lean-burn direct injection engines				
Conventional MPI	Stoichiometric GDI	Lean-burn GDI		
		1 st generation	2 nd generation	
 ✓ Port injection ✓ Stoichi. mixture ✓ TWC 	 ✓ Direct injection [side] → Knocking↓, Compression ratio↑, Power output↑, Fuel economy ~3% ✓ Stoichi. mixture ✓ TWC ✓ Mass production (SONA TA 2.4GDI, etc.) 	 ✓ Wall or air guided center injection ✓ Lean mixture ✓ 00'Lab. test (MISUBISHI, TOYOTA) 	 ✓ Spray guided injection → Fuel economy ~10% ✓ Lean mixture ✓ '07 BMW, Benz mass production → Cost & emission control s trategies 	
	Intake Valve	Straight Port		





Annex 7 - Nanoparticle Diagnostics

The following activity as undertaken by the Nanoparticles Diagnostics Task during the past year:

M. Ditaranto, C. Meraner, N.E.L. Haugen, and I. Saanum SINTEF: Effects of Fluence and Irradiance on LII Signal Using A variable Pulse Duration Laser

Highlights from the Task included the following:

Introduction

- Laser Induced Incandescence of soot:
- LII is a common technique to measure in-flame soot
- Locally and instantaneously measures soot in flames
- Not self-calibrating
- Single shot capability
- Soot vol fraction by integrating LII
 - Particle sizing by temp resol LII

Pertinent technique for use in both laboratory and industrial turbulent flames

Processes on the soot particle during LII:

- Absorption
- Conduction to surrounding gas
- Radiation
- Loss of mass by vaporization
- Internal energy rise
 - Annealing, oxidation

LII signal is the black body radiation from incandescent soot

Motivation

Practices in LII in terms of pulse duration:

- Use of Nd:YAG laser: 7-10 ns pulse
- Some ps pulse to study PAH at the very beginning of LII signal
- Tentative use of CW laser

Pulse duration is directly related to the absorption of heat at the soot surface and therefore interact with all other processes

The present work aims at filling the gap in terms of pulse durations 50ns - $1\mu m$

Summary

• Time resolved LII measurements showed an unexpected behaviour for pulses of approximately 100 ns and longer in the form of a secondary peak

• The phenomenon is seen to be only dependent on the time scale of the excitation and not on the energy absorbed.

• Although not validated yet, privileged hypothesis is formation of new particles

• Further work will focus on identifying the physical process responsible for that unexpected LII signal rebound and improve the predictive models used

• Measurement of soot volume fraction by LII is not impaired by the use of long pulse durations

• LII can be applied with a broad variety of laser,

• Interesting from the perspective of deploying LII as a monitoring method

Annex – 8 Hydrogen Enriched Lean Premixed Combustion for Ultra-Low Emission Gas Turbine Combustors

The objective of the Gas Turbine task is the generation of a data base for combustion properties of hydrogen-rich fuel gases and of hydrocarbon fuels burned in a $O_2/CO_2/H_2O$ atmosphere. Most important conditions to be met are elevated pressure conditions (up to 30bar) relevant for gas turbine operation. The operational envelope studied should also provide information on the flame stability characteristics of such gas turbine combustion systems being operated with quickly changing boundary conditions (pressure, air temperature, flow rates) representative for strong load gradients.

Following up on the previous collaborative efforts on "Hydrogen enriched Lean Premixed Combustion for Ultra-Low Emission Gas Turbine Combustors" the current collaborative task activities on gas turbine combustion issues should be linked to respective Zero Emission Power Plant concepts.

Fast response characteristics and large load gradients need to be additionally dealt with by gas turbine based power plants as such controllable power generation systems will be required to compensate fluctuating electricity production from renewable energy resources (wind, solar).

The following activities were undertaken within the Hydrogen Enriched Lean Premixed Combustion for Ultra-Low Emission Gas Turbine Combustors Task during the past year:

<u>Robert Barlow, Sandia:</u> Report from the TNF Workshop: Recent Progress on Stratified Combustion

<u>Tim Lieuwen, Georgia Institute of Technology:</u> Turbulent Burning Velocity Characteristics of High H₂ Fuels

<u>Yu-Chun Lin, S. Daniele, P. Jansohn, K. Boulouch, Paul Scherer Institute, Switzerland:</u> Turbulent Flame Speed as An Indicator for Flashback Propensity of Hydrogen-Rich Fuel Gases

R. Szasz¹, A. Lantz², E. Gutmark³, L. Fuchs¹, S.-I. Möller² 1 - Energy Sciences, Lund University, Sweden 2 - Combustion Physics, Lund University, Sweden 3 - University of <u>Cincinnati, USA:</u> Flashback Hysteresis in a Model Gas Turbine Combustor Highlights from the Task included the following:

Robert Barlow, Sandia: Report from the TNF Workshop: Recent Progress on Stratified Combustion









COMBUSTION RESEARCH FACILITY





COMBUSTION RESEARCH FACILITY

<u>Tim Lieuwen, Georgia Institute of Technology:</u> Turbulent Burning Velocity Characteristics of High H₂ Fuels



 Operational flexibility has been substantially crimped in low NO_X technologies because of high CO emissions at part load

28.5

29

Time (Days)

29.5

30

30.5

28

27.5

27

 Significant number of combined cycle plants being cycled on and off daily
 Georgia Tech

Transient Response Needs



- Locations with high penetration of wind and photovoltaic solar are seeing significant transient response needs
- Avoiding blowoff and flashback are key issues



Blowoff

 Low NO_X designs make flame stabilization more problematic





Motivation for Turbulent Flame Speed Study

Improve understanding of turbulent flame propagation characteristics of high hydrogen content fuels

Issues:

- Turbulent burning characteristics of thermo-diffusively unstable mixtures not well understood
- *S_T* is a key combustion parameter that impacts the performance of low emissions combustion systems
 Blow-off
 - Blow-on
 Flashback
 - Combustion instabilities
 - Emissions

Objective

Obtain turbulent flame speed data of HHC fuel blends at gas turbine realistic conditions and over a range of conditions:

- Pressure
- Fuel composition
- Turbulence intensities
- Equivalence ratio
- Turbulence length scale

Develop physics-based models to describe turbulent flame propagation



⁸ Georgia Tech

High Pressure Burner Facility

Pressure vessel

- Tested to 20 atm
- Optical access for diagnostics
- Cold and pre-heated flow
- Fully remotely operable



Design of Experiments

Constant $S_{L,0}$

- H_2/CO ratio and ϕ adjusted to maintain same $S_{L,0} = 34$ cm/s
- 12 and 20 mm burner
- 1, 5 and 10 atm
- $H_2/CO = 30/70 90/10$

Constant H₂/CO

- H_2/CO ratio held fixed while ϕ is varied
- 20 mm burner
- 1 20 atm
- $H_2/CO = 30/70 70/30$
- $\phi = 0.32 0.8$



Summary

Turbulent flame speed has strong, coupled fuel and pressure effects

- Manifestation of more fundamental sensitivity of flames to high stretch rates
- Pressure introduces additional length and time scale sensitivities, causing augmentation of turbulent flame speed with pressure for negative Markstein length mixtures



Yu-Chun Lin, S. Daniele, P. Jansohn, K. Boulouch, Paul Scherer Institute, Switzerland: Turbulent Flame Speed as An Indicator for Flashback Propensity of Hydrogen-Rich Fuel Gases









Mechanisms of Flashback*

- 1. Core flow flashback
- 2. Combustion induced vortex breakdown (CIVB)
- 3. Combustion instability induced flashback
- 4. Boundary layer flashback (BLF)

*Lieuwen, T., McDonell, V., Santavicca, D., and Sattelmayer, T., 2008, "Burner Development and Operability Issues Associated with Steady Flowing Syngas Fired Combustors," Combustion Science and Technology, **180**, pp. 1169-1192.

IEA Combustion Agreement, Task Leaders Meeting, July 21-25, 2013, San Francisco, CA, USA

PAUL SCHERRER INSTITUT

Laminar: $\mathbf{g}_{\mathbf{f}} = \partial u / \partial y = 8 \cdot \mathbf{u}_0 \cdot \mathbf{d}^{-1}$ $\mathbf{g}_{\mathbf{c}} = 3 \cdot \mathbf{S}_{\mathrm{L0}}^2 / (2 \cdot \mathbf{b}^{0.5} \cdot \alpha)$

Turbulent: $g_f = 0.03955 \cdot u_0^{1.75} \cdot v^{-0.75} \cdot d^{-0.25}$ $g_c = ?$



Summary (1/2)

- Compared to syngas mixtures, flashback occurs at even leaner conditions for H₂-rich fuel gases. A significantly reduced operational envelope is observed at elevated pressure (since the lean blow out limits are relatively independent of pressure).
- Flashback in the turbulent boundary layer occurs when the velocity gradient of the flame (g_c) exceeds that established by the flow (g_f). It is proposed that g_c can be described based on S_T divided by the product Le × δ_{L0}. The flashback limit (Φ_{FB}) at the respective pressure level is estimated as the equivalence ratio at which the two velocity gradients match.

IEA Combustion Agreement, Task Leaders Meeting, July 21-25, 2013, San Francisco, CA, USA

FAUL SCHERRER INSTITUT Summary (2/2)

- The derived flashback limits show that the present approach provides reasonable estimations on the operational limits for both H₂-rich and syngas fuel gases. The reduced operational range at higher pressure and the reduced flashback propensity by decreasing the preheat temperature (T₀) are well reproduced.
- The different flashback propensities between the H₂-rich and syngas mixtures are found to be justified by neither the adiabatic flame temperature (T_{ad}) nor the unstretched laminar flame speed (S_{L0}). Instead, the turbulent flame speed is capable of correlating the observed difference.
- The proposed flashback criterion could be implemented to qualify various burner designs.

IEA Combustion Agreement, Task Leaders Meeting, July 21-25, 2013, San Francisco, CA, USA

R. Szasz¹, A. Lantz², E. Gutmark³, L. Fuchs¹, S.-I. Möller² 1 - Energy Sciences, Lund University, Sweden 2 - Combustion Physics, Lund University, Sweden 3 - University of Cincinnati, USA: Flashback Hysteresis in a Model Gas Turbine Combustor



Flashback Hysteresis in a Model Gas Turbine Combustor

R. Szasz¹, A. Lantz², E. Gutmark³, L. Fuchs¹, S.-I. Möller²
1) Energy Sciences, Lund University, Sweden
2) Combustion Physics, Lund University, Sweden
3) Aerospace Engineering, University of Cincinnati, OH, USA

IEA 35thTLM Combustion, San Francisco, CA, USA, 2013-07-22

Background/Motivation

- Fuel flexibility is an increasing demand from GT users
- Instability issues
- Triple Annular Research Swirler (TARS)
- High-speed chemiluminescence of flashback and blowout events
- Continuation of previous studies of flashback using simultaneous PIV/PLIF



Objectives

- Investigate flashback and blowout limits for various Reynolds numbers
- · Investigate existence of bifurcation or hysteresis
- The possibility to detect flashback using modal decomposition techniques is discussed



Lund University / Faculty of Engineering LTH / Combustion Physics / Sven-Inge Möller/ IEA-TLM 2013



Fuel (natural gas) is injected 295 mm upstream the burner nozzle.

Combustion chamber (diameter = 102 mm, length = 400 mm)

Mixing tube (diameter = 49.2 mm, length = 100 mm)

TARS burner nozzle





Experimental setup (contd)



High speed chemiluminescence recording: Phantom V7.1 Hamamatsu image intensifier Nikkor f/2.5 f=105 mm Sampling rate: 1 kHz (1200 samples, pre-trigger 1000 samples) 300 Hz, 2000 samples for statistics Exposure time 100 μs



Lund University / Faculty of Engineering LTH / Combustion Physics / Sven-Inge Möller/ IEA-TLM 2013

Operating conditions

Case	Re	φ
C1	4000	1.24
C2	4000	1.05
C3	2600	1.28
C4	4000	1.09
C5	2600	1.44
C6	2600	1.25
C7	2600	0.91



Conclusions

- Flashback and blowout events were studied using highspeed chemiluminescence recordings
- A first attempt to detect flashback using DMD was reported



Annex 9 – Gas Engines

The following activities were undertaken within the Gas Engines Task:

<u>E. Tomita and N. Kawahara, Okayama University:</u> Effect of Split Injection of Pilot Diesel Fuel in a Dual-Fuel Gas Engine – Expansion of PREMIER Combustion Region

<u>A. Diequez-Alonso and F. Behrendt, Technical University of Berlin:</u> Fixed-bed Updraft Gasification Coupled to Gas Engines: A Possibility for Biomass Utilization

<u>D. Greenhalgh, Glasgow Caledonian University</u>: Research on Dual Fueling and its Advantages for Gas Fueled Engines

<u>K. Keskinen, O. kairo, M. Nuutinen, V. Vuorinen, Z. Kunscj, and M. Larmi, Aalto</u> <u>University</u>: Computational Studies in Gas-Air Mixture Formation for Lean Burn Dual-Fuel Applications

<u>S. Schlatter, B. Schneider, Y. Wright, and K. Boulouchos LAV, ETH Zurich:</u> Comparison of Ignition Systems for Lean Burn Gas Engines in an Optically Accessible Rapid Compression Expansion Machine

<u>B. Johansson, Lund University:</u> Prechamber Spark Plugs – A Way to Extend Lean or EGR Limit in an HD SI Natural Gas Engine

C. Bae and J. Jeon: Effects of diesel pilot injection pressure on Hydrogen CI engine

Highlights from the Task included the following:

E. Tomita and N. Kawahara, Okayama University: Effect of Split Injection of Pilot Diesel Fuel in a Dual-Fuel Gas Engine – Expansion of PREMIER Combustion Region

> IEA/TLM 2013 San Francisco July 23, 2013

> > Gas engine

Effect of Split Injection of Pilot Diesel Fuel in a Dual-Fuel Gas Engine – Expansion of PREMIER Combustion Region

Okayama University



Eiji TOMITA Nobuyuki KAWAHARA

Heat Power Engineering Lab.

Gas engine

Ignition

- Spark-ignition, Laser ignition?
- Pilot injection of liquid fuel (diesel fuel, gas oil)
- HCCI, PCCI
- Fuel supply
 - Intake port
 - Direct injection

Fuel

- Natural gas
- Biogas (Wood tips, , Producer gas)

Methane fermentation (Landfill gas, Food scraps, Sludge,

Sewage digester)

- Other gases

Usage

- Power generation (constant speed)

Car (haavv duty car haccondor car)



Pressure history in a natural gas engine ignited with diesel fuel

Lean burn gas engine ignited with diesel fuel

Features

- Higher thermal efficiency
- Lower HC
- Relatively higher NOx



Motivation of this study



PREMIER (Premixed Mixture Ignition in the End-gas Region) combustion in a natural gas dualfuel engine: Operating range and exhaust emissions, International Journal of Engine Research, Vol.12, (2011), 484-497. Effect of split injection on thermal efficiency and exhaust emissions (HC, CO and NOx) to expand the range of PREMIER combustion

under condition of no smoke

> Visualization of ignition process from bottom view

Effect of injection pressure on ignition and combustion

(P_{ini}=40 and 80 MPa)

Contents in this study

- In double injection, the operating range of PREMIER combustion is expanded by optimizing the second injection timing of diesel fuel (gas oil).
- In single injection, knock occurred. However, after the fuel spray of the first injection is ignited, the fuel spray of second injection make the combustion mild and PREMIER combustion was achieved.
- In single injection, normal combustion occurred. However, before the fuel spray of the first injection, the fuel spray of the second injection make the combustion active and PREMIER combustion was achieved.
- In double injection, the injection pressure is increased, HC and CO emissions are decreased with the same thermal efficiency.

Summary

A, Diequez-Alonso and F. Behrendt, Technical University of Berlin: Fixed-bed Updraft Gasification Coupled to Gas Engines: A Possibility for Biomass Utilization



Fixed-bed updraft gasification coupled to gas engines, a possibility for decentralized biomass utilization

A. Dieguez-Alonso, F. Behrendt Institute of Energy Engineering Technische Universität Berlin

2013 IEA 35th Task Leaders Meeting

Introduction



- Environmental protection policies require a drastic decrease of greenhouse gas emissions in the coming years, among which CO₂ is one of the main gases in terms of emission rate.
- Biomass is increasing in significance among the different renewable technologies due to the multiple applications that its conversion may have: chemicals, heat, power.
- Biomass gasification offers the possibility of producing a gas fuel adequate for fossil fuels substitution.
- Due to the fracking technology, allowing the production of a cheap natural gas, the economical viability of biomass gasification is in question. However natural gas will have an end.

Fixed-bed updraft gasification coupled to gas engines, ... | A. Dieguez-Alonso et al. | 2013 IEA 35th Task Leader Meeting Page 3



FVUR

Introduction

- Fixed-bed thermochemical conversion processes, such as gasification, may be a promising alternative for decentralized biomass energetic utilization and waste treatment.
- The gas product can be used for the production of synthetic natural gas, synthetic petroleum or other chemicals, as well as for heat and power generation, being combusted in boilers (heat), turbines and **engines** (heat and power).
- In this study the approach in consideration is a **gas engine** (heat and power), due mainly to:
 - Better performance at partial load
 - Higher efficiency for low power
 - · Lower requirements in gas cleaning
 - · Easier operation

in comparison with turbines

Fixed-bed updraft gasification coupled to gas engines, ... | A. Dieguez-Alonso et al. | 2013 IEA 35th Task Leaders Meeting Page 4




Introduction

Gas quality requirements for application in gas engines

- Tar content (including aerosol formation)
- · Particle matter content and particle size
- · Low heating value of the air/gas mixture
- Methane number
- · Laminar flame speed

Fixed-bed updraft gasification coupled to gas engines, ... | A. Dieguez-Alonso et al. | 2013 IEA 35th Task Leaders Meeting **EVUR**



Technisch Universitä Berlin

Objectives

What needs to be achieved?

	Reactor outlet		Gas engine inlet	
Tar	<u>Updraft</u> : 30 - 150 g/Nm ³ <u>Downdraft</u> : 0.1 g/Nm ³ <u>Fluidized</u> : 10 g/Nm ³ <u>Entrained</u> : negligible	\longrightarrow	~ 0.025 – 0.050 g/Nm³	
РМ	<u>Updraft</u> : Low <u>Downdraf</u> t: Low <u>Fluidized</u> : High <u>Entrained</u> : High		~ 0.025 g/Nm³	
Alkali metals Sulphur (H₂S) Ammonia			Limited by catalysts ' poisoning and emissions ' regulations	

Fixed-bed updraft gasification coupled to gas engines, ... | A. Dieguez-Alonso et al. | 2013 IEA 35^{h} Task Leaders Meeting Page 9



Objectives

How to achieve these quality requirements?

Cold gas cleaning

- Mature technology, proven reliability, simplicity
- High efficiency
- Combines PM, tar, other contaminants removal
- Efficiency of the plant \downarrow
- Waste streams $\uparrow \rightarrow \text{costs} \uparrow$



Wet scrubbing

Hot gas cleaning

• Increasing interest in recent years

Technische

Universität Berlin

- Waste streams $\downarrow \rightarrow \text{costs} \downarrow$
- Efficiency ↑, increase LHV of gas through tar conversion



UR

FV

Fixed-bed updraft gasification coupled to gas engines, ... | A. Dieguez-Alonso et al. | 2013 IEA 35th Task Leaders Meeting Page 10

Objectives of the study



"One of the **main technical hurdles** with the commercialisation of advanced biomass gasification syngas and energy production is to **meet the required gas quality**, in particular **tar** content/concentration and/or its composition."

" For the operation of gasification plants easy accesible values are needed without expensive machines that need highly skilled analysts. (...) **There is an unfilled demand for a continuous operating** tar-measurement or **tar-sensor** or a continuously measuring device which gives information about tar [1]".



→ An on-line, non-intrusive system, based on Laser Induced-Fluorescence, is proposed as tar-measurement device / tar sensor, applied in updraft gasification.

[1] Handbook Biomass Gasification, Second Edition. Edited by H.A.M. Knoef, 2012. Fixed-bed updraft gasification coupled to gas engines, ... | A. Dieguez-Alonso et al. | 2013 IEA 35th Task Leaders Meeting Page 11



Summary I



- Coupling of gasification with gas engines is a good approach for decentralized heat and power production: simplicity ↑, costs ↓, efficiency ↑, in comparison with turbines
- Control of the gas composition is required to meet the requirements in the gas engine.
- Updraft gasification is the easiest technology to control, admits the widest range of feedstock and presents higher efficiency for powers up to 10 MW_{th}. However it produces high tar quantity.
- An on-line tar-sensor is required to monitor the tar evolution. This is required for control of the process and to ensure the efficiency of the cleaning system.

Fixed-bed updraft gasification coupled to gas engines, ... | A. Dieguez-Alonso et al. | 2013 IEA 35th Task Leaders Meeting **EVUR**



Summary II

- An on-line, non-intrusive tar measurement device, based on Laser-Induced Fluorescence, has been developed and applied to tar characterization in updraft gasification
 - · On-line qualitative tar composition can be determined
 - Temporal evolution of the tar behavior during the process can be characterized.
 - Quantitative measurements with pure species have been done, showing a very high sensitivity (below 100 mg/Nm³)
- Further studies on on-line quantitative characterization have to be performed.

Fixed-bed updraft gasification coupled to gas engines, ... | A. Dieguez-Alonso et al. | 2013 IEA 35th Task Leaders Meeting **EVUR**

D. Greenhalgh, Glasgow Caledonian University: Research on Dual Fueling and its Advantages for Gas Fueled Engines



Research on Dual Fueling and its Advantages for Gas Fueled Engines

Presentation IEA TLM San Francisco 23rd July 2013

Doug Greenhalgh





Motivations

- It is now extremely obvious that new gas mining and recovery technologies (e.g. fracking) are transforming the availability worldwide of NG.
- IEA now predicts a new "Golden Age of Gas".
- It makes sense to utilise gas for transportation; this implies mainly land and marine – using compressed or liquefied NG for aircraft is much less likely for safety reasons.
- Many organisations are the looking at co-generation or combined heat and power technologies CHP [not to be confused with the California Highway Patrol]..
- We (GCU) installing installed a highly instrumented CHP gas fired system.
- We are also being offered access to a Marine Ship Engine (likely diesel) which we would like to configure to run in a dual-fuel format using NG.



Our Intended Research

Glasgow Caledonian University

lasgow Caledonian

> We have four (sub) projects which we will target.

- Using an installed and instrumented gas fuelled CHP engine based system to identify its real energy efficiency and to obtain real cost and CO₂ benefits.
- Seeking methods to reduce HC emissions from gas engines which may or may not be dual-fuelled.
- 4) Investigating particulate and soot precursor emissions from these engines

iea Large Dual-Fuelled Engines This is already a large scale international activity, we in this IEA IA needs to target carefully where we can impact.

PROJECT IMPACT



DUAL-FUEL ENGINES – WÄRTSILÄ 20DF, Wärtsilä 34DF and Wärtsilä 50DF

reference of the second second

IDF AND WARTSLEA SOOF, setto see hom MD to HFO and vic without power hom ND to HFO and vic without pow



E.S. Department of Energy
Energy Efficiency and Renewable: Energy
Energy Efficiency and Renewable: Levery
Energy Efficiency and Renewable: Levery

a part of the Next Generation Natural Gas ty, which is supported by the PCUT Program, at Air Quality Management Division, and the argy Commission. One goal of this activity dimende, commentally visible, and advance and dimensional commentation perspective O hanyy-being emission levels before 2007. O hany-being emission levels before 2007. A project was the domentation perspective and chaologies cophile of reduced schamat aministan to operating controls framery-data paratural gas

ISX G Natural Gas Engine

1,650 ft-lb peak torque
 450 hp rated power
 40% peak thermal efficiency
 0.5 g/bhp-hr NO₄ emissions
 0.1 g/bhp-hr NO₄ emissions

ENGINE AND VEHICLE RESEARCH & DEVELOPMENT

ROJECT GOALS

HeIG-HESSARE DIRECT-ALECTON SYSTEM project was led by DO: National Research Barger control (NEE2), Chaminas, Ear, and Watport Innovnet and State State (State State State State State and State State State State State State State and State State State State State State State Innovation (SPECIP) fairly other, is this project, and provide state State State State State State State Innovation (SPECIP) fairly other, is this project, and state and state State State State State State State State Innovation (SPECIP) fairly other This sublema is an approximate innovation (SPECIP) fairly other This sublema is a state state innovation (SPECIP) fairly other This sublema is a state innovation (SPECIP) fairly other than the state state innovation (SPECIP) fairly other than the state state is a state state of the state state state state state is a state is a state is a state sta

> GCU Glasgow Caledonian University

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HC Emissions from Dual-Fuel and Gas Engines

>HC emissions are dominated by unburnt gas trapped in the top piston crevice and first ring; this is why diesel engine HC emissions are low - the crevice is full of just air and not mixture.

>Options are:

- 1. Develop a HP Direct gas injection system for late injection – potential downside is lack of mixing time leading to enhanced NOx & particulates
- 2. Develop a method to purge the crevice.



Glasgow Caledonian University



Particulate Emissions from Dual-Fuel and Gas Engines

> There is strong evidence that gasoline particulate emissions are underestimated, NG engines will need to be lean burn!



FEVER: BC from Gasoline Vehicles is Underestimated



Conclusions

➢ The use of Gas in Dual Fuel engines presents an attractive option for a variety of large engine applications including land based (trucks, busses, plant) and marine based (ships, offshore generators etc.)

> Challenges remain in particular in ensuring that HC and especially CH_4 emissions are minimised.



K. Keskinen, O. kairo, M. Nuutinen, V. Vuorinen, Z. Kunscj, and M. Larmi, Aalto University: Computational Studies in Gas-Air Mixture Formation for Lean Burn Dual-Fuel Application



Computational Studies in Gas-Air Mixture Formation for Lean-Burn Dual-Fuel Applications

Karri Keskinen, Ossi Kaario, Mika Nuutinen, Ville Vuorinen, Zaira

Künsch* and Martti Larmi

Aalto University School of Engineering * ETH Zürich _____

Background (1/3): Today's Natural Gas-**Based Engines**

State of the art:

- Port gas injection
 - Spark ignition
 - Diesel spray ignition (Dual Fuel)
- Lean combustion, homogeneous mixtures

Why make research on new gas technologies?

- Growth •
- Ensuring competitiveness •



Wärtsilä 34SG spark-ignited gas engine (www.wartsila.com)



Wärtsilä 20DF dual-fuel marine engine (www.wartsila.com)



School of Engineering



Background (3/3): Challenges in Mixture Formation via Direct Injection of Natural Gas

- Part-load stratification
 - Mixture containment
- Local homogeneity
 - Mixing rate
 - Low momentum density of gas jets
 Tough Combination!
- Efficiency detriments from injection pressure
 - Low pressure \rightarrow timing constraints!



Research Objectives

Theoretical goals

- What are the potential mixing and containment mechanisms related to direct-injected gas jets?
- How can DI-NG mixture formation be feasibly and reliably simulated with various nozzle and combustion chamber configurations?

Practical goals

- How low can injection pressure be taken?
- What is required from injection equipment & control?
- What is required from combustion chamber geometry?



Study Plan

Stage / Timespan	Cylinder Geometry	Focuses	
1 / 2012-2013	Axisymmetric	Computational Methods Meshing Jet Mechanisms & Dynamics Optical Experiments Part Loads Stratified Mixtures	
2 / 2014-2015	Realistic Cylinder	Intake flow effects Injector Positioning & Orientation Engine Experiments Various Loads Stratified & Homogeneous Mixtures	



IEA TLM, San Francisco, CA 2/20/15

What We've Learned

- Sources of computational sensitivity
- Jet formation mechanisms
 - Particularly important (and sometimes unintuitive!) in complex jets
- Why Gas-DI mixture formation is challenging
 - "How not to do things"
- Promising mixture formation mechanisms
 - Importance of all in-cylinder flows, not just the jets



Future Objectives

Stage / Timespan	Cylinder Geometry	Focuses
1 / 2012-2013	Axisymmetric	Computational Methods Meshing Jet Mechanisms & Dynamics Optical Experiments Low Loads Stratified Mixtures
2 / 2014-2015	Realistic Cylinder	Intake flow effects Injector Positioning & Orientation Various Loads Stratified & Homogeneous Mixtures Engine Experiments



<u>S. Schlatter, B. Schneider, Y. Wright, and K. Boulouchos LAV, ETH</u> <u>Zurich:</u> Comparison of Ignition Systems for Lean Burn Gas Engines in an Optically Accessible Rapid Compression Expansion Machine

Background

Natural gas engines increasingly

popular due to: Abundant resources, low fuel price CH₄ high octane number -> high compression ratio -> high efficiency Substantial benefits w.r.t. particulate matter compared to Diesel CO₂ reduction compared to Diesel due to C/H ratio

Large bore engines: Used for power generation -> high reliability and TBO requirements Typically operated lean May use Miller valve timings and/or EGR to improve NOx

`adverse' conditions for initiating the combustion process

Motivation

Ignition in lean burn large bore engines can be challenging due to slow flame propagation (low reactivity of the lean mixture) and high ignition energy requirements

Different advanced ignition systems are applied which provide several benefits compared to conventional spark plug ignition such as high ignition energies and increased ignition «volumes»: Pilot injection (ignition of the methane/air mixture by means of autoignition of a directly injected «micro» Diesel pilot spray) Pre-chamber spark plug ignition (ignition in a

separate volume, generating flame jets entering the main combustion chamber)

Fundamental experimental data is sparse (most studies focus on engine performance investigations)

Conclusions

Increasing peak pressures with increasing amounts of methane in the system

For pilot injection, the ignition delays increase with increasing amounts of methane, decreasing temperature and pressure and the presence of EGR in the ambient mixture

Pilot injection with higher prail has more influence on the ignition delay for "hot" conditions where short ignition delays are observed where the atomization and evaporation processes contribute substantially to the ignition delay

Increasing methane equivalence ratios show a higher impact on the ignition delay for "cold" conditions than for higher temperatures and pressures, therefore suggesting that methane has an inhibiting effect on the low temperature reactions leading to high temperature ignition

The flame area evolution of the pre-chamber slows down considerably upon dissipation of the turbulence generated by the flame jets whereas the evolution of the combusting area with pilot ignition features a steadily steep slope even for very lean mixtures and low temperature and pressure conditions **B. Johansson, Lund University:** Prechamber Spark Plugs – A Way to Extend Lean or EGR Limit in an HD SI Natural Gas Engine

Prechamber Spark Plugs – A Way to Extend Lean or EGR Limit in an HD SI Natural Gas Engine

Bengt Johansson

Lund University

IEA Combustion Agreement Collaborative Task Leaders Meeting July 23, 2013, San Francisco



Outline

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- Background
 - Gas engine work in Lund
- Prechamber spark plug results
- Current prechamber work
- Future gas engine work



Gas engine project history

- 1990
 Flame propagation and turbulence (single-cylinder engine Volvo TD102)
- 1995 Combustion chamber effect on turbulence, combustion and emissions (single-cylinder engine Volvo TD102)
- 1997-2003
 Experiments on the multi-cylinder engine (6 cyl. Volvo TG103)
- 2006-2011 New Volvo 9.5 liter gas engine with lambda=1 and EGR
- 2012 Prechamber spark plugs
- 2013 Prechamber in Scania D13 engine geometry + Wärtsilä W34SG
- 2014-2017 Prechamber studies in Wärtsilä 20SG engine



Summary

- Been running gas engine research since 1990
- Mainly HD truck engine size range
- Topics:
 - Turbulence- flame speed interactions
 - Combustion chamber shape
 - Multi cylinder engine control
 - Cylinder balancing
 - Gas management (EGR, boosteyc.)
 - Dynamic control
 - Prechamber spark plugs
 - Fueled prechambers
- Recently also medium speed optical gas engine

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<u>C. Bae and J. Jeon:</u> Effects of diesel pilot injection pressure on Hydrogen Cl engine







	Fu	Fuel Properties at 25 ℃ and 1atm		
Properties	H2	CNG	Gasoline	
Research octane number	>120	140	91-99	
Flammability limits (Φ)	0.1-7.1	0.4-1.6	≈0.7-7	
Laminar flame velocity (m/s)	1.85	0.38	0.37-0.43	
Lower heating value (MJ/kg)	119.7	45.8	44.79	
Auto ignition temperature in air (K)	858	723	550	
Minimum ignition energy (mJ) ^b	0.02	0.28	0.24	
Stoichiometric volume fraction(%)	29.53	9.48	2(vapour)	
aLiquid at 0 ℃ bAt stoichiometry	Т	C.M. White, R.R. Steeper, A.E. Lutz The hydrogen-fueled internal combustion engine: a technical review International Journal of Hydrogen Energy 31 (2006) 1292-1305		

Motivation







Clean RCCI operation





With addition of diesel in hydrogen CI combustion, combustion occur s with two stages

• Diesel injection quantity

- First combustion stage increases with increasing of diesel injection quantity. Therefore, each stage is regarded as
- 1st stage : diesel premixed burn is dominant
- 2nd stage : hydrogen lean premixed combustion is dominant

• Diesel injection pressure

- As injection pressure is increased, IMEP is decreased because of decrease in combustion efficiency of hydrogen
- As injection quantity of diesel increased, dependence of diesel injection pres sure on hydrogen combustion efficiency increased
- From the exhaust emission results, higher IMEP with lower diesel injection p ressure comes from higher combustion efficiency of hydrogen

Annex 10 – Combustion Chemistry

The following activities were undertaken within the Combustion Chemistry Task:

V. Dias and H. Jeanmart, Catholic University of Louvain: Study of a Benzene Rich Premixed Flame in the Presence of Ethanol

W. J. Pitz, M. Mehl, and C. K. Westbrook, Lawrence Livermore National laboratory: Development of Chemical Kinetic Models for Surrogate Compounds and Surrogate Mixtures for Gasoline and Diesel Fuels

K. V. Puduppakkam, A. U. Modak, C. V. Naik and E. Meeks, Reaction Design: Prediction of Soot Particle Size Distributions and Fuel Effects in Flames

E. J.K. Nilsson, A. A. Konnov and Sven-Inge Moller, Lund University: Studies of premixed laminar flames of oxygenated fuels using the Heat Flux method

<u>T. Gerber. Paul Scherrer Institute:</u> Studies on Combustion Kinetics Based on Synchrotron VUV Spectroscopy

<u>D. Flowers, Lawrence Livermore National Laboratory:</u> Mulri-dimensional Engine Combustion Simulation using CFD and Detailed Chemical Kinetics for Complex Fuels

<u>A. Tezaki, University of Toyama:</u> Studies of premixed laminar flames of oxygenated fuels using the Heat Flux method

Highlights from the Task included the following:

V. Dias and H. Jeanmart, Catholic University of Louvain: Study of a Benzene Rich Premixed Flame in the Presence of Ethanol

Study of a Benzene Rich Premixed Flame in the Presence of Ethanol

Véronique Dias and Hervé Jeanmart Institute of Mechanics, Materials and Civil Engineering Université catholique de Louvain Belgium Veronique.Dias@uclouvain.be

Objectives

• The presence of oxygenated species in hydrocarbons combustion leads to

the reduction of soot and particulate matter.

• Ethanol is broadly used, either as a neat fuel, or blended with gasoline. It

can also be employed as an inhibitor of soot precursors formation.

Add ethanol in rich benzene flame to observe the effect of this oxygenated species.

Analyze and understand the kinetics of ethanol in the benzene combustion.

The UCL mechanism

• Validated against several flames

- CH4, C2H2, C2H4, C2H6, iC4H8, C6H6
 - → Understand the soot precursors formation
 - C3H8O2, C5H12O2, C2H5OH, CH3CHO, CH3COOH, CH2O
 - → Effect of oxygenated species on the soot precursors f ormation

→ Improvement and development of oxygenated species mechanisms

• Extended to heavier species up to pyrene (C₁₆H₁₀). It contains 183 chemical

species and 1015 reactions.

• Simulations are performed using the Cosilab software from SoftPredict and

an open source software (Cantera).

Conclusions

• The replacement of a fraction of C₆H₆ by a quantity of ethanol is responsible

for

- a decrease of the maximum mole fraction of the soot precursors

- an increase of the maximum mole fraction of the oxygenated species and

C₂H₄.

• The «UCL» model is extended to heavier hydrocarbons from naphthalene

(C10H8) up to pyrene (C16H10). It should be improved for some species,

especially C₂H₂ in the burnt gases.

• The present study preserves the equivalence ratio, and modifies the C/O

ratio: 0.80 in the FB flame and 0.77 in the FBE flame.

• The «UCL» model shows that the kinetics of ethanol does not act directly on

the formation of heavy hydrocarbons.

 \rightarrow We can conclude that this value of the C/O ratio is more important than

the nature of the additive itself for the hydrocarbons formation.

W. J. Pitz, M. Mehl, and C. K. Westbrook, Lawrence Livermore National laboratory: Development of Chemical Kinetic Models for Surrogate Compounds and Surrogate Mixtures for Gasoline and Diesel Fuels

Lawrence Livermore National Laboratory





35th Task Leaders Meeting of the International Energy Agency's Energy Conservation and Emissions Reduction in Combustion Implementing Agreement

LLNL-PRES-641082

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

Need fuel surrogate models for transportation fuels



Real diesel fuel requires the inclusion of many components in a fuel surrogate

AVFL-18 diesel surrogate palette¹ (9 components):



LLNL-PRES-641082

35th IEA Task Leaders Meeting





Chemical kinetic model development for practical fuels:

Fuel component and surrogate models validated by comparison to fundamental experimental data


Kinetic model development to represent aromatics: Comprehensive, well-validated base mechanism for aromatics



Extended model to represent higher molecular weight aromatics



LLNL-PRES-641082

Extension of the new aromatic basechemistry to alkylbenzenes, Collaboration with NUI-Galway





Extended model to represent higher molecular weight aromatics



LLNL-PRES-641082

Extension of the new aromatic basechemistry to alkylbenzenes, Collaboration with NUI-Galway





Rate constants for n-alkyl-benzenes developed based on analogy with n-alkenes



Developing surrogate for gasoline-ethanol mixtures: LLNL 4-component surrogate model for gasoline



Need to predict the formation of soot precursors



Mechanisms are available on LLNL website and by email



Summary

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K. V. Puduppakkam, A. U. Modak, C. V. Naik and E. Meeks, Reaction Design: Prediction of Soot Particle Size Distributions and Fuel Effects in Flames



The basis for a detailed soot model is a well validated Model Fuel Library

E	0			Fuel component	Gasoline	Diesel	Jet Fuel
Fuel component	Syngas	Natural gas		n-heptane	\checkmark	V	
Hydrogen	N			n-decane	\checkmark	\checkmark	\checkmark
00	N	1	Madal Eval	n-dodecane		\checkmark	\checkmark
Methane		N	wodel Fuel	n-hexadecane		\checkmark	
Ethane		N	Library	i-octane	\checkmark	\checkmark	\checkmark
Propane		N	aromatics	heptamethylnonane		\checkmark	\checkmark
n-Butane		N		Toluene	\checkmark	\checkmark	\checkmark
Iso-Butane		N	olefins	n-propylbenzene	\checkmark	\checkmark	\checkmark
Ethylene			c-paraffins	o-xylene	\checkmark	\checkmark	\checkmark
Acetylene				m-xylene	\checkmark	\checkmark	\checkmark
n-paramins				p-xylene	\checkmark	\checkmark	\checkmark
			naphthalene		\checkmark		
				1-methylnaphthalene	\checkmark	\checkmark	\checkmark
				Cyclohexane	V	\checkmark	\checkmark
Extensively validated				Methylcyclohexane	\checkmark	\checkmark	\checkmark
• Extensively valuated				Decalin	\checkmark	\checkmark	\checkmark
 Self-consistent kinetics 				1-pentene	\checkmark	\checkmark	
				2-pentene	\checkmark	\checkmark	
 Advanced emissions models 				1-hexene	\checkmark	\checkmark	\checkmark
				2-hexene	\checkmark	\checkmark	\checkmark
 – Fuel-NO_x sensitization 				3-hexene	\checkmark	V	\checkmark
PAH formation				2-methyl-2-butene	\checkmark	\checkmark	√.

reaction

A detailed soot-kinetics model was developed using CHEMKIN-PRO simulations

• Flame models replicate key experiments

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- Particle Tracking allows prediction of particle size distributions
- Fast solver allows fully detailed kinetics mechanisms to be used directly
 - No compromise on the fuel surrogate or fuel-chemistry
 - Allowed focus on the soot particle surface kinetics







We have tested the detailed soot-kinetics model in FORTÉ CFD

• Pressure, HRR, and average particle diameter results compare well with ORNL engine data*



Summary and Conclusions

• The sectional model in CHEMKIN-PRO enables mechanism testing against particle data

 Simulation times are typically ~ 2-5 minutes, allowing many parameter variations with detailed kinetics

- The detailed soot-kinetics model developed matches all observed trends in flame experiments
 - Based on scientific fundamentals, from the fuel chemistry to the soot surface kinetics
 - * Carefully validated for each step of the process
 - Provides details of particle size distributions and their dependencies on combustion conditions
 - Soot volume fractions also agree well with data



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E. J.K. Nilsson, A. A. Konnov and Sven-Inge Moller, Lund University: Studies of premixed laminar flames of oxygenated fuels using the Heat Flux method



Combustion kinetics

Experimental activities

- Heat flux setups for determination of laminar burning velocities
- Setups are designed to enable access with laser diagnostics
- · Laminar burning velocities of oxygenated biofuels
- Laminar burning velocities under • oxy-fuel conditions
- Laminar burning velocities of • mixtures of fuels

Modeling activities

Keywords

Chemical kinetics Biofuels Detailed models

Oxy-fuel conditions

Laminar burning velocities

- Detailed kinetics model: Konnov 0.6 including relevant C, O, H, and N chemistry
- Further development of kinetics • model for biofuel combustion
- Development of models for oxy-• fuel combustion
- Model evaluation and validation of in-house model and other models



Laminar burning velocities of esters: **Motivation**

- Esters are biodiesel fuels and fuel additives
- Experimental data are scarce
- We use a systematic approach to produce a large dataset
- · Valuable for model validation and understanding of how ester functionality affect burning velocity



(acetate)



ethyl methanoate (ethyl formate)

Figure 20 Final energy use of renewable motor fuels, 2000-2009





Laminar burning velocities of ester fuels: Summary and Conclusions

- Formates show higher laminar burning velocities than acetates
- Power exponent α describing the T-dependence is the same for all esters in this study



Prospects

- Further experimental studies of esters and other oxygenated fuels
- Studies on mixtures of oxygenates to further understand the combustion characteristics
- Development of the detailed chemical kinetics model to involve combustion of esters and other relevant oxygenates



<u>T. Gerber. Paul Scherrer Institute:</u> Studies on Combustion Kinetics Based on Synchrotron VUV Spectroscopy

For Details see TLM Proceedings

D. Flowers, Lawrence Livermore National Laboratory: Mulridimensional Engine Combustion Simulation using CFD and Detailed Chemical Kinetics for Complex Fuels

For Details see TLM Proceedings

A. Tezaki, University of Toyama: Studies of premixed laminar flames of oxygenated fuels using the Heat Flux method





Background : Understanding of chemical mechanism taking place in compression ignition



olefin and other intermediates

High temperature heat release (HTHR) = Final ignition

- Complete combustion at over 1000 K
- Chain reaction common to most hydrocarbons where $H+O_2 \rightarrow$
- OH + O is the rate limiting chain branching step.

Objectives



Conclusions

- CA resolved sampling technique with direct mass detection and exhaust gas analysis in hot ignition suppressed conditions have been applied to homogeneous compression ignition of PRF and n-heptane/toluene (NTF) systems.
- The additive effects of toluene to n-heptane LTO, in comparison with iso-octane, are summarized as;

At $x_{toluene} < 80\%$,

- Less consumption of toluene through the less rate constant with OH
- Less effect of reducing n-heptane LTO

At $x_{toluene} > 80\%$,

Total extinction of LTHR because of no OH reproduction of toluene