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LLNL-TR-741586

Cylinder Design for Reduced Emissions Final Report CRADA No. TC-1057-94

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November 13, 2017

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

Cylinder Design for Reduced Emissions

Final Report
CRADA No. TC-1057-94
Date Technical Work Ended: January 27, 1998

Date: May 3, 2001 Revision: 5

A. Parties

The work was a cooperative effort between the Low Emissions Technologies Research and Development Partnership formed under USCAR (herein referred to as the LEP), Sandia National Laboratories (herein referred to as Sandia), and Lawrence Livermore National Laboratory (herein referred to as LLNL).

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B. Project Scope

The technical objectives of the project were to:

(1) Investigate hydrocarbon species and flame propagation
(2) Obtain emission measurements, manipulate aromatic species reaction mechanisms, and research combustion variability
(3) Study spatial distribution of emissions, predict knock tendency, and develop combustion stability models

C. Technical Accomplishments

There were three phases to this project. The objective of this CRADA was to apply advanced diagnostics and computational modeling techniques to characterize the internal combustion in-cylinder processes that lead to hydrocarbon emissions. This report describes in detail only the work done by LLNL.

Phase I — First Year

Task 1: In-Cylinder Characterization
(Sandia was responsible for this task)

Objective: Observed the history of the hydrocarbon species distribution during expansion and exhaust strokes of a research engine.

Deliverables: Report detailing experimental results.

Task 2: Hydrocarbon Emissions Modeling
(LLNL was responsible for this task)

Objective: Predicted the emissions of hydrocarbon species during the expansion stroke of an engine.

Unburned hydrocarbon species that get trapped in piston-ring crevice volumes and absorbed in cylinder oil layers were believed to be responsible for much of the observed emissions from internal combustion engines. LLNL used available numerical models to examine this general problem by following the evolution of these unburned fuels. As unburned fuel air exited the ring-crevice volume during the expansion stroke of the engine cycle, it mixed with hot combustion products in the main combustion chamber. At sufficiently high bulk temperatures early in the expansion stroke, unburned fuel was rapidly consumed; as the chamber gas temperature fell due to expansion, the characteristic times for unburned fuel consumption rapidly became longer, and eventually the temperature became too low to oxidize the remaining fuel. The LLNL model calculations followed this process of fuel mixing with hot residual combustion products, predicted the temperature at which virtually no further fuel consumption was likely to take place, and predicted the resulting emissions of hydrocarbon species from the engine.

Deliverables: Report detailing simulation results.

Task 3: Flame Visualization
(LEP was responsible for this task)

Objective: Developed a qualitative understanding of flame propagation, including engine-operation marginal operating conditions.

Deliverables: Report detailing experimental results.

Phase II — Second Year

Task 4: Exhaust Port Analyses
(Sandia was responsible for this task.)

Objective: Obtained quantitative emission measurements in the exhaust port of the Sandia side-valve research engine.

Deliverables: Report detailing experimental results.

Task 5: Engine Combustion Chemistry Modeling
(LLNL was responsible for this task)

Objective: Incorporated aromatic species reaction mechanisms into existing models.

Previous kinetic modeling studies examined the roles that hydrocarbon fuel molecule size and structure played in determining overall combustion properties such as flame speed, rate of ignition, and the tendency to knock in internal combustion engines. Additional kinetic studies proposed reaction mechanisms to describe oxidation of aromatic hydrocarbon species such as benzene, toluene, and xylenes. These were all relatively simple examples of aromatic species with resonant ring structures. In this task, aromatic species reaction mechanisms were incorporated into existing models and used to simulate a variety of problems related to engine performance. Attention was focused on the observations that aromatic fuels did not exhibit peroxy radical isomerization reactions, which were common in many types of paraffinic fuels. This could explain the many differences in combustion properties for these fuels and those of paraffin and olefin fuels.

Task 6: Combustion Variability and Hydrocarbon Speciation
(The LEP was responsible for this task)

Objective: Improved the understanding of combustion variability, and to characterize design effects on hydrocarbon speciation.

Deliverables: Report detailing experimental results.

Phase III — Third Year

Task 7: Hydrocarbon Source Identification
(Sandia was responsible for this task.)

Objective: Determined how the various sources of unburned hydrocarbon emissions contribute to the spatial distribution of these species.

Deliverables: Report detailing experimental results.

Task 8: Engine Knock
(LLNL was responsible for this task)

Objective: Developed a computational means of predicting knock tendency and octane number for practical mixtures of fuels.

The efficiency and range of operation of conventional spark-ignition internal combustion engines were limited by the onset of knock. LLNL participated for some years in efforts to understand the fundamental chemical and physical processes that were responsible for knocking behavior, and to predict the octane rating of arbitrary mixtures of hydrocarbon fuels. However, virtually all past work was devoted to modeling the knock chemistry of paraffin and olefin species, and very little was established concerning the knock chemistry of aromatic species such as benzene, toluene, xylene, and others. These aromatic species provided a considerable fraction of the knock resistance of conventional gasolines, but also played a significant role in hydrocarbon emissions from engines, and their concentrations in automotive fuels could be limited in the future. The detailed chemical kinetic reaction mechanisms developed in Task 7 were used for a series of typical aromatic hydrocarbon fuels and integrated into existing engine knock models for paraffinic and olefinic fuels. This work developed a computational means of predicting knock tendency and octane number for practical mixtures of fuels. In addition to prediction capability for knock behavior, it was expected the chemical models could be used to examine such related applied problems of concern to automotive engine design such as Octane Requirement Increase (ORI).

Deliverables: Report detailing simulation results.

Task 9: Modeling and Application
(LEP was responsible for this task.)

Objective: Developed models of combustion stability at idle and deceleration, and of the oil layer hydrocarbon mechanism.

Deliverables: Report detailing experimental results.

D. Expected Economic Impact

This CRADA project was originally coordinated through the United States Council for Automotive Research (USCAR) and the SuperComputing Automotive Application Partnership (SCAAP) and the Automotive Composites Consortium. Later, this CRADA was coordinated with activities that were part of the "Partnership for a New Generation of Vehicles (PNGV)."

This project ensured work would be focused on issues that were of major importance to industry. There were frequent technical and program direction interaction with industry engineers, scientists, and managers. Industry representatives lent knowledgeable input and ensured timely review of technical progress. Ultimately, this project enhanced the return on investment of U.S. government funds by ensuring the work is relevant to practical industry needs and was commercially promising.

D.1 Specific Benefits:

This CRADA resulted in the development and application of new tools to diagnose the source and evolution of hydrocarbons during an engine cycle.

Benefits to DOE Program

This project developed models, concepts, and an understanding of the operation and performance of internal combustion engines. These were not technology transfer efforts, but were aimed at meeting a primary DOE goal and responsibility — to reduce fuel consumption and conserve energy while reducing or maintaining automotive emissions levels.

This CRADA was a direct part of the DOE program in Energy Conservation. Within the Energy Conservation program, it was part of the Heat Engine Development line item, which was part of the Transportation Sector. It was managed by the Advanced Propulsion Division. This division supported similar work for many years in order to meet DOE's energy conservation goals.

The techniques applied in this project applied to other DOE programs. The laser-based instrumentation techniques were also used for measurement of gas-handling performance in nuclear weapons systems. The numerical modeling techniques have been developed as solutions to problems in spray and jet formation, gaseous phase chemistry, and heat transfer. Each of these techniques had important application to nuclear weapons safety. Thus, the work described in this project improved the fluid mechanics, chemistry, heat transfer, and instrumentation expertise available for application to key weapons programs.

Relationship of CRADA to Other Work at Sandia National Laboratory

This CRADA was part of ongoing work at the Sandia, CA Combustion Research Facility (CRF). Programs at the CRF included work to measure, model, and understand the mechanisms of combustion engines, furnaces, burners, and flames. Fuels considered ranged from simple gaseous substances to complex, practical compounds like coal, gasoline, diesel fuel, and alcohols. This project related to piston engine combustion processes and controls, which were used in cars and trucks, and had been studied and measured at the CRF for many years.

This CRADA developed the capability to visualize, compute, and measure the generation of unburned hydrocarbon species during the engine combustion process. Particular emphasis was placed on understanding the interplay between fluid mechanics, chemical kinetics, and temperature as unburned hydrocarbons are created, stored, and expelled from the engine.

E. Partner Contribution

Phase I — Task 3: Flame Visualization

Objective: Developed a qualitative understanding of flame propagation, including engine-operation marginal operating conditions.

Deliverables: Report detailing experimental results.

Phase II — Task 6: Combustion Variability and Hydrocarbon Speciation

Objective: Improved the understanding of combustion variability, and to characterize design effects on hydrocarbon speciation.

Deliverables: Report detailing experimental results.

Phase III — Task 9: Modeling and Application

Objective: Developed models of combustion stability at idle and deceleration, and of the oil layer hydrocarbon mechanism.

Deliverables: Report detailing experimental results. Level of Effort

F. Documents/Reference List

Reports

None

Patent/copyright activity or pending applications

None

Subject inventions disclosed by either the industrial partner or LLNL

None

Licensing status of Background Intellectual Property (BIP) and subject inventions

No licensing of BIP and no subject inventions

G. Acknowledgement

Participant's signature of the final report indicates the following:

1) The Participant has reviewed the final report and concurs with the statements made therein.
2) The Participant agrees that any modifications or changes from the initial proposal were discussed and agreed to during the term of the project.
3) The Participant certifies that all reports either completed or in process are listed and all subject inventions and the associated intellectual property protection measures generated by his/her respective company and attributable to the project have been disclosed and included in Section E or are included on a list attached to this report.
4) The Participant certifies that if tangible personal property was exchanged during the agreement, all has either been returned to the initial custodian or transferred permanently.
5) The Participant certifies that proprietary information has been returned or destroyed by LLNL.

Ronald J. Herrin 5/21/01

Ron Herrin — Date
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Tom Kenney — Date
Ford Motor Company

Thomas W. Asmus — Date
DaimlerChrysler Corporation

Charles K Westbrook 6-21-01

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Attachment I – Final Abstract

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Thomas E. Kenney — May 18, 2001

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Attachment I – Final Abstract

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Final Abstract (Attachment I)
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E. Project Dates

January 27, 1995 – January 27, 1998