A national laboratory of the U.S. Department of Energy
Office of Energy Efficiency & Renewable Energy

National Renewable Energy Laboratory

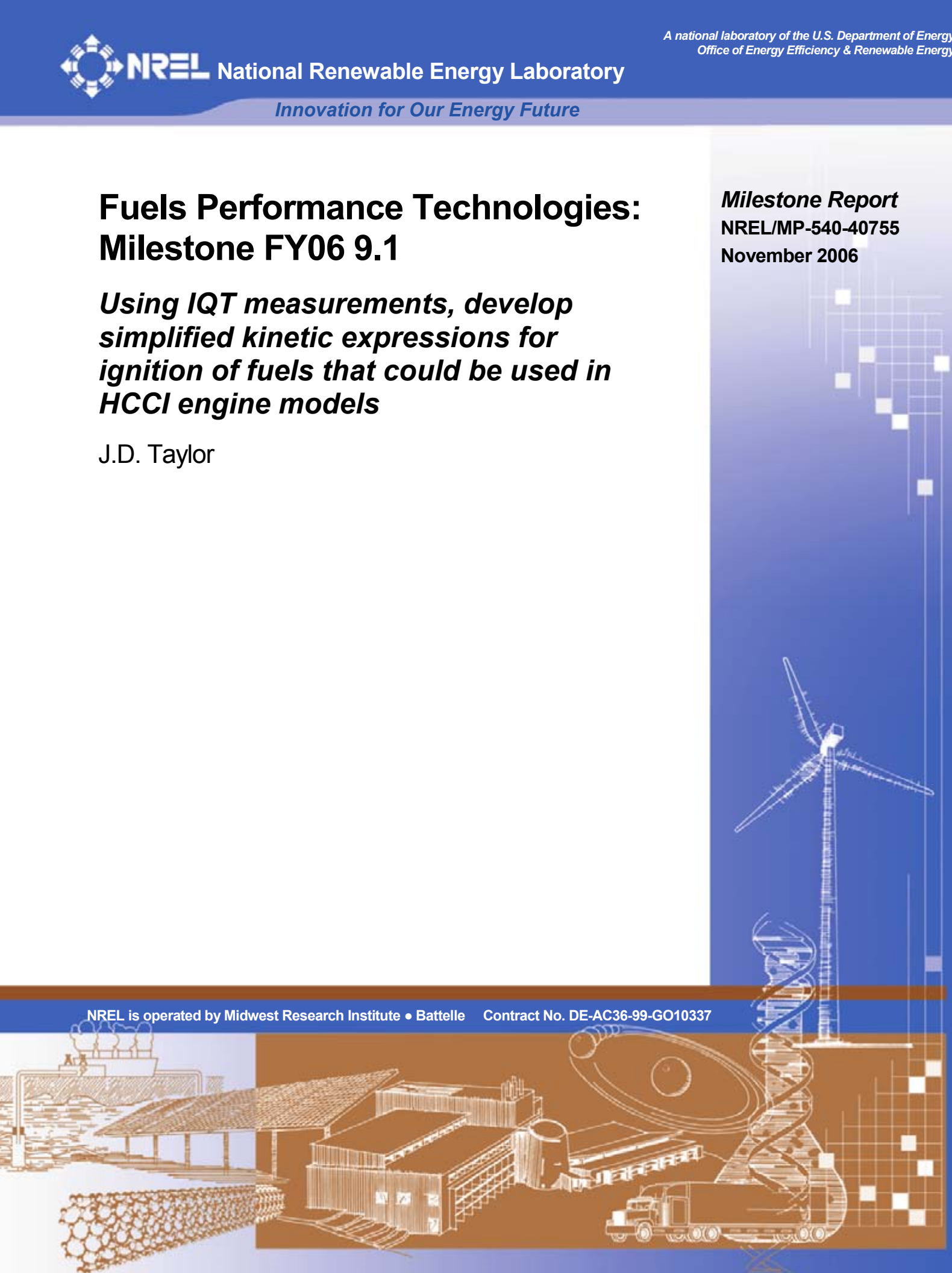
Innovation for Our Energy Future

Fuels Performance Technologies: Milestone FY06 9.1

Using IQT measurements, develop simplified kinetic expressions for ignition of fuels that could be used in HCCI engine models

J.D. Taylor

Milestone Report
NREL/MP-540-40755
November 2006



NREL is operated by Midwest Research Institute • Battelle Contract No. DE-AC36-99-GO10337

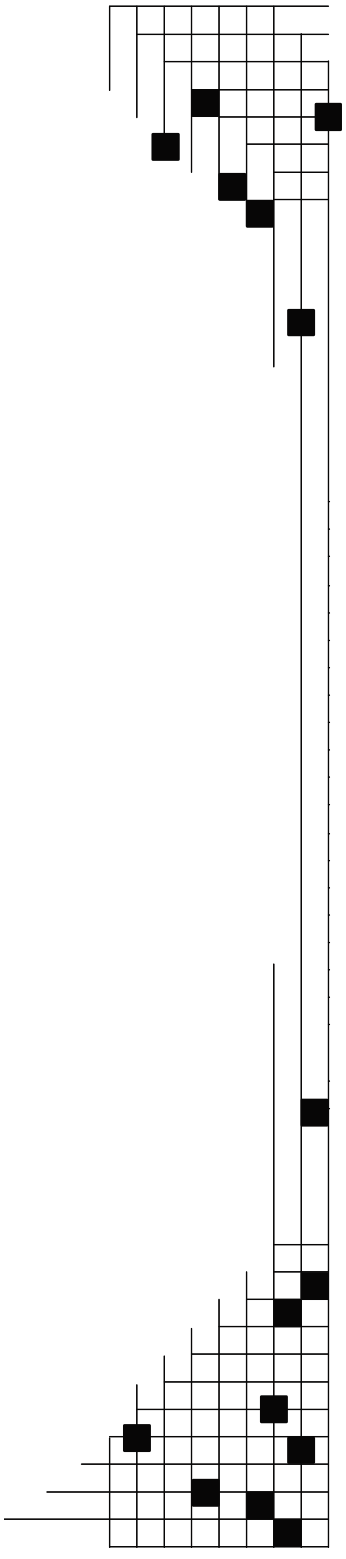
Fuels Performance Technologies: Milestone FY06 9.1

Milestone Report
NREL/TP-540-40755
November 2006

Using IQT measurements, develop simplified kinetic expressions for ignition of fuels that could be used in HCCI engine models

J.D. Taylor

Prepared under Task No. FC06.8000



National Renewable Energy Laboratory
1617 Cole Boulevard, Golden, Colorado 80401-3393
303-275-3000 • www.nrel.gov

Operated for the U.S. Department of Energy
Office of Energy Efficiency and Renewable Energy
by Midwest Research Institute • Battelle

Contract No. DE-AC36-99-GO10337

Table of Contents

List of Figures

List of Tables

List of Acronyms

CIDI	compression ignition direct injection
DCN	derived cetane number
EGR	exhaust gas recirculation
HCCI	homogeneous charge compression ignition
IQT	Ignition Quality Tester

Executive Summary

A new fuel characterization metric, based on a simplified kinetic expression, was developed to quantify ignition quality for low-temperature combustion applications. The ignition delay for a given fuel is measured over a range of temperatures, pressures, and concentrations of oxygen using the Ignition Quality Tester (IQT). An initial matrix of 27 test points was selected for testing on the IQT. Three parameters are derived from these measurements including the derived cetane number, the activation energy (sensitivity to temperature), and the reaction order on concentration of oxygen [sensitivity to pressure and exhaust gas recirculation (EGR)]. Since intake air temperature and EGR are both common control methods for low-temperature combustion, these fuel index parameters can be used to adjust the relative controller gain response in advanced combustion engines. Data from engine testing at Oak Ridge National Laboratory [1] corroborated results measured at the National Renewable Energy Laboratory for increased temperature sensitivity of biodiesel for homogeneous charge compression combustion.

[1] Szybist, J., B. Bunting, C. Wildman, and J. Tassitano, "Diesel Range Fuel Effects on Single Cylinder HCCI" Presented at the *2006 DOE Merit Review of Advanced Combustion, Emission Control, and Fuels Research at National Laboratories*, May 15-18, 2006.

Introduction

In light of strict emission requirements and demand for high fuel economy, vehicle and engine companies are focusing research efforts on advanced combustion engines. Advanced combustion engines, such as homogeneous charge compression ignition (HCCI) engines, offer the potential of high fuel efficiency and extremely low emissions due to better fuel-air mixing and lower peak combustion temperatures. However, these engines are difficult to operate due to challenges in controlling combustion phasing (i.e., ignition timing) and rate of pressure rise. Furthermore, it is difficult to assess which fuel properties are desirable in HCCI engines, and there is no agreed-upon index to rank fuels for HCCI.

In a compression ignition, direct injection (CIDI) engine, fuel is injected just slightly before top dead center, and the fuel ignites rapidly in the hot air environment. Fuels, then, can be ranked based on how quickly they ignite under a single set of representative conditions. This is the basis for ranking fuels by cetane number or derived cetane number (DCN) test methods. Even so, we have shown in past work that this single-point ignition measurement is not sufficient to predict the performance of a fuel under cold-start or other extreme variations in operating conditions for a CIDI engine. A benefit of CIDI engines over HCCI engines is that injection timing can be adjusted to correct ignition timing based on calibration maps. During the calibration phase for a CIDI engine, separate injection timing maps can be used for cold-start or other conditions. While variations in fuel properties will cause slight shifts in ignition timing, the effects are generally small in these types of engines.

A challenge for implementing HCCI engines is that any variations in fuel ignition quality have a much larger impact on ignition timing. The rate of pre-ignition chemistry is not only important at a single representative condition, but rather at all temperatures and pressures throughout the compression stroke. This is shown in Figure 1, where the temperature-pressure conditions are shown during the compression stroke where each point represents one crank angle degree. Because the fuel is mixed with the air throughout the compression stroke in an HCCI engine, the chemistry begins when the temperature-pressure conditions are sufficient for appreciable reaction rates. For this reason, it is important to understand how the ignition rate varies with temperature and pressure. Additionally, intake air temperature and EGR are both used as “knobs” to adjust combustion phasing in HCCI engines. Therefore, it is important to understand how much the ignition timing changes with temperature and composition.

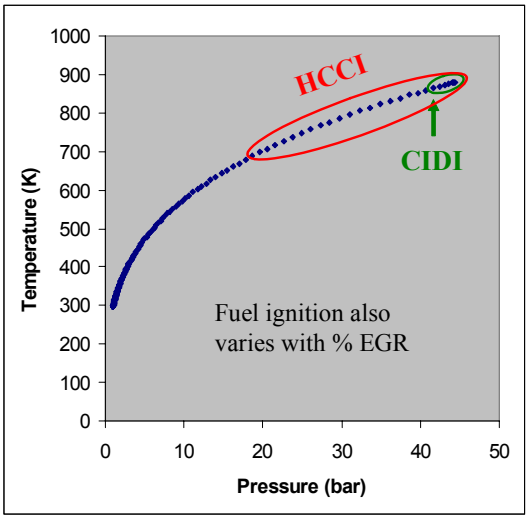


Figure 1: Temperature-pressure history through the adiabatic compression stroke of an engine

In this research, we aim to develop an index of fuel ignition quality that is applicable to HCCI and other advanced combustion engines. Our approach is to rank fuels based on their ignition delay at a representative condition (e.g., the DCN), but also to determine the sensitivity of the ignition delay to temperature and oxygen composition. These sensitivity parameters are derived from a simplified reaction rate expression for ignition delay based on activation energy for temperature dependence and reaction order of oxygen for EGR and pressure dependence.

Experimental

Ignition delays are measured using the Ignition Quality Tester (IQT), which is a constant volume combustion apparatus; this experimental apparatus has been explained in detail in a previous report [2]. Each experiment consists of 47 separate injections, of which 15 serve to equilibrate all temperatures, and 32 are used for a statistical measure of the ignition delay. The standard conditions to measure DCN are a temperature of ~550°C, a pressure of 22 bar, and 21% oxygen charge air.

In this set of experiments, conditions were selected to span a range of temperatures, pressures, and compositions. The conditions selected were as follows: T = 450, 500, and 550°; P = 10, 20, and 30 bar; and $[O_2]$ = 15%, 18%, and 21%. These compositions of oxygen correspond to EGR rates of 28%, 14%, and 0% respectively. In these experiments, exhaust gases were simulated by using compressed gas bottles that contained reduced concentrations of oxygen with the balance of nitrogen. Since the IQT does not operate using a compression stroke (where differing heat capacities affect the conditions), the effect of substituting nitrogen for CO_2 and H_2O is negligible. A full factorial design of the conditions was tested, resulting in 27 test points in addition to the DCN measurement.

Normal heptane was used to demonstrate the derivation of the sensitivity parameters for the fuel index. This approach can be applied to any real fuel or pure compound as long as the ignition delays are within the range measurable by the IQT. Additional testing will determine what those limits are, but it is expected that only very low cetane fuels (i.e., high-octane gasoline) will be excluded from this test method.

[2] Taylor, J., R. McCormick, and W. Clark, "Report on the Relationship Between Molecular Structure and Compression Ignition Fuels: Both Conventional and HCCI" *NREL Report #MP-540-36726* (http://www.nrel.gov/vehiclesandfuels/pdfs/mp36726.pdf) August, 2004.

Results

The results of the ignition delay measurements are shown in Figure 2. The data are shown on an Arrhenius-like plot where the representative reaction rate is plotted versus the inverse of temperature. A more appropriate reaction rate would be the inverse of ignition delay, which would result in the values all being multiplied by negative 1. The use of an Arrhenius plot was chosen because it facilitates the derivation of the activation energy, which is proportional to the slope of the plot.

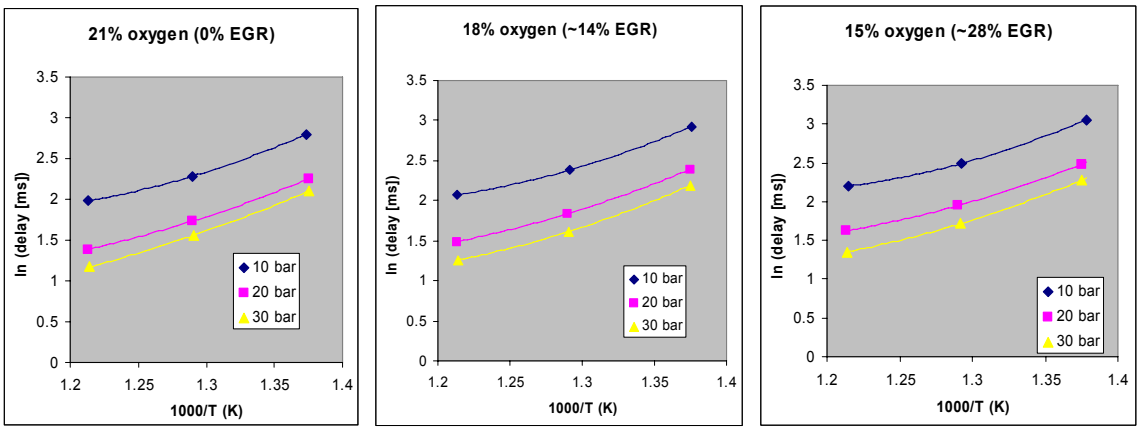


Figure 2: Experimental data of n-heptane ignition delay at 27 test point conditions using the IQT

These data show the expected trends in how ignition delay varies with each of the three variables. As the temperature decreases from 550°C to 450°C, the ignition delay increases. Although the curves are not straight lines, the activation energy can be approximated from the slope of the lines. As pressure increases from 10 to 30 bar, the ignition delay decreases. Finally, as the concentration of oxygen decreases from 21% to 15% (i.e., increasing EGR), the ignition delay increases slightly.

Discussion and Conclusions

A simplified global rate model was fit to the data in an attempt to deconvolute the effects of temperature and oxygen concentration on the measured ignition delay. In this model, the effects of charge pressure and oxygen fraction are coupled into a molar concentration of oxygen rather than treating them separately. The rate expression is shown in equation (1):

$$Rate = \frac{1}{\text{ignition delay}} = A \cdot \exp\left[\frac{E_a}{RT}\right] \cdot [O_2]^b \quad \textbf{(1)}$$

where A is the pre-exponential constant, E_a is the activation energy, R is the universal gas constant, and b is the reaction order for oxygen concentration. In equation 1, the concentration of oxygen is calculated by:

$$[O_2] = \frac{P}{RT} \cdot x_{O2} \quad \textbf{(2)}$$

where x_{o2} is the mole fraction oxygen in the charge air.

By applying this rate model, the ignition delay of a given fuel can be characterized by a three parameter fit. At first glance, it would appear that the three parameters should be A, E_a, and b. However, since A has little practical meaning, it is more convenient to use the DCN value as the constant. The two approaches are identical; and A can be calculated from DCN, E_a, and b using the correlation for DCN in the IQT literature.

The value of b is regressed by maximizing the R-squared value of the linear fit shown in Figure 3, and E_a is determined from the slope of the best fit line. It is clear from Figure 3 that the model is sufficient to allow for a good fit to the data, resulting in an R-squared value of 0.98.

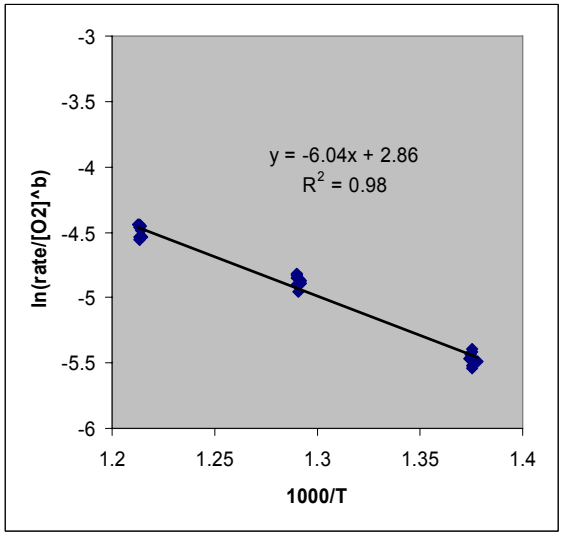


Figure 3: Regression of rate parameters to 27 data points of ignition delay data for n-heptane

The values determined for heptane are shown in Table 1.

Table 1. Kinetic Parameter Values Determined for Heptane

DCN	E_a	b
52.5	50.2 kJ/mol	0.74

A plot of the experimentally measured ignition delay versus the predicted value using the model is shown in Figure 4. These parameters are a quantitative metric of how the fuel ignition responds to changes in temperature, pressure, and EGR. The activation energy can be used to adjust the gain value on an intake air temperature controller for a given fuel. Similarly, reaction order (b values) can be used to adjust relative boost (intake air pressure) or EGR levels. Furthermore, using the rate expression and correcting the pre-exponential value for engine specific conditions, it is feasible that this type of formulation can be used to predict ignition timing over a wide range of conditions in an HCCI engine model.

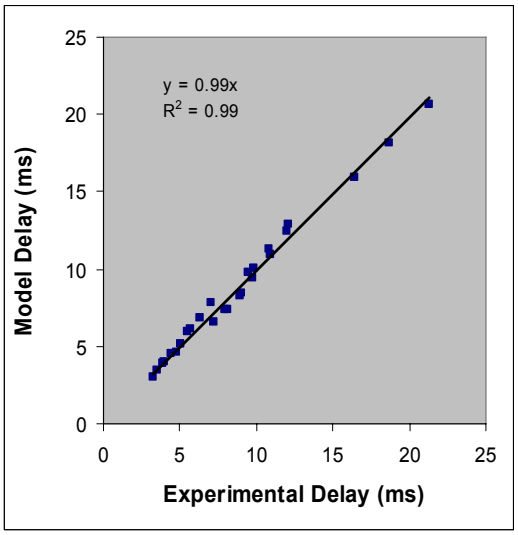


Figure 4: Comparison of experimental values with predictions from the simplified rate model

Currently, we have only applied the complete model approach to n-heptane, but we will use this approach for other pure compounds and real fuels. In past research, we have shown that different fuels (or pure compounds) can have significantly varied activation energies, such as the higher activation energy shown by biodiesel (which was confirmed in engine experiments at Oak Ridge National Laboratory). This work shows that we can now quantify the effects of activation energy independent from the change in oxygen density that is inherently coupled in the IQT.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ORGANIZATION.

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
November 2006	Milestone report	11/2005 - 9/2006

4. TITLE AND SUBTITLE
Fuels Performance Technologies: Milestone FY06 9/1—Using IQT measurements, develop simplified kinetic expressions for ignition of fuels that could be used HCCI engine models

5a. CONTRACT NUMBER
DE-AC36-99-GO10337

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
J.D. Taylor

5d. PROJECT NUMBER
NREL/MP-540-40755

5e. TASK NUMBER
FC06.8000

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
National Renewable Energy Laboratory
1617 Cole Blvd.
Golden, CO 80401-3393

8. PERFORMING ORGANIZATION REPORT NUMBER
NREL/MP-540-40755

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSOR/MONITOR'S ACRONYM(S)
NREL

11. SPONSORING/MONITORING AGENCY REPORT NUMBER

12. DISTRIBUTION AVAILABILITY STATEMENT
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22161

13. SUPPLEMENTARY NOTES

14. ABSTRACT *(Maximum 200 Words)*

A new fuel characterization metric, based on a simplified kinetic expression, was developed to quantify ignition quality for low-temperature combustion applications. The ignition delay for a given fuel is measured over a range of temperatures, pressures, and concentrations of oxygen using the Ignition Quality Tester (IQT). An initial matrix of 27 test points was selected for testing on the IQT. Three parameters are derived from these measurements including the derived cetane number, the activation energy (sensitivity to temperature), and the reaction order on concentration of oxygen [sensitivity to pressure and exhaust gas recirculation (EGR)]. Since intake air temperature and EGR are both common control methods for low-temperature combustion, these fuel index parameters can be used to adjust the relative controller gain response in advanced combustion engines. Data from engine testing at Oak Ridge National Laboratory corroborated results measured at the National Renewable Energy Laboratory for increased temperature sensitivity of biodiesel for homogeneous charge compression combustion.

15. SUBJECT TERMS
fuels; fuel characterization; simplified kinetic expression; ignition quality; low-temperature combustion; exhaust gas recirculation; IGR; IQT

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			19b. TELEPHONE NUMBER *(Include area code)*
Unclassified	Unclassified	Unclassified	UL		

Standard Form 298 (Rev. 8/98)
Prescribed by ANSI Std. Z39.18