Real Fuel Modeling for Gasoline Compression Ignition Engine

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Abstract

Increasing regulatory demand for efficiency has led to development of novel combustion modes such as HCCI, GCI and RCCI for gasoline light duty engines. In order to realize HCCI as a compression ignition combustion mode system, in-cylinder compression temperatures must be elevated to reach the autoignition point of the premixed fuel/air mixture. This should be co-optimized with appropriate fuel formulations that can autoignite at such temperatures. CFD combustion modeling is used to model the auto ignition of gasoline fuel under compression ignition conditions. Using the fully detailed fuel mechanism consisting of thousands of components in the CFD simulations is computationally expensive. To overcome this challenge, the real fuel is represented by few major components of create a surrogate fuel mechanism. In this study, 9 variations of gasoline fuel sets were chosen as candidates to run in HCCI combustion mode. A study detailing the development of the gasoline real fuel model was performed and various surrogates for gasoline fuel were investigated. The gasoline real fuel model will be used in subsequent CFD modelling activities for the development of an advanced mixed mode combustion system as part of the Department of Energy funded project DE-EE0008478.

Introduction

Development of advanced gasoline compression ignition (GCI) engines requires the use of engine CFD modeling with a robust gasoline fuel model that captures the physical properties as well as the chemical reactions accurately without excessive computational effort. The gasoline fuel is represented by few well understood components of the desired fuel and assembled together into what is known as a real fuel surrogate model. Real fuel modeling consists of modeling the physical properties (e.g. evaporation) using the spray model and the kinetic properties (e.g. combustion) using the chemistry model. Anand et al. [1] studied the fuel's chemical and physical properties with two sets of surrogate components. They validated the surrogate fuel by comparing H/C ratio, distillation profile, specific gravity, cetane index and lower heating value of model with experimental data.

In this study, nine variations of gasoline fuel sets are chosen as candidates to run in homogeneous charge compression ignition (HCCI) combustion mode simulation. The fuel sets differentiate in the number and concentration of components containing in the set and they are between 10 and 20 components. Initial modeling for the individual components showed alterations in prediction of the ignition delay time over a wide range of temperature from 700K to 2000K for each component which contributes to the final combined surrogate model consisting of these components [2]. A wide research on primary reference fuel (PRF) has been done using constant volume reactors, engines and RCM. Reuillon et al [3] studied oxidation products of PRF (iso octane and n heptane) in a jet stirred reactor, while Filipe et al [4] studied oxidation products of iso octane bends with varying percentage of n heptane in a motored engine. The study found that reactivity of PRF increased as % of n heptane in blend was increased. Figure 1 shows the ignition delay experimental results for actual 13 component surrogate PRF fuel. Heptane (nC7H16) and IsoOctane (iC8H18) showed best match for real fuel versus experimental ignition delay. [5]

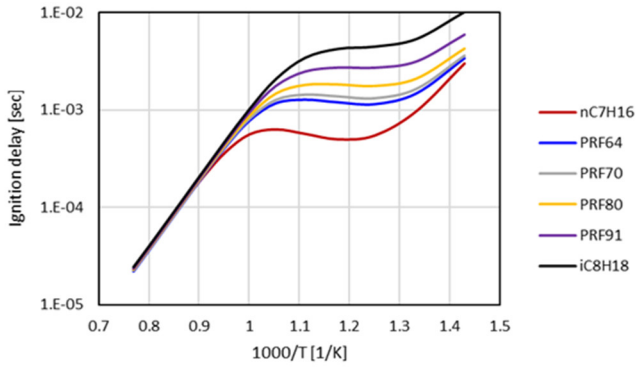


Figure 1 Figure 1: Ignition Delay time simuation at 1bar and phi=1 for several primary reference fuels (n-heptane, PRF64, PRF70, PRF80, PRF91 and isooctane)

Fuel Spray Modeling

The authors in collaboration with Michigan Technological University have developed techniques to model both physical and chemical properties, and combustion of multi-component fuels and studied surrogate models for diesel and gasoline fuels [6]. The detailed mechanism for n heptane and iso octane has been developed to describe the oxidation of the mixture of n-heptane and iso-octane at low and high temperature ranges by S.S Ahmed et al. [7]. Real fuel model described in this paper consists of modeling the physical properties using the spray model and the kinetic properties using the chemistry model.

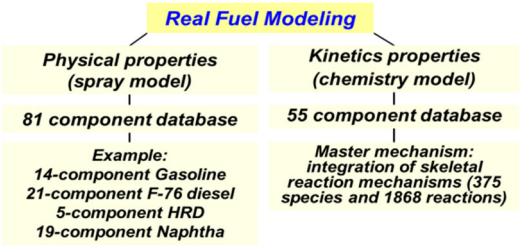


Figure 2: Real Fuel Modeling (spray & chemistry)

The spray model is constructed using a 81 component physical properties database which covers the range of possible fuel property combination referenced in Table 1. Multi-component fuel spray models are constructed from this database to represent a real fuel. For example, 14-component gasoline, 21-component F-76 diesel, 5-component HRD and 19-component Naphtha.

Kinetic properties will be modeled using a 55 component database. The database for the master mechanism consists of the integration of skeletal reaction mechanisms with 375 species and a total of 1868 reactions. This master mechanism database is extensive and can be used to cover a wide range of fuel properties and types.

Table 1: Typical gasoline blend feedstock properties

No.	Physical Property	No.	Physical Property
P1	Liquid Density	P7	Vapor heat capacity
P2	Vapor Pressure	P8	Vapor diffusivity
P3	Surface tension	P9	Vapor viscosity
P4	Liquid viscosity	P10	Vapor thermal
P5	Liquid thermal conductivity	P11	Liquid heat capacity
P6	Heat of vaporization	P12	Critical properties

Multi-Component Spray Behavior

Initially, the component profile concentration is plotted with the red dots as seen in Figure 3. During the spray break-up phase the low carbon number components C5H12 dominates the vaporized mixture at 80% (as shown in Figure 3 left) this is because low carbon fuels tend to vaporize more readily than higher carbon fuels. At spray jet tip penetration, the mixture concentration profile transitions towards high carbon number components C818, C9H20 and C10H22 (as shown in Figure 3 right). As a multi-component fuel is injected the lighter (lower carbon) components are mixed with air first and while the heavier component fuels are left to mix further down-stream during the injection process.

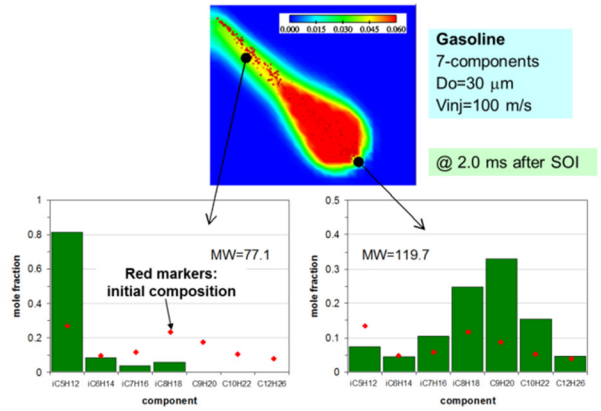


Figure 3: 7-Component gasoline fuel spray modeled using CFD

Surrogate Fuel Model Development

Multi-component gasoline surrogate fuel model was developed using the procedure listed in Figure 5. Real properties of real fuels are measured, as well as measured concentrations of hydrocarbon classes and measured distillation profiles. These are all used to combine to provide an initial choice of concentration type and number of surrogates.

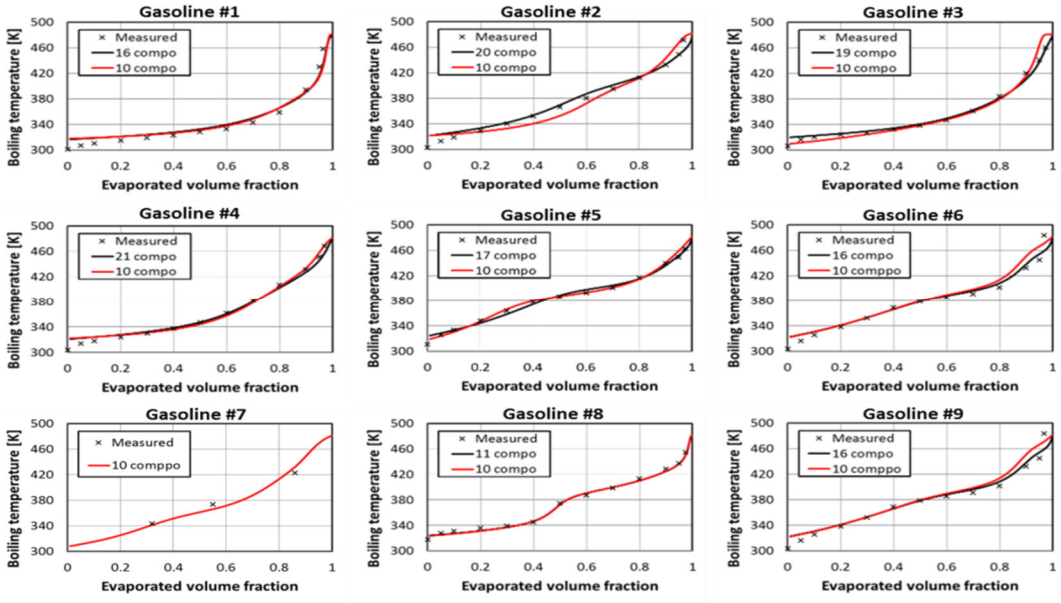


Figure 4. PSGCR gasoline surrogate fuel models versus experimental data for boiling temp

In the study, a 7-component gasoline fuel was modeled and characterized to study the change in composition of the fuel spray during various stages of the injection, break-up and mixing processes.

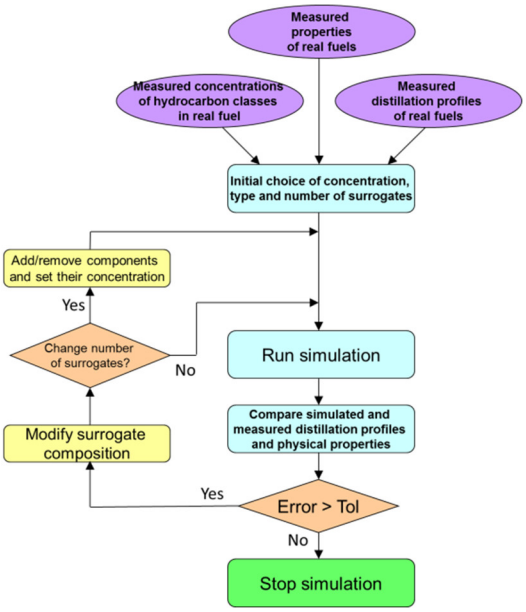


Figure 5: Surrogate Fuel Model Development

A chemical simulation is run and the simulated results are compared with the measured distillation profiles and physical properties. If tolerance Tol > error term, then the composition of the surrogate fuel is modified, by changing the number of surrogates and adjusting concentrations and the simulation can be run again [8]. If the error term is minimal then simulation is stopped and the surrogate fuel composition is found.

The gasoline fuels matrix for 9 different gasoline samples was modeled using MTU Physical Surrogate Group Chemistry Representation (PSGCR) combustion model [8]. The composition of each of the 9 gasoline surrogate models are listed in Appendix A. Experimental data for boiling temperature was compared with 10 component and maximum component surrogates of each of the 9 gasoline fuels and presented in Figure 4. In some cases the 10 component surrogate fuel (such as Gasoline 1) has the same distillation curve as the 16 component surrogate, and validated experiment data well therefore surrogate with 10 components is sufficient. Whereas, for Gasoline#2, the 20 component fuel is likely needed because the 10 component fuel has a larger deviation from experimental mid-range temperature. In general a 10 component fuel has a relatively low deviation from, measured distillation curve. Figure 4 shows the effect of multi-component surrogate kinetic mechanism on boiling point and comparison with experimental data. The result show that a 3-component fuel has a nearly constant linear boiling temperature as evaporated volume fraction is increased and does not adequately represent the property.

E10 Gasoline Compression Ignition Reaction Kinetics Development:

Ethanol (E10) was added to multi-component gasoline surrogate fuel to create the kinetics model for RD5-87 E10 gasoline and validated under compression ignition conditions. A 14-Component ideal mechanism which includes ethanol and other fuel components is listed in Table 2.

Table 2: E10 14-component surrogate gasoline composition

Component	Mass fraction	Activity coefficient
C2h5oh	0.0995	4.211
C4h10	0.02	1.088
ic5h12	0.12	1.154
c5h10	0.02	1.096
ic6h14	0.1	1.201
nc6h14	0.09	1.190
nc7h16	0.0555	1.201
ic8h18	0.06	1.197
mch	0.08	1.229
toluene	0.05	1.357
c8h16	0.029	1.131
ic9h12	0.115	1.287
ic10h22	0.117	1.137
tetralin	0.044	1.506

This mechanism adequetly predicts the boiling temperature at higher evaporated volume fractions but tends to over predict for volume fractions less than 50% as shown in figure 6.

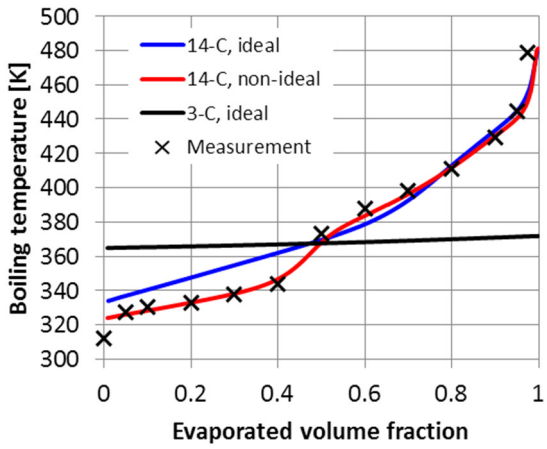


Figure 6: Effect of number of components on distillation curve model prediction.

The difference between the three mechanisms 3-component ideal, 14-component ideal and 14-component non-ideal is most noticeable in Figure 7 which plots the fuel fraction versus crank angle degrees. Ideal model is the ideal mixture model based on Rault's rule [9]. Non-ideal model is the non-ideal mixture model that considers the interaction among molecules of different species. The initial injected liquid and volume fractions are almost identical immediately after SOI from -28 degATDC to -23 degATDC, after which we begin to see a deviation in vapor and liquid fraction.

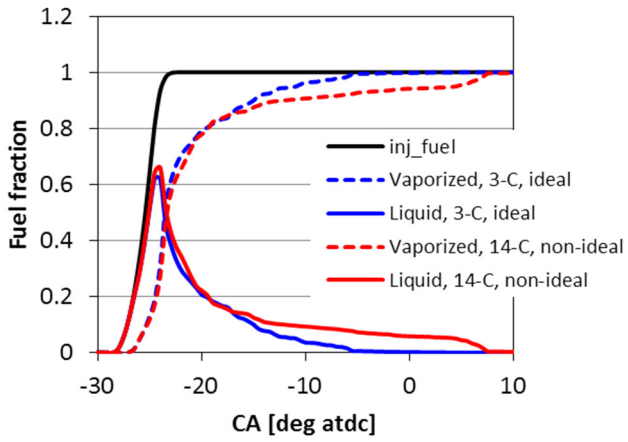


Figure 7: Effect of number of components on distillation curve model prediction.

The 14-component ideal model predicts all of the spray vaporization occurs at before -5degATDC ignition. Whereas the 14-component non-ideal mechanism continues to vaporize the fuel to after TDC where ignition has taken place and combustion temperature is the hottest. This is critical for accurate prediction of fuel spray characteristics and wall wetting as well as predicting auto-ignition and emissions.

The 14-component non-ideal does a much better job of matching the cylinder pressure and heat release trace compared to the 3-component ideal mechanism which is observed to be noticeably delayed as shown in figure 8. Simulation studies are conducted on GM 1.9L small bore high speed diesel engine. engine specifications are listed in table 3. Therefore, the non-ideal 14-component mechanism is the best option for distillation curve prediction as well as in-cylinder vaporization prediction and start of combustion and combustion phasing prediction.

It follows that 14-component non-ideal mechanism would be useful for validation of other properties for advance compression ignition (CI) engines including: auto-ignition time, flash point, thermo-physical properties such as; RON, Octane sensitivity, flame speed- from surrogate fuel mechanisms, heat of vaporization, and particulate matter index. However these would need to be investigated further.

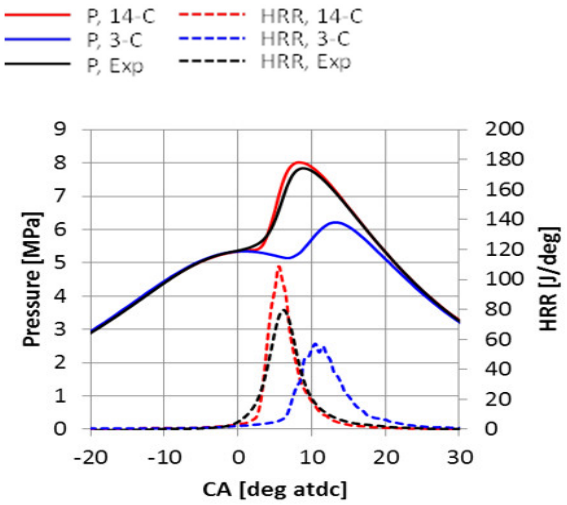


Figure 8: Effect of multi-component fuel composition on combustion and boiling temp.

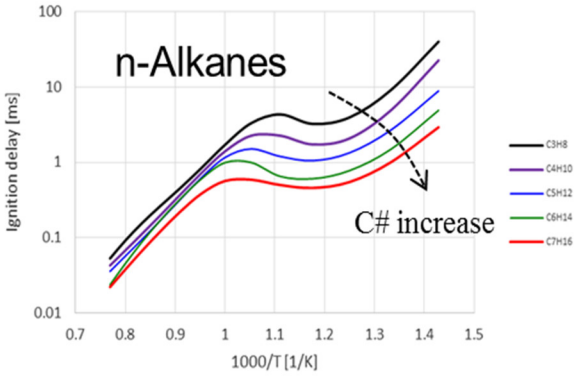
Table 3: Engine specifications and operating conditions

Engine type	Light duty, reentrant bowl piston
Bore ✕Stroke [mm]	82 ✕90.4
Connecting rod length [mm]	161
Compression ratio	16.5:1
Valve timing	IVO=340, IVC=-132 EVO=112, EVC=388
Injector	
Number of holes	7
Included angle	155
Nozzle hole diameter [µm]	141.4
Injection timings [°ATDC]	1st pulse: -350 2nd pulse:-31
Injection pressure [bar]	500
Operating conditions	
ENgnie speed [RPM]	2000
Engine NMEP [bar]	4
Fuel	Gasoline (ON=87)

Effect of Chemical Groups on Ignition

The effect of chemical groups on ignition delay is shown in Figure 9. The effect of carbon number increase on Alkanes showed that ignition delay was shortened as carbon number increased. Ignition delay is defined as the lapsed time when the temperature rise from the initial temperature exceeds 400 K. the stoichiometric air fuel mixture is pressurized at 40 bar pressure in a constant volume chamber. Aromatics content was varied using alkyl chain length with the shortest ignition delay coming from longest Alkyl chain length, heptylbenzene (HpB) as shown in Figure 10.

Naphthenes were varied (CHX, MCH, Decalin) to determine the effect on ignition delay with the results shown in Figure 11. The addition of Decalin is showing the shortest ignition delay.



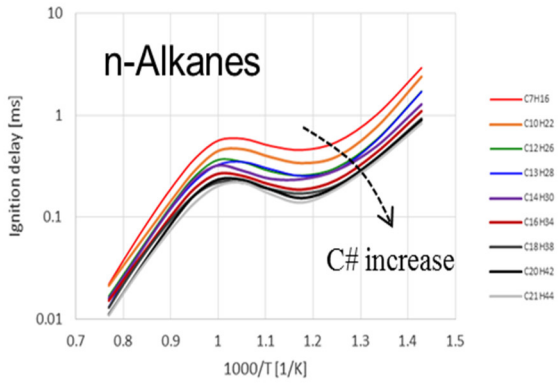


Figure 9: C3 to C7 alkane (top) C7 to C22 alkanes.

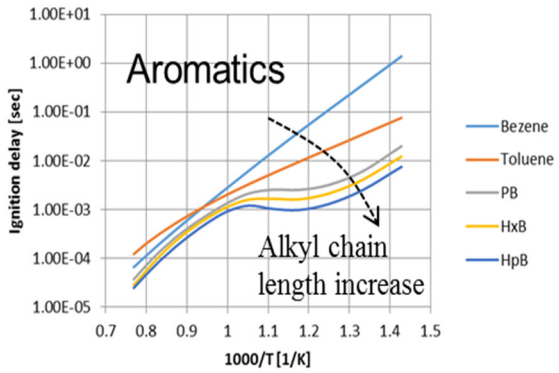


Figure 10: Aromatics effect on Ignition delay

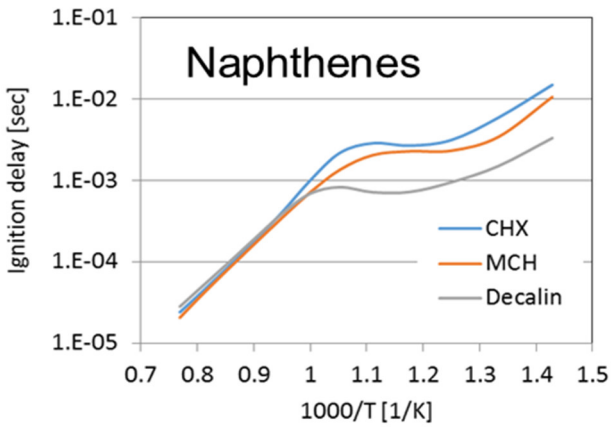


Figure 11: Naphthenes effect on Ignition delay

Conclusions

A gasoline real fuel model was developed with a 14-compoent non-ideal fuel with E10. The fuel was developed using a surrogate modeling process. The fuel mechanism was used to correctly predict both distillation curve and boiling temperature as well as injector vaporization and ignition delay. The fuel mechanism showed good sensitivity on ignition delay to carbon number in alkanes, aromatic chain length, and naphthenes. Future work will include the measured properties of fuels matrix to be used on the "Co-optima mixed mode GCI engine project (DE-EE0008478) consisting of 4 fuels with varying RON number from 60 to 91, and inputting these properties into the simulation process for composition. The final mechanism can be validating using the HCCI model and should cover a wide range of operational points. An advanced compression ignition fuel merit function will be developed.

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Definitions and Abbreviations

HCCI: Homogeneous Charge Compression Ignition

SI: Spark Ignition

BMEP: Brake Mean Effective Pressure

AFR: Air Fuel Ratio

SOI: Start of Injection

GDI: Gasoline Direct Injection

EGR: Exhaust Gas Recirculation

COV: Coefficient of Variation

IMEP: Indicated Mean Effective Pressure

CAD: Crank Angle Degree

Deg ATDC: degrees after top dead center

CA50: Crank Angle at 50% fuel burn

Tol: Tolerance

HpB: heptylbenzene

HxB: Hexylbenzene

PB: propylbenzene