

Numerical Study of RCCI and HCCI Combustion Processes Using Gasoline, Diesel, *iso*-Butanol and DTBP Cetane Improver

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ABSTRACT

Reactivity Controlled Compression Ignition (RCCI) has been shown to be an attractive concept to achieve clean and high efficiency combustion. RCCI can be realized by applying two fuels with different reactivities, e.g., diesel and gasoline. This motivates the idea of using a single low reactivity fuel and direct injection (DI) of the same fuel blended with a small amount of cetane improver to achieve RCCI combustion. In the current study, numerical investigation was conducted to simulate RCCI and HCCI combustion and emissions with various fuels, including gasoline/diesel, *iso*-butanol/diesel and *iso*-butanol/*iso*-butanol+di-tert-butyl peroxide (DTBP) cetane improver. A reduced Primary Reference Fuel (PRF)-*iso*-butanol-DTBP mechanism was formulated and coupled with the KIVA computational fluid dynamic (CFD) code to predict the combustion and emissions of these fuels under different operating conditions in a heavy duty diesel engine. The results show that RCCI combustion is achievable by applying a single low reactivity fuel combined with small amount of DTBP cetane improver over wide operating conditions, and that the performance of the *iso*-butanol-DTBP fuel is comparable to that of gasoline-diesel and *iso*-butanol-diesel fuels. However, due to the low reactivity of *iso*-butanol, a relatively high amount of DTBP is needed to enhance the reactivity of the DI *iso*-butanol+DTBP mixture. The simulations were extended to also model homogeneous charge compression ignition (HCCI) combustion under similar operating conditions with the various fuels. Comparisons between HCCI and RCCI show that although comparable performance can be obtained with HCCI under low to medium load conditions, RCCI shows advantages under higher load conditions.

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INTRODUCTION

Currently thermal efficiency and emissions are two major concerns in the internal combustion (IC) engine research community due to energy and environmental concerns. Many novel combustion concepts, such as HCCI, partially premixed compression ignition (PPCI) and RCCI have been proposed to achieve clean and high efficiency combustion [1, 2]. Among these concepts, HCCI combustion is attractive due to its high thermal efficiency and very low NO_x and soot emissions. However, since the HCCI combustion is controlled by chemical kinetics, there is no direct way to control the combustion rate (pressure rise rate and heat release rate (HRR)), especially under high load conditions. Therefore, HCCI combustion has been limited to low-to-medium load conditions, which restricts the wide application of such combustion concepts. PCCI was proposed to overcome the drawbacks of the limited operating range

of HCCI by introducing concentration stratification to control the combustion rate. However, advanced injection timing is usually needed in order to get satisfactory mixing to avoid soot emissions, which results in high unburnt hydrocarbon (UHC) and carbon monoxide (CO) emissions. In addition, although the combustion phasing shows some response to the injection timing, there is still no effective measure to directly control the combustion phasing.

Dual fuel HCCI combustion, which utilizes variable fuel reactivity by changing the ratio between two fuels with different reactivities, offers another way to control the combustion phasing. For example, DME and methanol have been applied to improve the controllability of the HCCI combustion process [3]. It was found that the combustion

phasing can be effectively tuned by altering the ratio of these two fuels. However, similar to single fuel HCCI, the operating range of dual fuel HCCI is still limited to medium load conditions.

The RCCI combustion concept has been proposed to utilize both concentration and reactivity stratification to optimize the combustion process [4, 5]. A low reactivity fuel (i.e., gasoline) was premixed through port injection and a high reactivity fuel (i.e., diesel) is directly injected into the combustion chamber to serve as the ignition source. Since both concentration and reactivity gradients exist in the chamber, the ignition timing and combustion phasing can be controlled by the direct injection timing and fuel mass, and the combustion rate can be controlled through both concentration and reactivity stratification. In addition, thermal stratification can also be created due to the cooling effect of the directly injected fuel, which is also helpful to lower the reaction rate. Therefore, this concept can overcome the disadvantages of HCCI, and thus much higher loads can be achieved. For example, an indicated mean effective pressure (IMEP) of 21 bar has been demonstrated through direct injection of both gasoline and diesel in simulations [6].

Theoretically, RCCI can be achieved as long as the two fuels have quite different reactivities. This motivated the idea of using a single low reactivity fuel as the premixed fuel and the same fuel blended with a small amount of cetane improver as the DI high reactivity fuel to achieve RCCI combustion. DTBP and 2-ethylhexyl nitrate (EHN) are two of the most widely used cetane improvers in IC engine research. Splitter et al. [7] applied port injection gasoline and direct injection gasoline mixed with DTBP to explore their ability to achieve RCCI combustion. It was found in their study that addition of only 2% volume fraction of DTBP was capable to obtain stable RCCI combustion. Kaddatz et al. [8] found that the reactivity of E10 (10% ethanol+90% gasoline) mixed with 3% volume fraction of EHN was less than conventional diesel fuel, thus more direct injected E10+EHN was needed to improve the overall reactivity.

Dempsey et al. [9] conducted HCCI combustion experiments with both PRF and methanol and ethanol mixed with EHN and DTBP cetane improvers. A reference HCCI combustion phasing map for the PRF fuel and effective combustion phasing maps for alcohol-cetane improvers were generated to characterize the reactivities of alcohol-DTBP and alcohol-EHN mixtures. The combustion phasing of the alcohol-DTBP mixtures could then be linked to the combustion phasing of a PRF mixture, thus providing an effective PRF number (i.e., octane number) for the tested fuel. This provides a method for characterizing the enhancement of fuel reactivity with cetane improvers in alcohol fuels by linking back to the PRFs used for standardized octane number tests. The results showed that the reactivities of both ethanol and methanol could be enhanced, but the response of the both methanol and ethanol to EHN additive was higher than that of DTBP. However, similar to Kaddatz et al.'s finding [8], EHN was found to have a potential disadvantages due to its nitrate group, which contributes to NO_x emissions, i.e., about one third of the NO_x emission came from the fuel-bound NO in the EHN molecule. It was also found that the response of the DTBP and EHN

in methanol was higher than that in ethanol with the same additive percentage and fixed global equivalence ratio. Dempsey et al. [9] further conducted RCCI experiments with methanol mixed with cetane improvers. In order to find the reasons for the different response behaviors for DTBP in methanol and ethanol, based on kinetic studies, Wang et al. [10] formulated a reduced PRF-methanol-ethanol-DTBP kinetic mechanism and coupled the proposed mechanism with the KIVA CFD code [11] to explore the reactivity enhancement and different behaviors of DTBP in methanol and ethanol. It was found that both thermal and chemical effects contribute to the reactivity enhancement, and the different response behaviors of DTBP in methanol and ethanol can be attributed to the different absolute DTBP mass if both the equivalence ratio and DTBP mass fraction were fixed.

In addition to methanol and ethanol, butanol, the four carbon atom alcohol, has also attracted attention in past years [12]. Among the four butanol isomers, *n*-butanol is currently the most widely used isomer due to its advantages compared to methanol and ethanol. *n*-butanol has an octane number of 96 [12], which is comparable to that of gasoline. Many experimental and numerical studies have been conducted to investigate butanols' oxidation kinetic mechanisms and effects on both diesel and gasoline engine's performance and emissions [13, 14, 15, 16, 17, 18]. *Iso*-butanol, another butanol isomer, has an octane number of 113 [12], which is higher than gasoline, and thus can be regarded as a potential candidate for RCCI application. Therefore, it is of interest to assess the possibility of applying *iso*-butanol as the low reactivity fuel in RCCI combustion. As mentioned above, it is also of interest to evaluate the performance of RCCI combustion achieved using *iso*-butanol as the low reactivity fuel and diesel and/or *iso*-butanol mixed with cetane improver to act as direct injected high reactivity fuels. The higher latent heating value of *iso*-butanol compared to gasoline can also be helpful to enhance the cooling effect created by both port injection and direct injection of *iso*-butanol, which is also thought to be beneficial for extending RCCI operating loads. In addition, oxygen content can be introduced by applying oxygenated alcohol for soot reduction. Applying oxygenated bio-derived alcohol fuels can also be helpful for energy security and reducing dependency on petro-derived diesel/gasoline fuels.

In the current study, numerical studies are conducted to explore and compare the performance of RCCI and HCCI combustion achieved using gasoline/diesel, *iso*-butanol/diesel and *iso*-butanol/*iso*-butanol+DTBP cetane improver under different conditions. A reduced PRF-*iso*-butanol-DTBP kinetic mechanism was formulated and coupled with the KIVA CFD code to simulate RCCI and HCCI combustion processes in a heavy-duty diesel engine. Validation of the proposed mechanism was first conducted by comparing with available RCCI engine experimental data, and then the simulations were further extended to predict the combustion characteristics of both RCCI and HCCI combustion modes under three different engine load conditions. Information about the in-cylinder evolution processes and comparisons among these tested fuels are extensively discussed.

EXPERIMENTAL AND MODELING SETUP

Experimental Setup

RCCI experiments with gasoline/diesel, *iso*-butanol/diesel and *iso*-butanol/*iso*-butanol+DTBP were conducted by DeVescovo et al. [19] in a heavy-duty diesel engine. Details about the test engine and the experimental setup can be found in work [19], thus only a brief introduction will be presented here. The specifications of the test engine are shown in Table 1. The major properties of the tested fuels are shown in Table 2. As mentioned above, three different fuel groups were tested in the experiments. Different fuel combinations to achieve both RCCI and HCCI combustion under different conditions are shown in Table 3. Gasoline and *iso*-butanol were applied as the premixed low reactivity fuels and diesel and mixtures of *iso*-butanol and DTBP were applied as the direct injection high reactivity fuels in RCCI combustion.

Table 1. Engine specifications

Engine Type	CAT SCOTE 3401
Bore*stroke [mm]	137.2 x 165.1
Displacement [L]	2.44 L
IVC [CA ATDC]	-143.0
EVO [CA ATDC]	130.0
Compression ratio	14.88:1-RCCI piston 16.1:1-Stock piston
Combustion chamber	Shallow-RCCI piston Mexican Hat piston-stock piston
Fuel injection type	Premixed-Port injection Direct injection-Common rail
Injector	6 holes

The engine operating conditions in the experiments are shown in Table 4. A bath-tub-shaped RCCI piston with compression ratio of 14.88 was used in DeVescovo et al.'s experiments. The geometries of both the RCCI and stock pistons are shown in Figure 1. As can be seen in Table 4, at the 6.5 bar indicated mean effective pressure (IMEP) condition, four different intake pressures were tested for all three fuels, which are marked in **bold** font in Table 4. Simulations were conducted firstly to guide the setup of the engine experiments. It was found that due to the relatively low reactivity of the *iso*-butanol-DTBP mixture, 20% volume fraction of DTBP needed to be blended with the *iso*-butanol to serve as the direct injection high reactivity fuel in the *iso*-butanol/*iso*-butanol+DTBP fuel group.

Table 2. Properties of gasoline, diesel, *iso*-butanol and DTBP

	diesel	gasoline	<i>iso</i> -butanol	DTBP
Molecule formula	C ₁₂ -C ₂₅	C ₄ -C ₁₂	C ₄ H ₉ OH	C ₈ H ₁₈ O ₂
Cetane number	48	10	-	-
RON	20-30	97	113	-
Oxygen content (% weight)	-	-	21.6	21.88
Density (g/cm ³ @20°C)	0.8179	0.7371	0.802	0.796
Lower heating value (MJ/kg)	42.6	42.8	32.96	33.80
Boiling point (°C)	180-370	25-215	107.89	109-111
Latent heat (kJ/kg@25°C)	270	380-500	579.9	-

Table 3. Tested fuels

Mode	RCCI		HCCI
Fuels	Premixed	DI	Premixed
gasoline/diesel (GD)	gasoline (<i>iso</i> -octane)	diesel (<i>n</i> -heptane)	gasoline diesel
<i>i</i> -butanol/diesel (BD)	<i>iso</i> -butanol	diesel (<i>n</i> -heptane)	<i>iso</i> -butanol diesel
<i>i</i> -butanol/DTBP (iBD)	<i>iso</i> -butanol	<i>iso</i> -butanol 20% DTBP	<i>iso</i> -butanol DTBP

Table 4. Engine operating conditions [4, 19]

IMEP [bar]	6.5	9.0	14.6
Piston geometry	RCCI	Stock	Stock
Engine speed [rev/min]	1300	1300	1300
Intake pressure [bar]	1.35, 1.50 1.65, 1.80	2.0	2.34
Intake temperature [°C]	40	32	32
EGR ratio [%]	0	45%	55%
Total fuel mass [mg/cycle]	GD: 75 BD: 92.2 iBD: 97	GD: 94.21 BD: 121.0 iBD: 127.0	GD: 160.85 BD: 210.0 iBD: 217.0
Premixed fuel mass fraction [%]	GD: 86.8 BD: 67.9 iBD: 39.8	GD: 89.0 BD: 85.0 iBD: 40.0	GD: 90.0 BD: 90.0 iBD: 35.0
DI SOI-1 [CA ATDC]	-58	-58	-58
DI SOI-2 [CA ATDC]	-37	-37	-37
Injection pressure [MPa]	600	800	800
DI fuel in 1 st injection [%]	67	67	37

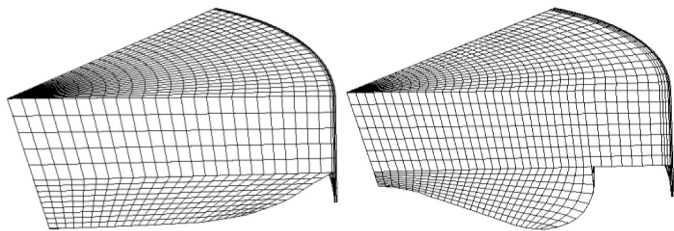
Two higher load conditions were also chosen in the current numerical study as listed in Table 4, with IMEPs of 9.0 bar and 14.6 bar, respectively [4]. The stock piston with compression ratio of 16.1 was applied in these experiments, also shown in Figure 1. Only gasoline/diesel fuels were used under these two conditions in the experiments. However, in order to thoroughly evaluate the capability of the other two fuel groups, *iso*-butanol/diesel and *iso*-butanol/*iso*-butanol+DTBP fuels were also applied under these conditions in the simulations to assess the engine performance.

Modeling Setup

In the current study the KIVA CFD code was applied and coupled with the proposed chemical kinetic mechanism to predict RCCI and HCCI combustion and emissions. The sub-models applied in the simulations are listed in Table 5. The computational grids are shown in Figure 1, and 60-degree sector meshes for both the stock and RCCI pistons were applied to improve the computational efficiency.

Table 5. Sub-models used in the simulations

Phenomenon	Model	Reference
Spray breakup	KH-RT instability	[20, 21]
Evaporation	Discrete multi-component fuel (DMC)	[22]
Turbulence	Renormalized k-ε model	[23]
Combustion	Sparse analytical Jacobian (SpeedChem)	[24]
Droplet collision	Radius of influence (ROI) model	[25]
Near nozzle flow	Gas-jet model	[26]



(a) RCCI piston (b) Stock piston

Figure 1. Computational grids applied in the simulations

HCCI combustion simulations with the various fuels were also conducted in the current study to provide comparisons between RCCI and HCCI. 2-dimensional (2D) sector meshes were applied and homogeneous charge mixtures were assumed at intake valve closing (IVC) timing. Closed cycle simulations were conducted, i.e., from IVC (−143.0 CA ATDC) to exhaust valve opening (EVO, 130.0 CA ATDC) in all cases. The simulations were initialized with uniform concentrations, flow fields and temperature at IVC timing, when the simulations start, thus no gradient were imposed for the initialization.

The combustion efficiency is a measure of the completeness of the combustion process and is calculated as:

$$\eta_{comb} = \frac{E_{fuel} - E_{comb loss}}{E_{fuel}} = \frac{E_{fuel} - m_{OHC}^{EVO} LHV_{fuel} - m_{CO}^{EVO} LHV_{CO}}{E_{fuel}} \quad (1)$$

The LHV_{fuel} is calculated based on the relative amounts of port injected fuel and direct injected fuel. The LHV_{CO} is taken to be 10 MJ/kg. The AHRR is determined from a first law of thermodynamics balance on the cylinder contents. It is essentially the chemical heat release rate minus the heat loss rate to the combustion chamber walls, and is given by:

$$AHRR = \frac{dQ}{d\theta} |_{chem} - \frac{dQ}{d\theta} |_{wall} = \frac{1}{\gamma-1} V \frac{dQ}{d\theta} + \frac{\gamma}{\gamma-1} P \frac{dQ}{d\theta} \quad (2)$$

where P is the average in-cylinder pressure, V is the cylinder volume, and γ is the ratio of specific heats for the in-cylinder gas mixture. In this work γ was taken to be a constant of 1.35 when calculating all the AHRR.

Mechanism

A reduced PRF-methanol-ethanol-DTBP mechanism was used to simulate the combustion processes of both PRF and alcohol-DTBP mixture fuels [10]. In the current study the mechanism was further extended to include a reduced *iso*-butanol sub-mechanism. Details and validations of the base PRF and PRF-methanol-ethanol-DTBP can be found in [10, 27], thus only brief introduction of the *iso*-butanol sub-mechanism is shown here.

The detailed mechanism proposed by Sarathy et al. [14] contains the four butanol isomers' oxidation mechanism, and was taken as the baseline mechanism. Direct Relation Graph Error Propagation (DRGEP) [28, 29], reaction pathway analysis and sensitivity analysis were applied to do the mechanism reduction. After the reduction, the standalone *iso*-butanol sub-mechanism contained 61 species and 293 reactions, and was merged with the base PRF-DTBP mechanism to formulate the PRF-*iso*-butanol-DTBP mechanism. Duplicated species and reactions from the reduced *iso*-butanol mechanism were removed from the integrated mechanism. A reduced NO_x sub-mechanism with 4 species and 12 reactions was also incorporated to the base mechanism [30]. The final mechanism contains 92 species and 388 reactions. Validations were conducted to ensure that the addition of the *iso*-butanol sub-mechanism did not affect the prediction abilities of the baseline PRF and DTBP sub-mechanisms. The validation of other sub-mechanisms, including the PRF and DTBP sub-mechanisms, can be found in [10, 27].

Since experimental ignition delay data was not available for the validation of the proposed mechanism under low temperature conditions, the detailed mechanism was taken as the reference for the validation. Comparisons of the ignition delay between the detailed and reduced *iso*-butanol mechanisms are shown in Figure 2. (Ignition delay was defined as the timing when a 400K-temperature increase was reached compared to the initial temperature and the validations were conducted with the CHEMKIN Pro package [31]). It is seen that the reduced mechanism predicts quite close ignition delays compared to the detailed mechanism over a wide range conditions.

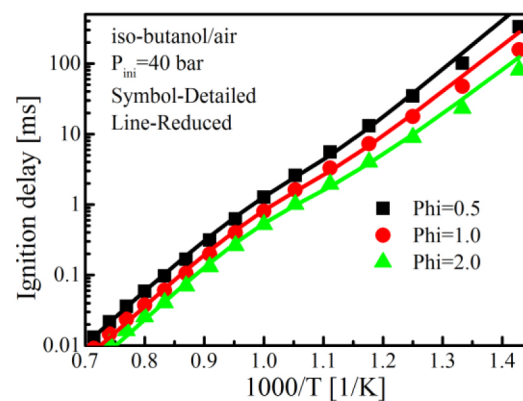
Figure 2. Comparisons of ignition delay between the detailed and current reduced *iso*-butanol sub-mechanism.

Figure 3 shows comparisons of the ignition delays between *iso*-octane and *iso*-butanol under 40 bar initial pressure conditions with different equivalence ratios. It is seen that the ignition delays of *iso*-butanol are much longer than *iso*-octane when the initial temperature is less than 900 K, thus it is expected that higher DI fuel amounts will be needed to achieve similar combustion phasing in RCCI combustion.

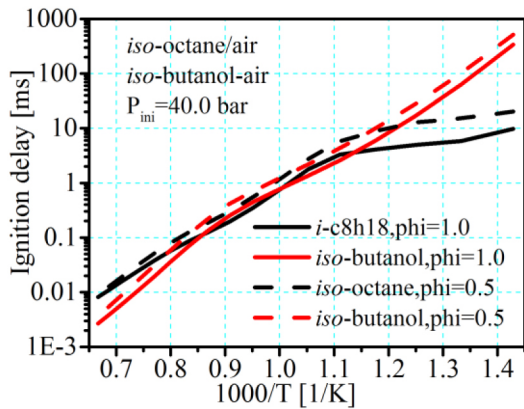


Figure 3. Comparisons of ignition delays between *iso*-octane and *iso*-butanol under 40 bar initial pressure conditions.

Figure 4 shows the predicted effect of the DTBP cetane improver additive on the ignition delay of *iso*-butanol-DTBP mixtures. The operating condition was chosen to be a representative condition in a typical RCCI combustion engine prior to ignition. It is observed that similar to methanol and ethanol, the reactivity response of *iso*-butanol to DTBP also depicts a non-linear behavior, and that small amounts of DTBP can greatly shorten the ignition delay, while further increasing the DTBP amount in the mixtures only yields limited reactivity enhancement. Addition of 10% DTBP in the *iso*-butanol-DTBP mixture yields a reactivity similar to that of PRF45 (45% *iso*-octane and 55% *n*-heptane), which is much lower than diesel (PRF0). Even so, it is seen that compared to the neat *iso*-butanol, the ignition delay is shortened by more than three times if 10% mass fraction of DTBP is applied. Noting that usually the DI fuel mass is small in RCCI engines, the DTBP only takes about 1-5% of the total fuel mass consumed per cycle in RCCI operation.

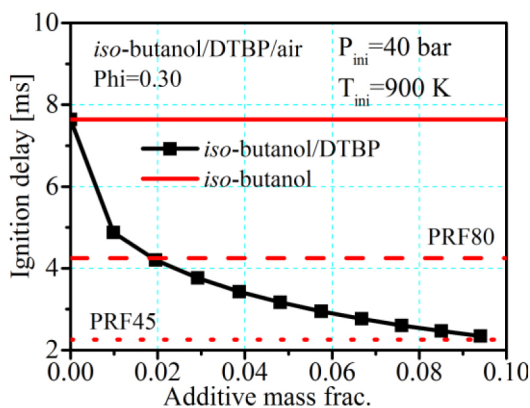


Figure 4. Effects of DTBP cetane improver additive on the reactivity of the *iso*-butanol-DTBP mixtures.

In the simulations, the physical properties of gasoline and diesel were represented by *iso*-octane and *n*-tetradecane, while the *iso*-octane and *n*-heptane mechanisms were applied as single component surrogate models for these two fuels [30]. The physical and chemical reaction mechanisms of both *iso*-butanol and DTBP fuels were applied in the simulations.

In the following sections, comparisons of RCCI combustion between experiments and simulations at the 6.5 bar IMEP condition will be presented first to serve as validation of the proposed mechanism. Then HCCI combustion simulations were conducted under the same condition and compared with the RCCI experimental and simulation results. The operating loads of both RCCI and HCCI were extended to 9.0 bar and 14.6 bar IMEP based on the gasoline/diesel RCCI experiments, and comparisons between RCCI and HCCI with various fuels under different load conditions are presented and discussed.

RESULTS AND DISCUSSION

6.5 Bar IMEP Condition

In DelVescovo et al.'s [19] experiments, the intake pressure was varied while the IMEP was kept at 6.5 bar. As mentioned above, the three fuel groups, GD, BD and iBD, specified in Table 3 were applied in the experiments. In the case of applying a mixture of *iso*-butanol and DTBP as the high reactivity fuel, 20% volume fraction of DTBP was blended with neat *iso*-butanol to improve the reactivity of the DI fuel. Since the alcohol's latent heat values are much higher than conventional gasoline, the intake cooling effect should be taken into consideration. The approach adopted by Dempsey et al. [9] was applied to account for the cooling effect of *iso*-butanol. Corrections were made to the intake temperature when using the alcohol fuels based on estimates from one dimensional cycle simulations which accounted for the charge cooling from port injected alcohols. The engine intake temperature (T_{in}) is measured at the exit of the intake surge tank, just prior to the point of port fuel injection. The intake temperature, amount of fuel port injected, intake runner wall temperature, and in-cylinder wall temperatures are all boundary conditions for the cycle simulation. Details about the cyclic simulations can be found in Dempsey et al.'s work [9].

Figure 5 shows comparisons of in-cylinder pressures and apparent heat release rates (AHRR) between the experiments and simulations at the 1.5 bar intake pressure condition. The thin gray lines in these plots are in-cylinder pressures and AHRRs of 250 individual cycles taken from the experiments, while the thick black lines indicate the ensemble-averaged results from the experiments, and the red lines are the results predicted by the simulations. It is seen that although discrepancies exist between the experiments and simulations, the general characteristics of RCCI combustion achieved using the various fuels are captured by the simulations. Cyclic variations exist in the experiments, indicated by the thin grey lines, and the predicted pressures and AHRRs are within the shadow except for the BD case. There are several possible reasons for the discrepancy observed in BD cases. The first is uncertainty in the mechanism. Currently there are limited available experimental measurements for the validation of *iso*-butanol mechanism under low temperature conditions. The second is that interactions between *n*-heptane/diesel and *iso*-butanol