A Detailed Study of Boost Pressure and Injection Timing on an RCCI Engine Map Fueled with Iso-Octane and N-Heptane Fuels

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ABSTRACT

By using two types of different fuels and changing the ratios of these fuels, Reactivity Controlled Compression Ignition Engine (RCCI) is able to provide a more effective control over combustion phase at different loads and speeds. In a typical RCCI engine which could be considered as a type of homogeneous charge compression ignition (HCCI) engine, a low reactive fuel is injected into the intake port and a high reactive fuel is directly injected into the combustion chamber. In this study, a multi-dimensional model coupled with chemical mechanism is developed to simulate an RCCI engine operation fueled with iso-octane as the low reactive fuel and n-heptane as the high reactive one. Initially, the engine map was derived using different quantities of total above-mentioned fuels at different ratios and then engine inappropriate operating points were detected and improved by changing intake air pressure and injection timing strategies. The improved criteria to extend engine map are ringing intensity limit, NO_x formation standard and gross indicated efficiency. It was concluded that high ringing intensity and NO_x formation can be reduced by increasing intake air pressure; also badfire and misfire points can get improved by retarding the injection timing.

NOMENCLATURE

ATDC	After Top Dead Center	PM	Particulate Matter
BMEP	Brake Mean Effective Pressure	PMEP	Pumping Mean Effective Pressure
BSFC	Brake Specific Fuel Consumption	PPRR	Peak Pressure Rise Rate
BTDC	Before Top Dead Center	PRF	Primary Reference Fuel
CA50	Mass Fraction Burned of 50%	RCCI	Reactivity Controlled Compression Ignition
CNG	Compressed Natural Gas		
CO	Carbon Monoxide	RI	Ringing Intensity
CO2	Carbon Dioxide	SOC	Start of Combustion
DTBP	Di-tert-butyl peroxide	SOI	Start of Injection
EGR	Exhaust Gas Recirculation	UHC	Unburned Hydrocarbon
ERC	Engine Research Center		
EPA	Environmental Protection Agency		
EVO	Exhaust Valve Opening	Notations	
GIE	Gross Indicated Efficiency	r	drop radius
GISFC	Gross Indicated Specific Fuel Consumption	Y_1	vapor mass fraction
		Ω_{KH}	calculated frequency
HCCI	Homogeneous Charge Compression Ignition	P_{max}	peak pressure
		Λ_{KH}	calculated wavelength
ISFB	In-cylinder Fuel Blend	R	ideal gas constant
IMEP	Indicated Mean Effective Pressure	B_1	adjustable parameter
IVC	Intake Valve Close	Sh_d	Sherwood number
KH-RT	Kelvin-Helmholtz Rayleigh-Taylor	C_b	adjustable parameter
LTC	Low Temperature Combustion	T_{max}	peak temperature
MFB	Mass Full Burn	D	mass diffusivity of liquid vapor in air
PCCI	Premixed Charge Compression Ignition	α	collision angle

D_0	sac diameter		$\frac{L}{D}$	ratio of the nozzle length to the nozzle diameter
γ	specific heat ratio			
d_0	parent parcel diameter		σ	surface tension
ρ_a	air density		Y_1^*	vapor mass fraction at the drop's surface
d_2	diameter of the smaller droplet			
ρ_l	liquid density			

1. INTRODUCTION

The importance of fuel economy and tighter restrictions of environmental standards on emissions such as NO_x and particulate matters have shifted the compression ignition engines toward low-temperature combustion (LTC) strategies.

The LTC has promising features with higher thermal efficiency and much lower emission level due to improved air-fuel mixture and combustion criteria (Curran *et al.,* 2013). What can be ultimately understood from numerous researches on variant alternative fuels and combustion strategies is the fact that HCCI and premixed charge compression ignition (PCCI) engines have this such capability to enhance efficiency and reduce pollutants formation simultaneously (Hardy and Reitz, 2006; Zheng *et al.,* 2015). Using two fuels with different reactivities is one of the strategies that can be used to control combustion in HCCI engines. In addition, emission production and efficiency are placed at the acceptable level. A lot of previous researches have demonstrated that this type of combustion can have a good control over the combustion phasing and heat release rate (Kokjohn *et al.,* 2011a; Splitter *et al.,* 2011a).

Some researchers have investigated the effects of several operating parameters on RCCI engines. These are injection timing, Diesel fuel quantity, gasoline to diesel fuel rate, exhaust gas recirculation, fuel additives and alternatives and intake charge conditions (Hanson *et al.,* 2010; Kokjohn *et al.* 2009; Paykani *et al.,* 2015). Splitter *et al.* (2014) employed a single cylinder heavy duty RCCI engine fueled with E85 and 2-ethylhexyl nitrate (EHN) and applied a constant cycle thermodynamic conditions with constant CA50 and net IMEP to maximize the gross thermal efficiency (GTE) by experimentally testing various intake and charge conditions. They observed points with high GTE in which relatively highly diluted mixtures were burned with a combustion efficiency of 97% and heat release rate of 12bar/CA. They also reached to a clear insight of losses based on global and premixed equivalence ratios.

Ma *et al.* (2013) evaluated the effects of multiple injection strategies on combustion phase in an RCCI engine in diverse operation conditions and reported high efficiency and low engine-out pollutants. The second injection in a double injection strategy was also introduced as a practical way to expand the engine operation limits to higher loads. A parametric study carried out by Li *et al.* (2014) on the effects of 1st and 2nd start of injection (SOI) timing and injection duration, diesel fuel mass fraction and natural gas mass fraction on a CNG/diesel RCCI engine. The second SOI timing and injection

duration were found out to be the most crucial factors which can well improve indicated power output. Splitter *et al.* (2011b) have investigated the effects of injection timing with single and double injections in a low load RCCI engine. With later single injection timing of diesel-type fuel, they observed up to 50% reduction in CO and HC as well as slight improvements in thermal efficiency. However, the best case was the one in which n-heptane fuel was introduced into the air-isooctane mixture of 0.22 equivalence ratio via a double injection strategy. In this case they reported thermal efficiency and combustion efficiency as high as 50% and 98% respectively. By developing a 3D model, Poorghasemi *et al.* (2017) simulated the operation of a CNG/diesel light duty RCCI engine and investigated the effects of numerous parameters such as split and single injections. In split injection strategy, they retarded the SOI1 toward top dead center (TDC) and calculated higher combustion temperature which more NOx production and lower HC and CO emissions were concluded, however, the results for retarding the SOI2 were quite vice versa.

Using adaptive injection strategies, Hanson *et al.* (2016) studied parameters such as main and pilot SOI timing, EGR rate, port fuel injection mass fraction and rail pressure to extend the RCCI engine operation limit to higher loads. Also, they realized that conventional diesel combustion and RCCI combustion have same sensitivities toward direct injection parameters. Except for NOx formation, almost all emissions were seen to be benefited from using no EGR. Besides, thermal efficiency was slightly improved. Walker *et al.* (2012) fueled an RCCI engine with a low pressure gasoline direct injection fueling system which is economically justifiable and compered the results with a high pressure (common rail injection) system. The results were observed to be comparable in emissions except for unburned hydrocarbons due to hampered mixture formation and combustion efficiency. Fajri *et al.* (2017) evaluated different characteristics of combustion phasing such as start of combustion, combustion duration, and 10% to 90% of mass fraction burned (MFB) for iso-octane/n-heptane fuels by varying fuels ratio, engine load and speed, injection timing, equivalence ratio, exhaust gas recirculation (EGR) application, boost pressure, injection pressure as well as combination of these different parameters toward acquiring the best engine operating points from higher engine performance and lower NOx production point of view. They specified that decreasing equivalence ratio and increasing EGR were the most effective ways to reach to this goal. In another experimental work, Benajes *et al,* (2015) found the diesel injection timing, EGR rate, and fuel blending ratio as the key

variables to reach to stable RCCI engine operation. They observed great dependency of NOx and soot production to engine speed and diesel SOI, respectively. It was claimed that lowering the compression ratio from 14.4:1 to 11:1 can result in great improvements in UHC, carbon monoxide and soot emissions.

Lim and Reitz (2014) evaluated the possibility of achieving to high load RCCI combustion by implementing computational tools. A dual injection strategy was optimized for introducing isooctane within the combustion chamber and a single n-heptane was set to ignite the mixture. They concluded that the first iso-octane injection timing has the main role in emissions while the ringing intensity could get minimized with an optimized iso-octane second SOI. The n-heptane injection mass and timing was introduced as the most effective tool to control the combustion phase.

Using multi-dimensional CFD simulations combined with engine testing, Molina *et al.* (2015) analyzed performance and emissions of an RCCI engine at low, medium and high loads to find out the effective parameters in order to extend its operation range. They observed that at low loads, double direct injection strategies with high amounts of in-cylinder fuel blend (ICFB) and at high loads, single injection strategies could work properly to attain adequate and stable combustion phase. Wang *et al.* (2016) experimentally compared the neat diesel LTC operation with RCCI regimes at low loads in a heavy duty engine and reported much lower HC and CO emissions as well as fuel consumption in LTC regime. However, RCCI emitted lower NOx and soot pollutants. Then they evaluated the RCCI operation in different speeds. They found out that high gasoline/diesel proportion and EGR rate with slightly advanced diesel injection are of the major importance for extending the RCCI operational limit at high speeds. The effects of fuel reactivity gradients in a gasoline/diesel RCCI engine was investigated by Li *et al.* (2015) via developing new chemical mechanisms. They realized that the fuel reactivity gradient could reduce heat release rate and mitigate peak pressure rise rate as well as NOx production due to retarding the ignition timing. DelVescovo *et al.* (2017) investigated different equivalence ratio between 0.28 and 0.35 and different SOI between -140º and -35º ATDC and showed peak gross efficiency was achieved between -60º and -45º SOI while NOx emission peaked around -25º SOI. By developing a 3D-CFD combustion model, Nazemi and Shahbakhti (2016) optimized the effects of four different parameters including: spray angle, SOI timing, injection pressure and pressure rise rate on combustion and performance of an RCCI engine and found out that spray angle and injection pressure have the most and the least effects on RCCI combustion and performance.

The surrogate fuels have been widely attempted in RCCI engine research. The works cover a wide range of octane and cetane numbers providing diverse reactivity levels. In some works done, the surrogate fuels have been used as additives (or as an alternative to gasoline and diesel fuels) where ethanol and hydrous ethanol fuels are among the common fuels used (Curran *et al.,* 2014; Splitter *et al.,* 2011c). Splitter *et al.* (2011a) experimentally used E85 (85% Ethanol fuel and 15% gasoline fuel) instead of gasoline in a gasoline/diesel fueled RCCI engine and reported an increase in IMEP from 14.5 bar to 16.5 bar. It was also realized that by replacing gasoline with E85, the engine thermal efficiency can get improved by 3% due to less EGR demand. Curran *et al.* (2012) elucidated that employing ethanol fuel in the RCCI engine results in further retard in the start of low-temperature reactions and consequently in combustion phase. The UHC pollutant was seen to get reduced by injecting more amount of diesel fuel. According to DelVescovo *et al.* (2015), three fuel blends, EEE/diesel, iso-butanol/diesel and iso-butanol/ iso-butanol + DTBP were evaluated and concluded by using iso-butanol fuel as a high octane fuel, more direct injection reactive fuel was required to match combustion phasing similarly to using gasoline fuel as primary fuel, therefore, NOx and CO emissions were increased due to using high direct injection fuel and low premixed equivalence ratio.

In an RCCI engine, varying the rate of gasoline to diesel fuels changes the mixture reactivity, so combustion phasing is controlled by changing the air-fuel mixture reactivity. Diesel fuel is used as a tool for changing the mixture reactivity so that using diesel fuel in different conditions can drive the combustion process to regions with more or less produced pollutants and worse or better performance.

As specified, studying a wide range of various injection strategies and evaluating their effects to improve the engine performance and the level of engine-out emission were at the center of major attention of previous researchers. Whereas making appropriate reactivity stratification is not possible in low load conditions (and especially when the diesel fuel is less than gasoline fuel), varying injection strategies is a plausible way to improve these engine operating points. In this research, the engine operating map for different total amount of fuel and variant ratios of iso-octane to n-heptane fuels were derived in a constant speed and as a novelty, different injection strategies were utilized directly into the engine map to refine and extend the engine operating points in low loads and high levels of PRFs and also the possibility of boost pressure and making lean mixture were evaluated in high loads and in an extensive region of engine operating points. Finally, improved engine map was obtained for the different total amount of fuel and different iso-octane to n-heptane fuels ratios.

2. EXPERIMENTAL AND SIMULATION RESULTS

In this study, the experimental results of a single cylinder heavy duty diesel engine obtained from conducted tests in the University of Wisconsin-Madison Engine Research Center, were used in order to validate the developed CFD model.

This engine is modeled by using the CONVERGE CFD tool (Richards *et al.,* 2014). The engine uses

two fuel injectors, first injector injected low reactivity fuel into the port which mixed to air, and the second injector injected high reactivity fuel into the in-cylinder mixture, this is located horizontally at the center of cylinder. Further specifications of the engine and also specifications of these two injectors are tabulated in Table 1 and Table 2, respectively.

Table 1 Specification of Wisconsin – Madison ERC diesel engine (Splitter, 2010)

Cat® 3401E SCOTE engine geometry	
Cylinder Volume (Liter)	2.44
Cylinder Bore (cm)	13.72
Connecting Rod Length (cm)	21.16
Geometrical Compression Ratio	16.1
Number of Valve in cylinder	4
Intake Valve Closing (ºATDC)	-143 and -85
Exhaust Valve Opening (ºATDC)	130

Table 2 Specification of Low and High pressure injector(Splitter, 2010)

Low pressure injcetor	
Injection Pressure (bar)	5.17
High-Pressure Injector	
Number of Nozzle at Injector	6
Nozzle Bore (μm)	250
Injector Pressure (bar)	800
Included Spark Angle (Degree)	145

In-cylinder pressure was measured by a pressure sensor (Kistler Model 6067C1). Setup results were based upon the average values of engine 500 cycles to minimize the effects of cyclic variations. The intake air flow rate was measured by a chocked flow orifice, intake and exhaust air chamber were equipped with a proportional integral-derivate controller. Also, PM in the exhaust gases were measured by AVL devices (Splitter, 2010).

The experimental engine test set-up specifications along with the main outputs of the tests are listed in the Table 3 and Table 4, respectively. According to the experimental results, NO$_x$ formation level is lower than Environmental Protection Agency 2010 [0.268 gr/kW-h for NO$_x$ formation].

Together with the primary and secondary fuel breakup, respective spray models such as collision, coalescence, evaporation and wall impingement are necessary in order to simulate the spray atomization formation.

In this simulation, a developed model was used to simulate the fuel evaporation (Amsden *et al.*, 1989). Schmidt and Rutland (2000) developed spray collision model was used to simulate the fuel collision. To simulate coalescence of fuel droplets, a model by Post and Abraham (2002) was utilized. A model which includes two impingement regimes based on the Weber number (GONZALEZ D *et al.,*

1992; Naber and Reitz, 1988), was applied for simulation of wall impingement phenomena. The Kelvin-Helmholtz Rayleigh-Taylor (KH-RT) model has been applied to simulate fuel droplets breakup (Reitz and Bracco, 1986; Reitz, 1987). In order to include detailed chemistry in combustion applications, the SAGE model has been used in this study (Senecal *et al.*, 2003), iso-octane and n-heptane fuels have been used as a representative of gasoline and diesel fuels respectively which are known as primary reference fuels. The model uses a reduced mechanism to simulate the n-heptane and iso-octane chemical reactions with 108 species and 435 reactions (Wang *et al.*, 2015).

It is shown quite reasonable to use iso-octane fuel as gasoline-type fuel and n-heptane fuel as diesel type one (Ra *et al.*, 2009). A Nitrogen oxides mechanism including 12 reactions was used to predict NO$_x$ formation (Sun, 2007). Also, Hiroyasu model was employed to predict soot formation (Hiroyasu and Kadota, 1976; Lavoie *et al.*, 1970).

Table 3 Engine Test Conditions (Kokjohn *et al.*, 2011b; Splitter, 2010)

Engine characteristics	Specifications	
	Case1	Case2
Engine Speed (RPM)	1300	1300
EGR Rate (%)	0	41
Equivalence Ratio	0.24	0.51
Intake Air Temperature (ºC)	32	32
Intake Air Pressure (bar)	1.37	1.74
Total Fuel (mg)	60.1	94
Percent Gasoline by Mass (% by mass)	68	89
Diesel Injection Pressure (bar)	800	800
Start of Diesel Injection in Pulse1 (ºATDC)	-58	-58
First Injection Duration (ºCA)	5.07	3.9
Percent of Diesel Fuel in Pulse1 (% by mass)	62	67
Start of Diesel Injection in Pulse2 (ºATDC)	-37	-37
Second Injection Duration (ºCA)	2.34	2
Intake Valve Closing (ºATDC)	-143	-143

Table 4 Experimental Results (Kokjohn *et al.*, 2011b; Splitter, 2010)

Engine characteristics	Case1	Case2
GI Power (kW)	13.63	24.6
GI SFC (gr/kW-h)	172	150
GI MEP (bar)	5.16	9.3
GI NOx (gr/kW-h)	0.015	0.01
GI Soot (gr/kW-h)	0.005	0.011

Due to geometrical symmetry of combustion chamber, only a 60º sector of engine cylinder has been considered to improve computational efficiency which is depicted in Fig. 1.

Aiming a more precise comparison, the developed model results for in-cylinder pressure and heat release rate at the same engine operating conditions and the experiments results are depicted in Figs. 2 and 3. The simulation results are in a good agreement with the experimental curves in both trends and values. Also, A comparison between predicted and practical levels of emissions, which is depicted in Fig 4. demonstrates almost reasonable coincidences.
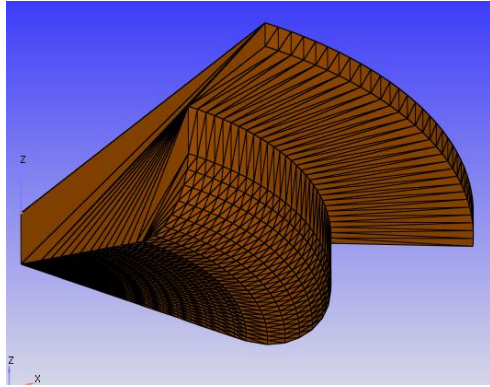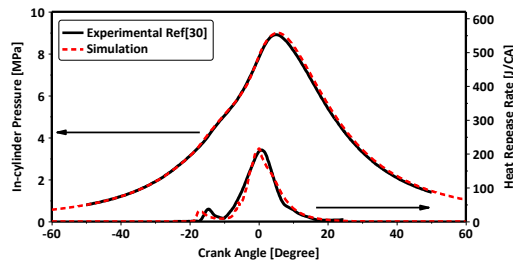

Fig. 1. A 60º Sector of Engine Cylinder Geometry.

Fig. 2. Comparison between Experimental and Simulation Results of In-cylinder Pressure and Heat Release Rate for Case1.
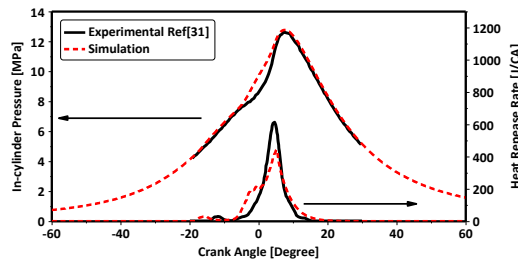
Fig. 3. Comparison between Experimental and Simulation Results of In-cylinder Pressure and Heat Release Rate for Case2.

The small discrepancies can be due to lower heating value of PRFs in comparison with diesel and gasoline fuels. furthermore, the octane number of iso-octane fuel is more than gasoline fuel and the cetane number of n-heptane fuel is more than diesel fuel, so there would be some differences in the formation and consumption of species during the reaction which does affect the pressure, heat release rate and pollutant formation in the model simulation. For example, in case 2, NOx formation can be seen was predicted over experimental data, this is due to using EGR in simulation, obtaining the correct EGR

components and temperature at IVC are fairly difficult, differences in the modelling of EGR has caused early heat release rate and high NOx formation. Since the model was simulated the interval between the IVC to EVO and pumping loss were not considered, the final results of future simulations will be based on the gross IMEP. Boost pressure can affect the PMEP as a result of increase in back pressure. When the turbocharged engine needs more boost pressure, the waste-gate valve or VGT vanes have to be closed and this can exceedingly have impacts on the PMEP. More optimizations will be needed when the PMEP and FMEP can be calculated in the real test setup.
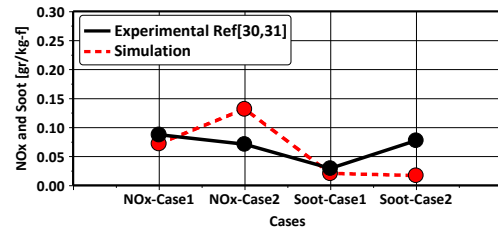
Fig. 4. Comparison between Simulation and Experimental Results of In-cylinder Emissions.

3. BASIC EQUATIONS

Spray primary and secondary breakups is modeled by KH-RT model. KH model is applied for primary breakup after injection and RT model is referred to the secondary breakup. The time of Primary breakup is calculated by Eq. (1):

$$\tau_{KH} = \frac{3.726B_1 r}{\Omega_{KH} \Lambda_{KH}} \tag{1}$$

Where, B_1 is an adjustable parameter, r is drop radius and Λ_{KH}, Ω_{KH} are the calculated wavelength and frequency of the fastest growing wave, respectively. Fast breakup and better air to fuel mixing can be achieved by smaller B_1 (Dempsey, 2013).

After a certain breakup length L_b, RT model continues the breakup process which this length is calculated by the empirical following equation:

$$L_b = C_b d_0 \sqrt{\frac{\rho_{fuel}}{\rho_{air}}} \tag{2}$$

d_0 is the parent parcel diameter and C_b is an adjustable parameter. KH-RT model has many adjustable parameters to set the appropriate penetration length and predict the time of evaporation which they are applicable for calibrating primary model.

Droplet collision model affects the dense spray region in proximity to the injection nozzle. The region near the injection nozzle increases the probability of collisions. Collision events depend on the ratio of droplet sizes, gas density, gas velocity, the fuel-air ratio of the gas around the droplets. The final impact of collision would affect the process of break-up. the most important dimensionless parameters governing the collision process is the

Weber number, differences in Weber number can result in the different type of collision process, as an example, in low Weber number, coalescence can happen when two small droplets collide and make a bigger droplet after collision and once the Weber number is high, these two small droplets can separate temporarily after collision (Baumgarten, 2006).

$$We_{coll} = \frac{\rho_l d_2 v_{rel}^2}{\sigma} \qquad (3)$$

$$v_{rel} = |\bar{v}_2 - \bar{v}_1| = \sqrt{v_1^2 + v_2^2 - 2v_1 v_2 \cos\alpha} \qquad (4)$$

ρ_l is the liquid drop density, σ is the surface tension, d_2 is the diameter of the smaller droplet, α is the collision angle between the trajectories of both drops and subscripts 1 and 2 refer to the larger and the smaller droplet, respectively.

Wall impingement process happens when the spray penetration is high enough to reach to the cylinder wall and the piston crown. This collision can affect the performance and emission of direct injection engine especially in cold start process and it would be a problem by using high pressure injectors and injection in low density of air-fuel mixture (Baumgarten, 2006).

Weber number is defined to represent a measure of the droplet kinetic energy based on the droplet diameter and its velocity normal to the wall (Stiesch, 2013).

$$We_{in} = \frac{\rho_l d_{in} v_{in}^2}{\sigma} \qquad (5)$$

$$We_{out} = 0.678 We_{in} \exp(-0.044 We_{in})$$
$$5 < We_{in} < 80 \qquad (6)$$

In $We_{in} \leq 5$, the drop sticks to the wall. Within the range $5 < We_{in} < 80$ the drop rebounds and for incident Weber numbers more than 80 the drops slide along the wall in the manner of a liquid jet.

For modelling spray evaporation, the Frossling model (Amsden *et al.*, 1989) was used. In this model, the rate of varying droplet diameter is calculated by the Eqs. (7) and (8).

$$\frac{dr_0}{dt} = -\frac{\rho_g D}{2\rho_l r_0} B_d Sh_d \qquad (7)$$

$$B_d = \frac{Y_1^* - Y_1}{1 - Y_1^*} \qquad (8)$$

Where D is the mass diffusivity of liquid vapor in air, Y_1^* is the vapor mass fraction at the drop's surface, Y_1 is the vapor mass fraction, and Sh_d is the Sherwood number.

The spray cone angle is calculated using Eq. (9). The angle is one of the most important parameters in simulating fuel atomization process and spray penetration; therefore, a model developed by Hiroyasu and Arai (Hiroyasu and Arai, 1990) was

employed in this study in order to predict the spray cone angle.

$$\theta = 83.5 \left(\frac{L}{D}\right)^{-0.22} \left(\frac{D}{D_0}\right)^{0.15} \left(\frac{\rho_a}{\rho_l}\right)^{0.26} \qquad (9)$$

Where, $\frac{L}{D}$ is the ratio of the nozzle length to the nozzle diameter, D_0 is the Sac diameter, ρ_a and ρ_l are the density of air and liquid, respectively.

To predict NOx emission, the following 12 reactions were used (Sun, 2007).

N + NO = N2 + O

N + O2 = NO + O

N + OH = NO + H

N2O + O = N2 + O2

N2O + O = 2NO

N2O + H = N2 + OH

N2O + OH = N2 + HO2

N2O + M = N2 + O + M

HO2 + NO = NO2 + OH

NO + O + M = NO2 + M

NO2 + O = NO + O2

NO + H = NO + OH
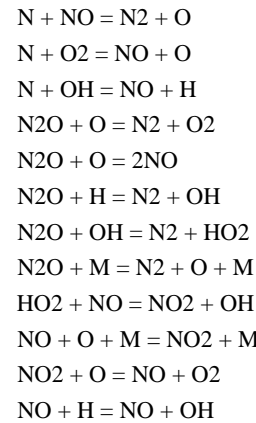
Equation (10) represents the RI (Ringing Intensity) correlation. Since the engine operates under the boosted condition, the peak pressure rise rate is not a representative of knock; therefore, the RI correlation is used based on the model developed in (Eng, 2002).

$$RI\left[\frac{kW}{m^2}\right] = \frac{1}{2\gamma} \frac{\left(\beta \frac{dP}{dt}|_{max}\right)^2}{P_{max}} \sqrt{\gamma R T_{max}} \qquad (10)$$

Where, γ is the specific heat ratio, $\frac{dP}{dt}|_{max}$ is the PPRR, P_{max} is the peak pressure, R is the ideal gas constant, T_{max} is the peak temperature and β is a constant which is taken to be 0.05 ms. Dec's studies (Dec and Yang, 2010) show that the RI below 5 MW/m2 yields an acceptable engine noise. Therefore, this will be used as the maximum acceptable value in this study.

In this paper, the Eq. (11) is used to express the ratio of two fuels.

$$PRF = \frac{m_{Iso-Octane}}{m_{Iso-Octane} + m_{N-Heptane}} \qquad (11)$$

4. RESULTS AND DISCUSSION

4.1. Evaluation of Changing Iso-Octane to N-Heptane fuels Ratio

This study seeks for extending engine operating points through increasing intake air pressure and changing injection timing in an extended map with
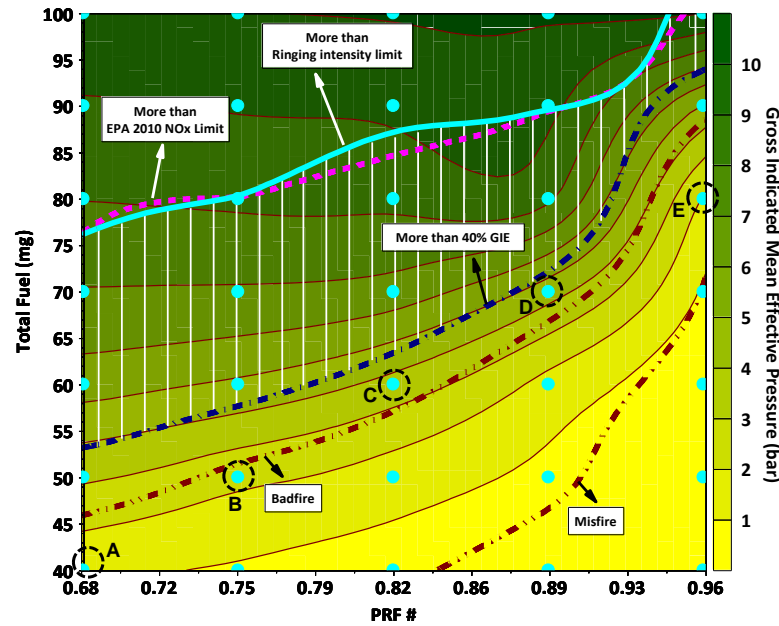
Fig. 5. RCCI Engine Performance Map Displaying NOₓ Formation and RI Limits, GIE, Badfire and Misfire Limit.

varied total fuel and also iso-octane to n-heptane fuels ratio. The total amount of fuel has been increased from 40 to 100 mg per cycle and also the iso-octane to n-heptane fuels ratio has been changed from 68% to 96%.

Also 35 engine operating points have been selected based upon changing loads and fuels ratio at the same speed to obtain a complete view of the engine under different operating conditions. The simulation parameters have been kept unchanged at all mentioned points except for injection duration of n-heptane fuel which has been solely changed due to constant injection pressure. It is also worthy to note that all cases are studied with use of no EGR.

Figure 5 shows a complete view of the results of these 35 engine operating points. In this engine map, indicated mean effective pressure (IMEP) is a representative of badfiring and misfiring regions, also the curves of RI and NOₓ formation are visible. In the present work, remaining 50% to 85% of fuel energy as unburned fuel has been considered as a criterion for determining badfiring regions while existence of more than 85% of fuel energy in unburned fuel has been considered as a criterion to indicate misfiring regions.

The specified regions in Fig. 5 (vertical lines in sequence) represents the best operating condition in terms of performance parameters such as low RI, low NOₓ formation and high GIE.

The results show that by reducing the amount of total fuel and increasing the percentage of iso-octane fuel, combustion moves toward badfiring and misfiring regions, since there would be no possibility to maintain acceptable fuel stratification in terms of reactivity within the combustion chamber by reducing the amount of n-heptane fuel, therefore, iso-octane fuel in the cylinder would have no chance to

participate in combustion and consequently, leading to badfiring.

The duration between start of n-heptane fuel injection in pulse 1 and the location of 5% mass fuel burn (MFB of 5%) can be observed in Fig. 6. Increasing the amount of n-heptane fuel improves fuel reactivity, so causes advance in combustion phasing and shortens combustion duration. The NOₓ formation rate is increased by reduction in combustion duration.

As shown in Fig. 5, in-cylinder temperature and NOₓ formation are decreased by increasing iso-octane due to retardation of combustion phasing. Abnormal combustion takes place in the region of of low amounts of total fuel and high amounts of PRF as a result of weak fuel stratification.

The gross indicated specific fuel consumption (GISFC), Fig. 7, is increased by moving to the region of weak fuel stratification and this is because of badfiring combustion.

Table 5 illustrates the comparison between different engine operating points to demonstrate in-cylinder temperature and n-heptane and iso-octane fuels mass fractions, the information is related to the following points: 1- total fuel is ranged from 40 to 100 mg in which PRF is 0.82, 2- total fuel is equal to 70 mg and PRF is changed from 0.68 to 0.96.

4.2. Improvement of Engine Operating Points to Extend the Range of Operation

It is proven that RCCI engines are capable to operate with good performance but within a limited range. Accordingly, extending this efficient and reliable operating range is a pivotal necessity in the way of RCCI engines development. The two available engine parameters that are injection timing and inlet air pressure were used to improve the engine
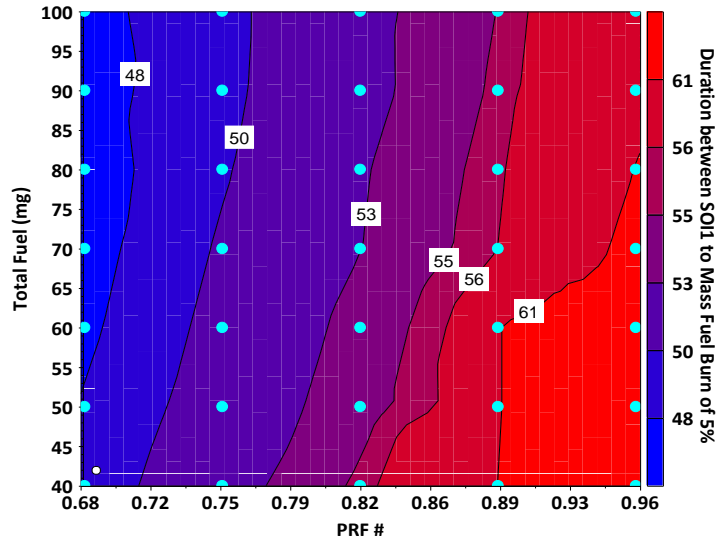
Fig. 6. Duration between Start of N-heptane Fuel Injection and MFB of 5%.
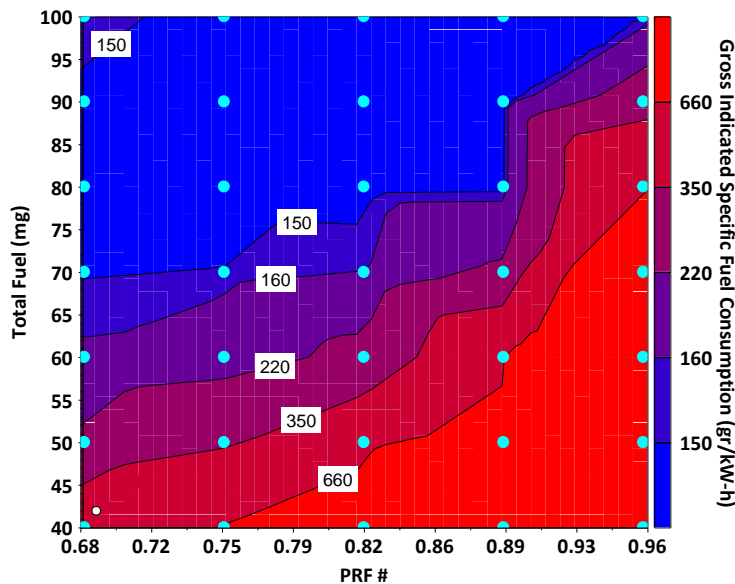

Fig. 7. Comparison of Gross Indicated Specific Fuel Consumption in Different Engine Operating Points.

inappropriate operating points which are corresponded with high emission production, high RI and low engine efficiency.

Injection timing has a great impact on the combustion phasing since it changes fuel reactivity within combustion chamber which this is important in initiating combustion phase. Retarding n-heptane fuel can accumulate fuel with high reactivity in closer points within the cylinder, therefore, combustion phasing is advanced and heat release rate is drastically increased, owing to the fact that the injected n-heptane fuel has less opportunity to mix with primary mixture. Enhanced mixing of n-heptane fuel with in-cylinder mixture and reduction of high reactivity regions are made by advancing n-heptane fuel injection timing. This results in further delay in start of combustion phasing.

Intake air boost pressure is a parameter that can easily improve the upper region of engine operating point. By increasing intake air pressure and making mixture leaner, several events take place. The first one, oxygen molecule concentration is increased and this is an obstacle against fuel spray penetration. This can accumulate n-heptane concentration in regions near injectors, so increasing reactivity regions and finally this will be able to advance the start of combustion. Excessive air, the second event, can reduce the temperature in combustion chamber and then remarkably decrease NO_x formation, although excessive air can provide the opportunity for NOx to form, nevertheless, decreasing in temperature has a deeply key role to reduce thermal NOx formation and finally, the engine-out NOx is reduced. The third one is combustion duration, increasing boost pressure can prolong the combustion duration, due to reduction of heat release rate, and adiabatic flame temperature.
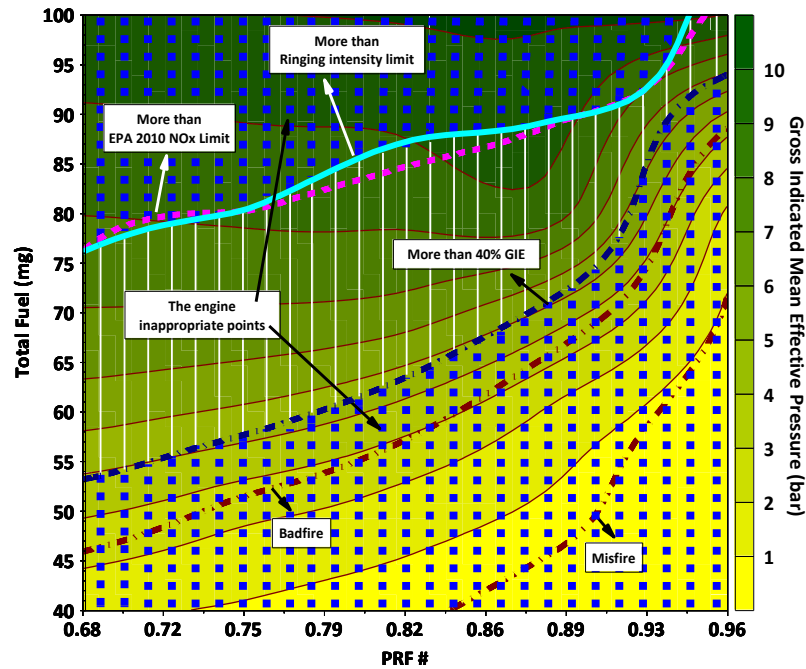
Fig. 8. Upper and Lower Regions for Engine Inappropriate Operating Points.

The upper and lower regions of engine inappropriate operating points are shown in Fig. 8. These regions were improved by varying intake air pressure and n-heptane fuel injection timing.

As shown in Fig. 9, two typical points representing engine inappropriate operating conditions with 90 mg of total fuel and PRF equal to 0.68 and 0.75 were selected to study the effects of increased intake air pressure.
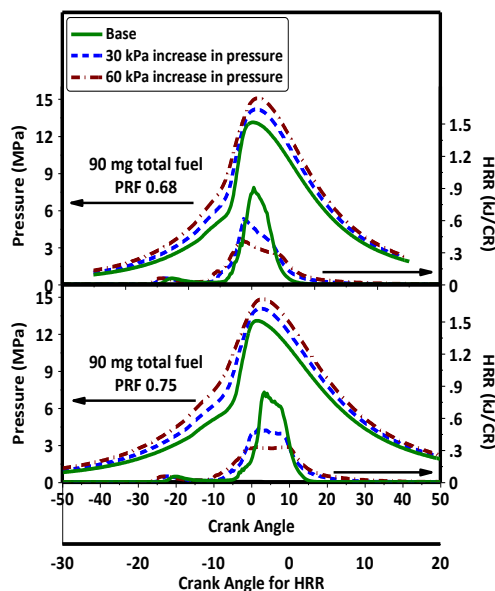

Fig. 9. In-cylinder Pressure and Heat Release Rate With Increasing 30 and 60 [kPa] in Intake Air Pressure for Two Engine Inappropriate Operating Regions.

The start of heat release is advanced by increasing intake air pressure which can prolong the duration of heat release, too. As a result, the point of peak pressure within the cylinder is retarded and RI is decreased which is obvious in Fig. 9. Also, the number of points with high temperature inside the combustion chamber and consequently, amount of NO_x formation are reduced.

Increasing intake air pressure by 30 and 60 [kPa] eliminates the upper region of inappropriate operating points. Figs. 10 and 11 clearly show these effects. Therefore, by increasing intake air pressure to 60 [kPa], the upper region of inappropriate operating points were added to the proper-functioning region.

The lower regions of engine inappropriate operating points with less than 40% indicated efficiency are made of the results of low n-heptane fuel amount. Therefore, the mixture is unable to initiate a good combustion and this leads to greater badfiring and misfiring regions. In order to improve these operating points, increasing the reactivity of primary ignition kernel is an effective way, subsequently, double injection strategy of n-heptane fuel has been converted to the single injection and also injection timing is delayed to reduce duration between SOI and SOC. Retarded single injection is one of the best choices in order to prevent n-heptane fuel from being entirely mixed which means more accumulation of reactive fuel everywhere within the chamber. In diesel engine, retarding of diesel fuel can delay in combustion phasing, on the contrary, RCCI engines operate with differences, fuel stratification in terms of reactivity is changed with retardation of high reactive fuel and causes high reactivity gradient and high possibility of combustion initiation.

Table 5 Comparison of engine operating points in different total amounts of fuel

TDC	Temperature (°K)	Y_{IC8H18}	Y_{NC7H16}
PRF 0.82 / T.Fuel 40 mg			
PRF 0.82 / T.Fuel 50 mg			
PRF 0.82 / T.Fuel 60 mg			
PRF 0.82 / T.Fuel 70 mg			
PRF 0.82 / T.Fuel 80 mg			
PRF 0.82 / T.Fuel 90 mg			
PRF 0.82 / T.Fuel 100 mg			
PRF 0.68 / T.Fuel 70 mg			
PRF 0.75 / T.Fuel 70 mg			
PRF 0.82 / T.Fuel 70 mg			
PRF 0.89 / T.Fuel 70 mg			
PRF 0.96 / T.Fuel 70 mg			

temp: 1000 1250 1500 1750 2000

yIC8H18: 0.001 0.00325 0.0055 0.00775 0.01 0.01225

yNC7H16: 0.0001 0.00046 0.00082 0.00118 0.00154 0.0019

For a closer look at this topic, two engine operating points at the region with poor performance in engine map were selected with the total amount of fuel equal to 60 mg and PRF equal to 0.82 and 0.89. In Fig. 12, variations of the cylinder pressure, heat release rate and total amount of heat release at these points are displayed. It is clearly shown that by increasing high reactivity regions in the combustion chamber, the possibility of complete combustion in the engine increases. As a result, heat release is advanced and more fuel is burned before the start of expansion phase and these points are set far from badfiring or misfiring regions.

Although retarding single injection timing up to 22o [BTDC] results in improvement of heat release rate and causes normal combustion in the region of badfiring area, nevertheless, the retardation of n-heptane fuel injection can increase the NOx formation due to increasing the number of high temperature regions.

As it can be seen in Figs. 13 and 14, the injection timing in all parts of the lower region of engine inappropriate operating points, has been affected by implementing single injection at 37° and 22° [BTDC], respectively. According to these figures, retarding fuel injection has created some improvement in these operating points.

Injection timing was changed in order to keep injection pressure constant, but the rest of injection parameters were not altered.

Figure 15 shows the start of combustion vs. n-heptane fuel injection timing for the indicated cases of Fig. 5 to extend the fact of the improving effects of n-heptane fuel retardation on in-cylinder reactivity and then combustion behavior. As always, once the fuel stratification is not efficient for initiating combustion, retarding injection timing and varying double injection to single injection can be effective for this issue. Meanwhile, more retardation would not influence on the complete combustion and just advanced the start of combustion.

5. CONCLUSION

Reactivity controlled compression ignition strategies are known to be the most effective way ever to reduce NOx and soot formation in internal combustion engines. The challenge of controlling combustion initiation and reaching to lower emissions levels at the same time is adequately met by changing the total reactivity of the fuels used in these engines.

The simulation results have been derived and assessed for 35 set point of engine running map under wide operating range in different loads. The outcome resulted in a detailed view of engine loading which is controlled by varying the iso-octane to n-heptane fuels ratio, so the combustion phasing is managed by adding a high reactivity fuel to the primary air-fuel mixture.

The results of engine operating maps clearly indicate that the combustion process has a tendency to enter badfiring and misfiring regions in case of reducing the amount of total fuel and increasing the percentage of iso-octane to n-heptane fuels ratio, therefore, the possibility of perfect combustion is diminished when engine runs with very lean mixture or comparatively
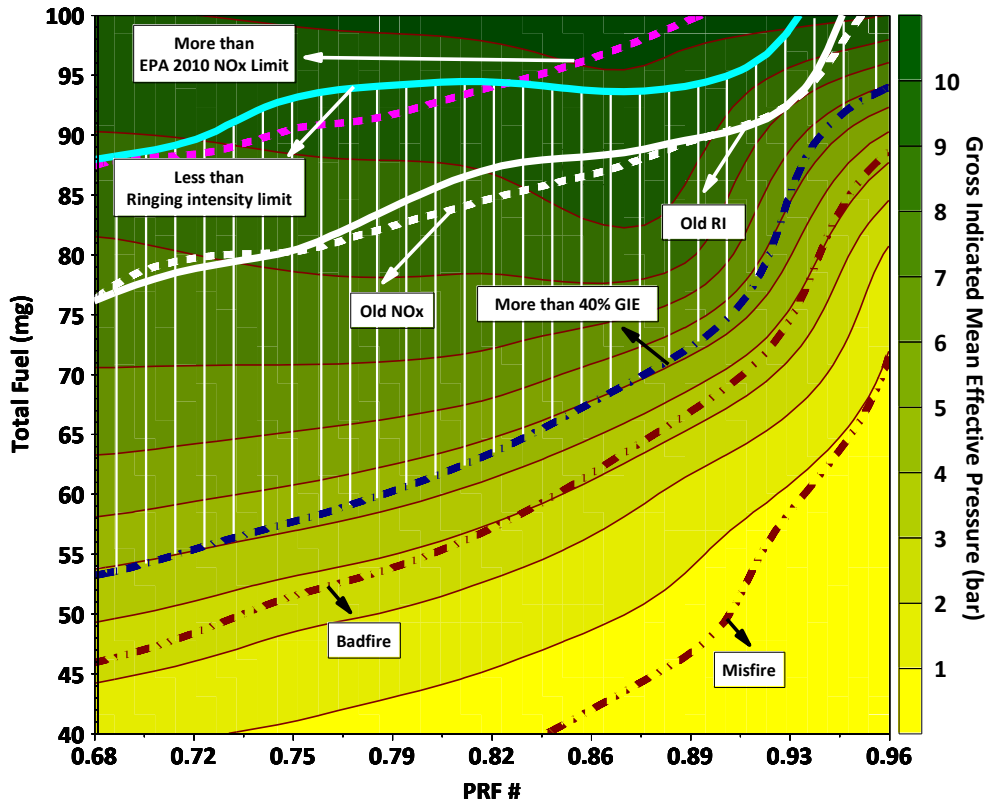
Fig. 10. Improving Upper Region of Inappropriate Operating Points by Increasing Intake Air Pressure in 30 [kPa].
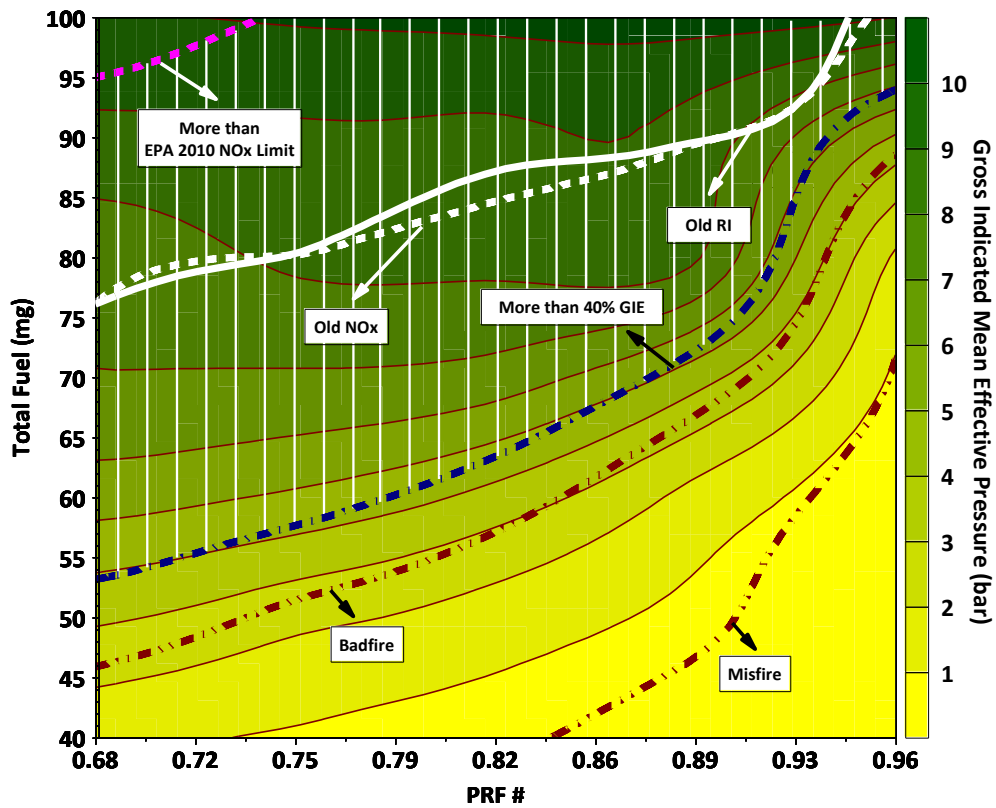

Fig. 11. Improving Upper Region of Inappropriate Operating Points by Increasing Intake Air Pressure in 60 [kPa].
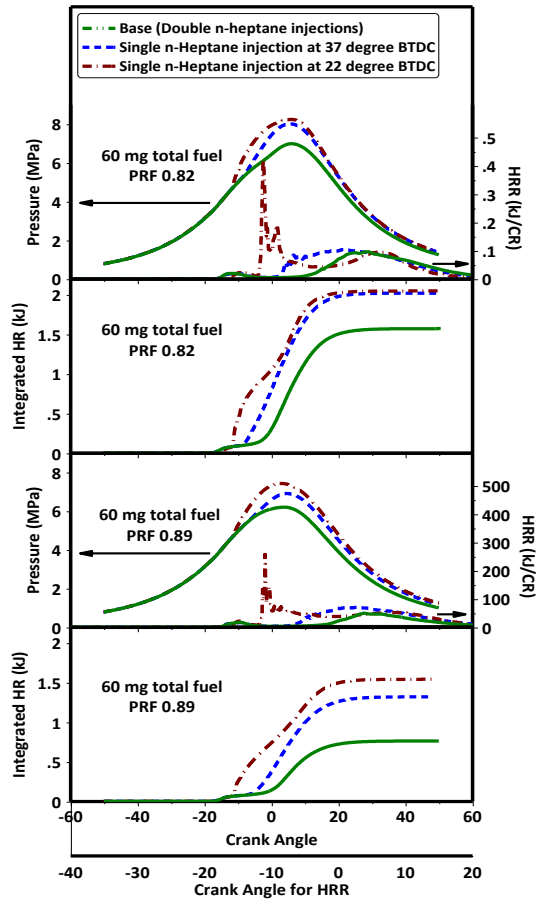
Fig. 12. In-cylinder Pressure and Heat Release Rate with Retarding Injection Timing and Switching Double to Single Injection.
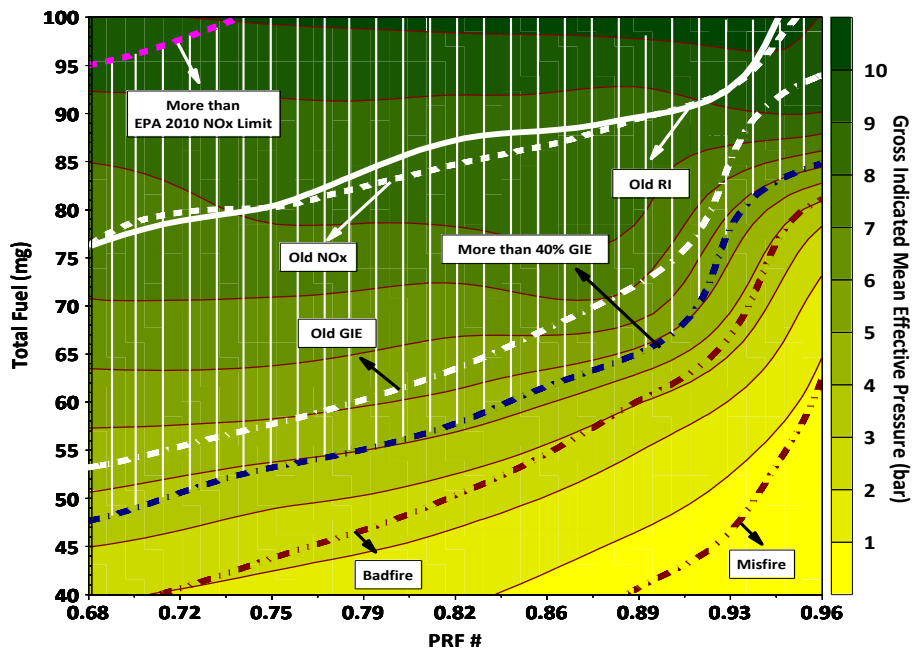

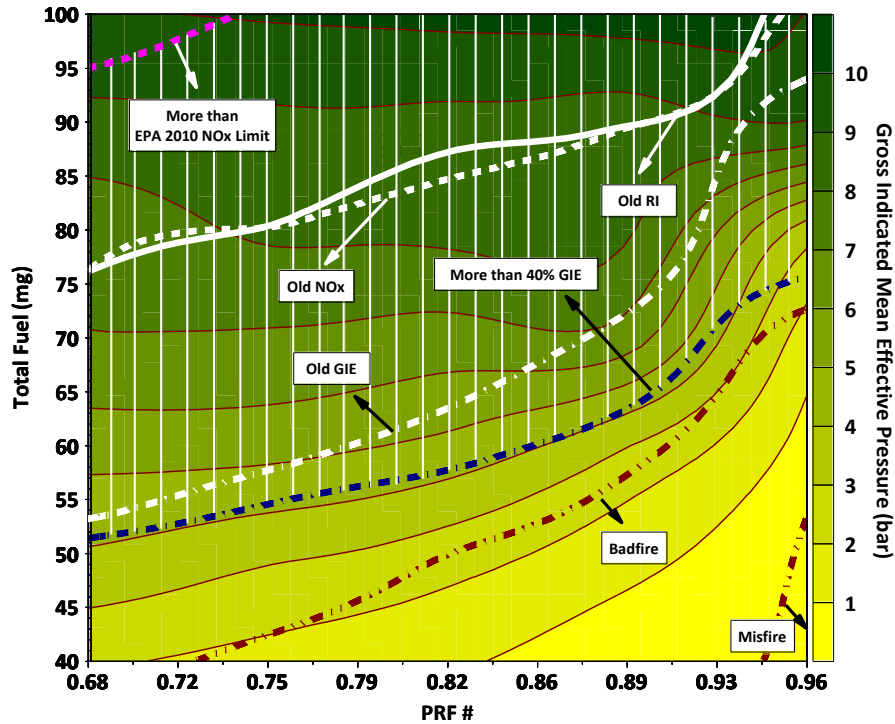**Fig. 13. Improving Lower Region of Engine Inappropriate Operating Points With Retarding Single Injection Timing to 37º [BTDC].**

Fig. 14. Improving the Lower Region of Engine Inappropriate Operating Points with Retarding Single Injection Timing to 22º [BTDC].
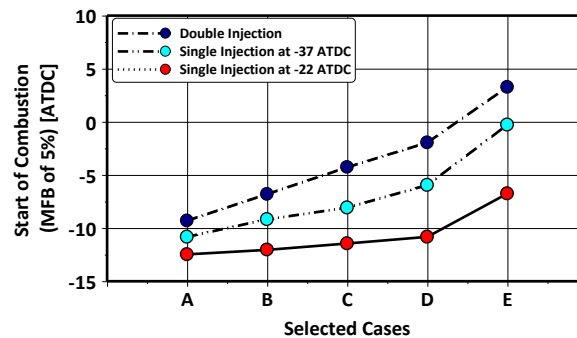

Fig. 15. Start of Combustion vs. N-heptane Fuel Injection Timing for Selected Cases from Fig. 5.

low amount of n-heptane fuel rather than iso-octane fuel. The reason is that it is very difficult to effectively change the reactivity of fuel delivered to the combustion chamber when the amount of n-heptane fuel has been reduced, therefore, iso-octane fuel that is present in cylinder would have no chance to initiate combustion so it is shifted to badfire.

In the region with more excess n-heptane fuel than iso-octane fuel, engine exceeds RI limit and NO_x formation standards as a result of providing a mixture with higher reactivity.

Investigating the duration between start of n-heptane fuel injection in pulse 1 and the location of mass fraction burned of 5% indicates that advance in combustion phasing and decrease in combustion duration versus increase in the amount of n-heptane fuel is achieved. Consequently, rate of NO_x formation is increased by lowering combustion durationExtending range of operation and improving appropriate engine operating points was revealed to

be possible by means of enhancing intake air pressure and retarding the injection timing. Through increasing intake air pressure, leaner mixture is formed, start of heat release is delayed and duration of heat release is prolonged. As a result, the occurrence of peak pressure within the cylinder is retarded and RI is mitigated. Also, high temperature points inside the combustion chamber is decreased so the amount of NO_x formation is reduced. Increasing the reactivity of primary ignition kernel is selected as a feasible alternative to improve lower region of inappropriate operating points, therefore, double injection of n-heptane fuel has been converted to the single injection and also injection timing is delayed to reduce duration between SOI and SOC. According to this method, retarding fuel injection got obvious to result in notable improvements in characteristics of these points.

By enlarging the range of engine operation, an extensive map with large range of different amount of total fuel and variant iso-octane to n-heptane fuels

ratios is obtained.

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