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Multi-Objective Optimization of a RCCI Engine Fueled with Diesel Fuel and Natural Gas Enriched with Hydrogen

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Abstract: The present study seeks to conduct the optimization of a heavy-duty diesel engine under RCCI combustion fueled with diesel fuel and natural gas enriched with hydrogen. Since NOx emission is one of the most important concerns of using hydrogen as a sole fuel or an additive to hydrocarbon fuels in an internal combustion engine like RCCI engine, thus, the main goals of this study are to overcome the NOx challenge, enhance the RCCI combustion characteristics, and reduce the fuel consumption when the conventional hydrocarbon fuels are substituted with hydrogen. In order to conduct the optimization process, an artificial neural network coupled with the design of the experiment concept was employed to identify the RCCI combustion mathematical model and provide the required population for two optimization algorithms, namely genetic algorithm, and particle swarm optimization algorithm. The results from the optimization process show that by advancing the diesel fuel injection along with the appropriate amount of exhaust gas recirculation and nitrogen as diluents, the level of EURO VI for NOx can be met. However, the losses in the RCCI engine output power is less than 5% meanwhile the gross indicated efficiency is over 50% and the reduction in hydrocarbon fuels consumption is about 40%.

keywords: RCCI combustion; Heavy-duty diesel engine; Hydrogen; Artificial neural network; optimization.

Nomenclatures

ANN	Artificial neural network	LHV	Lower heating value
ATDC	After top dead center	N2	Nitrogen
CA	Crank angle	NG	Natural gas
CA10	The crank angle of 10% fuel burned	NOx	Nitrogen oxides
CA50	The crank angle of 50% fuel burned	P	In-cylinder Pressure
CA90	The crank angle of 90% fuel burned	PCCI	Premixed-charged compression-ignition
CFD	Computational fluid dynamic	PLTC	Premixed low-temperature combustion
CNG	Compressed natural gas	PPRR	Peak pressure rise rate
CO	Carbon monoxide	PRF	Primary reference fuel
Cp	Heat capacity at a constant pressure	PSO	Particle swarm optimization
Cv	Heat capacity at a constant volume	R	Gas constant
DOE	Design of experiment	RCCI	Reactivity-controlled compression-ignition
EGR	Exhaust gas recirculation	RI	Ringing intensity
EPA	The U.S. Environmental Protection Agency	SOI	Start of diesel fuel injection
EURO	European emission standard	t	Time
GA	Genetic algorithm	T	In-cylinder temperature
H2	Hydrogen	TDC	Top dead center
HCCI	Homogeneous charge compression-ignition	UHC	Unburned hydrocarbon
HRR	Heat release rate	α	Weight coefficient
IMEP	Indicated mean effective pressure	γ	the Cp / Cv ratio

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1. Introduction

Heavy-duty diesel engines have a great contribution to the development of human life, industries, transportation, and so on. However, one of the obstacles to the development of the use of this type of engine is its high contribution to air pollution. Researches were shown that the use of new combustion technologies such as PLTC can overcome the challenge of the diesel engine emissions like nitrogen oxides and soot. Among these new combustion technologies, HCCI combustion, PCCI combustion, and RCCI combustion strategies can be mentioned (Reitz & Duraisamy, 2015). Although, HCCI and PCCI combustion strategies have the potential to reduce the engine emissions significantly, , the disadvantages of their use in an engine are weakness in controlling the combustion phasing and faster heat release rate in the combustion process which causes to reduce the combustion duration (Kokjohn, Hanson, Splitter, Kaddatz, & Reitz, 2011). Therefore, the RCCI combustion strategy was introduced to overcome the HCCI and PCCI combustion strategies' disadvantages by using two fuels with different reactivity. In this combustion strategy, during the intake stroke, a low reactive fuel such as gasoline gets injected into the engine intake port, thus, a low reactive air-fuel mixture will be formed in the engine combustion chamber. Then, at the end of the engine compression stroke, a highly reactive fuel such as diesel fuel (as an ignition source) is directly injected into the combustion chamber to ignite the available low reactive air-fuel mixture. RCCI combustion strategy has not only been able to overcome the HCCI and PCCI combustion disadvantages, but also it has the potential to reduce engine emissions, drastically. Several experimental and simulation works have been conducted in the RCCI combustion field with a wide variety of fuels with different reactivity (low reactivity/high reactivity) like gasoline/diesel fuel (Kokjohn, Hanson, Splitter, Kaddatz, & Reitz, 2011), hydrated Ethanol/diesel (Dempsey, Adhikary, Viswanathan, & Reitz, 2012), natural gas/biodiesel (Gharehghani, Hosseini, Mirsalim, Jazayeri, & Yusaf, 2015), natural gas/diesel fuel (Walker, Wissink, DelVescovo, & Reitz, 2015; Ebrahimi, Najafi, Jazayeri, & Mohammadzadeh, 2018; Nieman, Dempsey, & Reitz, 2012), isobutanol/isobutanol with the addition of Di-Tert Butyl Peroxide (DelVescovo, Wang, Wissink, & Reitz, 2015), and so on. Moreover, in many research related to RCCI combustion strategy, the effect of different parameters on a heavy-duty diesel engine performance under RCCI combustion mode was evaluated. Some of these evaluated parameters were intake charge temperature and pressure, diesel fuel injection timing in a single or double injection strategy, low reactive or high reactive fuel type, engine speed, equivalence ratio, exhaust gas recirculation percentage (Reitz & Duraisamy, 2015), piston bowl geometry type (Splitter, Wissink, Kokjohn, & Reitz, 2012), and so on. Also, the engine output parameters which were evaluated under RCCI combustion mode are the engine output power, the engine fuel consumption, the engine emissions, diesel knock occurrence, and so on (Reitz & Duraisamy, 2015). Due to the limited use of hydrocarbon fuels resulted from global warming and the need to replace them with green fuels, in recent researches, the use of hydrogen as a sole fuel or as an additive to hydrocarbon fuels such as natural gas has become attractive to researchers in the RCCI combustion field (Kumar, Gupta, & Kumar, 2015). Among these researches, the use of natural gas enriched with hydrogen and diesel fuel in a RCCI engine (Mabadi Rahimi, Jazayeri, & Ebrahimi, 2020), landfill gas enriched with hydrogen and diesel fuel in a RCCI engine (Ebrahimi & Jazayeri, 2019), hydrogen addition to a diesel engine with conventional diesel combustion (Ahmadi & Hosseini, 2018), natural gas-hydrogen mixture in a RCCI engine (Kakoee, Bakhshan, Motadayen Aval, & Gharehghani, 2018), CNG enriched with hydrogen and diesel fuel in an engine (Kalsi & Subramanian, 2017), di-methyl ether-methane-hydrogen mixture in a dual fuel RCCI engine (Liu, Yang, Wang, & Ouyang, 2012), methane-hydrogen mixture in compression ignition engine (Talibi, Balachandran, & Ladommatos, 2017), natural gas-hydrogen blend in a spark-ignition engine (Hu, Huang, Liu, Zheng, & Gu, 2009; Huang, Hu, Huang, Zheng, Liu, & Jiang, 2009), methane-hydrogen-oxygen-argon mixture in a spark-ignition engine (Zhang, Huang, Wei, Zhang, & Law, 2012), premixed methane-hydrogen in a spark-ignition engine (Hu, Huang, He, Jin, & Zheng, 2009; Huang, Zhang, Zeng, Liu, Wang, & Jiang, 2006), and so on can be mentioned. The main objective of these researches is to reduce fossil fuel consumption along with achieving more complete combustion in order to reduce engine emissions. But, despite the favorable characteristics of hydrogen, the main challenge related to the use of hydrogen as a fuel in an engine is the high level of NOx emission (Kumar, Gupta, & Kumar, 2015) so that the EURO VI level of this emission cannot be met (Mabadi Rahimi, Jazayeri, & Ebrahimi, 2020). It should be noted that the most experimental or simulation works in the RCCI combustion field were conducted based on the traditional method. In the sense that, in each, engine test step, all the effective parameters on the engine performance are kept constant except one. Thus, based on the variation of this single variable parameter, the engine output parameters are evaluated. In the literature of the DOE, the traditional method is known as the one-factor-at-a-time approach (Hicks & Turner, 1999). In contrast, there is another method, known as the factorial approach; in which all of the engine effective parameters can allow being variable at the same time, of course, in a completely randomized manner (Hicks & Turner, 1999; Montogomery, 2001; Wilson & Kumar, 2012).

Recently, some researches show that to implement combustion optimization through a multi-objective optimization method, the use of an ANN can be an efficient approach (Parlak, Islamoglu, Yasar, & Egrisogut, 2006; Ebrahimi, Najafi, & Jazayeri, 2018). An optimization algorithm needs an initial population to conduct the optimization process, thus, an ANN has the potential to provide the required initial population by identifying the mathematical model for the combustion. Since the combustion like the RCCI combustion strategy has an unknown function or mathematical model, therefore, the factorial method is able to provide the input-output data pairs of the combustion for an ANN (Ebrahimi, Najafi, & Jazayeri, 2020). Moreover, some limited studies related to the optimization of a RCCI engine performance were conducted like the performance optimization of a heavy-duty diesel engine operation at high load (Shi & Reitz, 2009), a RCCI engine performance optimization fueled with natural gas/diesel fuel (Nieman, Dempsey, & Reitz, 2012), optimization of a RCCI engine operating fueled with methanol/diesel fuel (Li, Jia, Chang, Liu, Xie, Wang, & Zhou, 2014), optimization of a diesel-natural gas RCCI engine performance, combustion noise and emissions using response surface method (Borjian Fard, Gharehghani, & Bahri, 2021), computational optimization of RCCI combustion (Jain, Krishnasamy, & Pradeep, 2021), multiple-objective optimization of methanol/diesel dual-fuel RCCI engine at low loads (Li, Jia, Xu, & Song Bai, 2020), experimental optimization of RCCI combustion in a light-duty diesel engine (Pandian & Anand, 2018), and optimization of RCCI combustion fueled with diesel and hydrous ethanol using response surface methodology (Fang, Kittelson, & Northrop, 2015).

Based on the aforementioned researches, although in recent years, the use of optimization methods for improving the RCCI engine performance fueled with different fuels have been studied, however, no investigation to use optimization methods to improve an RCCI engine performance fueled with diesel fuel and natural gas enriched with hydrogen has been published in the literature to date. Since NOx emission is one of the most important concerns of using hydrogen in an internal combustion engine, therefore, the aim of this current optimization study is to overcome the main challenge of the hydrogen addition to the hydrocarbon fuel in a heavy-duty diesel engine under RCCI combustion (i.e. NOx emission) through multi-objective optimization of combustion. Also, this study seeks to maintain the RCCI engine power output, reduce the hydrocarbon fuel consumption, reduce the engine emissions, and have lower combustion noise (or diesel knock). For this purpose, a heavy-duty diesel engine with bathtub piston bowl geometry is considered to operate at 9.4 bar gross IMEP. Six the engine effective input parameters include the start of diesel fuel injection timing (single injection), the mass ratio of H2 to NG or methane, the mass ratio of hydrogen to diesel fuel, the percentage of EGR, volumetric ratio of CO to hydrogen, and volumetric ratio of N2 to hydrogen are considered as the input signals in the optimization process. The DOE concept-fractional factorial method is used to combine all the mentioned input parameters' levels in a randomized manner and gather the required input-output data pairs for the artificial neural network. The used ANN is trained to identify the RCCI combustion mathematical model for providing the required database for optimization algorithms. Two different optimization algorithms include GA and PSO algorithms are employed to optimize the RCCI combustion strategy fueled with diesel fuel and natural gas enriched with hydrogen. Moreover, the obtained optimal conditions will be assessed in terms of the optimal operation of the selected heavy-duty diesel engine under RCCI mode.

2. Heavy-Duty Diesel Engine Specifications and Operating Conditions

In the current work, the technical specifications of the selected heavy-duty diesel engine which is used to optimize RCCI combustion were listed in Table 1. Also, a set of the operating conditions of this engine under RCCI combustion fueled with diesel fuel and natural gas were presented in Table 2 (Walker, Wissink, DelVescovo, & Reitz, 2015). As mentioned earlier, a RCCI engine uses two fuels with different reactivity.

Table 1: Heavy-duty diesel engine specifications (Walker, Wissink, DelVescovo, & Reitz, 2015)

Caterpillar 3401E SCOTE– Single Cylinder	
Compression ratio	14.88:1
Bore x Stroke	137.2 mm x 165.1 mm
Connecting rod length	261.6 mm
Piston bowl geometry [8]	Bathtub
Intake/Exhaust valves number	2
Intake valve closing (IVC)	-143° ATDC
Exhaust valve opening (EVO)	130° ATDC
Swirl ratio	0.7
Injector holes number	6
Injector hole diameter	250 μm
Included spray angle	145°
Engine speed	1300 rpm

Table 2: Set of the engine operating conditions (Walker, Wissink, DelVescovo, & Reitz, 2015)

	Engine gross IMEP (bar)					
	Low- Load range			Mid-Load range		
Parameter type	5.6	6.3	7.7	9.4	11.5	13.5
Intake pressure (bar)	0.97	1.08	1.32	1.6	1.9	2.2
Intake temperature (K)	313					
Diesel fuel (mg)	13 mg (per cycle)					
Methane (mg)	42	49	62	76	96	108
Total fuel (mg)	55	62	75	89	109	121
SOI (° ATDC)	-35	-39	-42	-45	-48	-51

In the present study, natural gas as a low reactivity fuel gets injected into the intake port during the engine intake stroke. Since a significant percentage of natural gas belongs to methane (about 89% by volume), thus, in this simulation study, methane with the LHV of 50 MJ/kg is considered as representative of natural gas. Also, in order to ignite the available air-methane mixture, n-heptane with the LHV of 44.6 MJ/kg as representative of diesel fuel is directly injected into the combustion chamber as a high reactivity fuel. Moreover, when natural gas is enriched with hydrogen, the LHV of hydrogen is considered to be 119 MJ/kg (Kumar, Gupta, & Kumar, 2015).

3. Computational Model

As mentioned in Table 1 and depicted in Fig. 1, since the engine's diesel fuel injector has six holes on it, thus, due to the symmetry, one-sixth segment of the engine combustion chamber is used as three-dimensional computational grids.

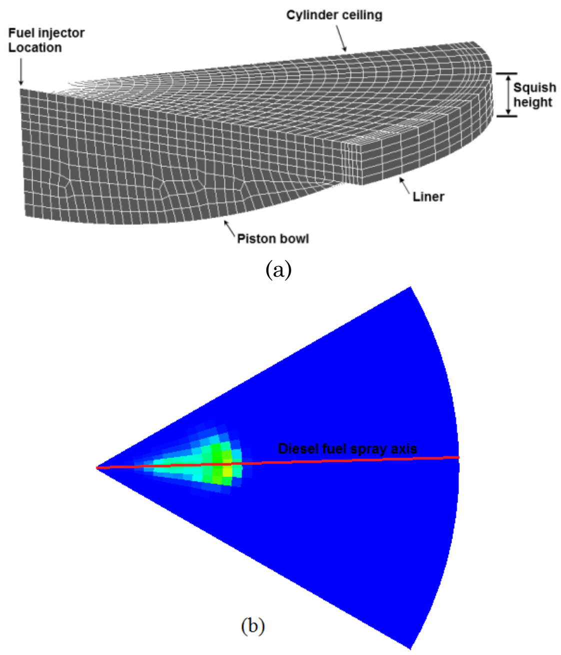


Figure 1: (a) Three-dimensional computational grid of the selected engine (b) Diesel fuel spray axis displaying (Mabadi Rahimi, Jazayeri, & Ebrahimi, 2020)

In order to verify the combustion simulation results with the experimental data (Walker, Wissink, DelVescovo, & Reitz, 2015); based on a set of the engine operating conditions listed in Table 2, the RCCI combustion simulation is conducted by the AVL FIRE CFD tool coupled with CHEMKIN chemistry tool. It should be noted that, for implementing the RCCI combustion simulation, some sub-models listed in Table 3 were used for modeling diesel fuel spray, and also, in order to predict the reactions between methane and n-heptane, a reduced PRF mechanism include 76 species and 464 reactions were used (Rahimi, Fatehifar, & KhoshbakhtiSaray, 2010).

For the set of the engine operating conditions mentioned in Table 2, the obtained RCCI combustion simulation results were validated with the engine experimental data (Walker, Wissink, DelVescovo, & Reitz, 2015) as depicted in Figs 2 and 3. Figure 2 shows the rate of heat release during RCCI combustion for the set of engine loads (Table 2). For better illustration, the heat release rate was divided into two ranges of the engine operation, Low-Load, and Mid-Load. In terms of the occurrence of cool flame and the time of the start of the main combustion, Fig. 2 shows that the three-dimensional computational models used in the RCCI combustion simulation had the potential to precisely predict the heat release rate compared to the experimental results (Walker, Wissink, DelVescovo, & Reitz, 2015).

Also, compared to the experimental data (Walker, Wissink, DelVescovo, & Reitz, 2015), Fig. 3 depicts that accurate predictions of the engine in-cylinder peak pressure can be achieved by the used computational model. It should be noted that, in a heavy-duty diesel engine, to avoid the diesel knock occurrence, the PPRR value should be limited to less than 15bar/º (Reitz & Duraisamy, 2015). As depicted in Fig. 3, the obtained PPRR values from the RCCI combustion simulation fueled with diesel fuel and natural gas are in the acceptable level like the experimental data (Walker, Wissink, DelVescovo, & Reitz, 2015) which indicates that the used computational model can predict the engine operation under RCCI combustion without the exposure to diesel knock.

Table 3: Diesel fuel spray modeling sub-models

Description	Sub-model type
Particles interaction with the individual turbulent eddies	Turbulence Dispersion (Gosman & Ioannides, 1983)
Diesel fuel spray/Cylinder wall interaction	Wall Jet Model (Naber & Reitz, 1988)
Diesel fuel droplets evaporation	Dukowicz Model (Dukowicz, 1979)
Diesel fuel droplets break-up	Wave Standard Model (Liu & Reitz, 1999)
Diesel fuel injection nozzle flow simulation	Diesel Nozzle Model (Kunsberg-Sarre, Kong, & Reitz, 1999)

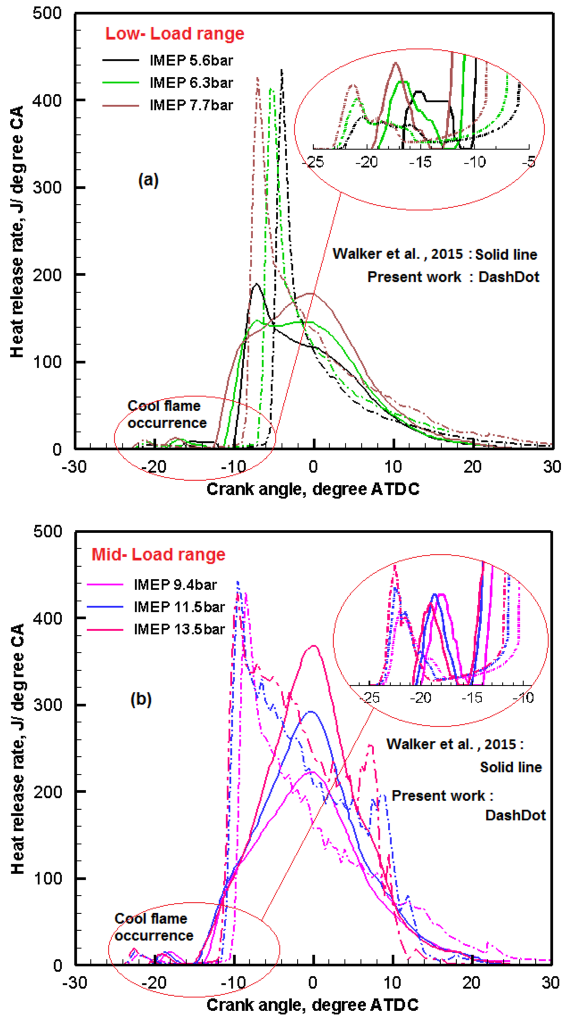


Figure 2: The heat release rate validation for: (a) Low- Load range and (b) Mid- Load range

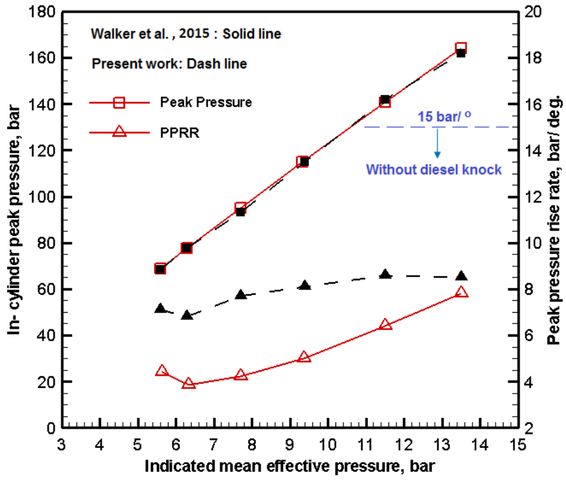


Figure 3: The engine in-cylinder peak pressure and the PPRR validation

4. Optimization Process

In the present study, in order to implement the RCCI combustion optimization process at 9.4bar gross IMEP, the effects of six effective input parameters on the engine performance are considered to be evaluated. These six input parameters as the input signals in the optimization process include the start of diesel fuel injection timing (single injection), the mass ratio of H2 to NG or methane, the mass ratio of H2 to diesel fuel, the percentage of EGR, volumetric ratio of CO to H2, and volumetric ratio of N2 to H2.

According to the aim of this study in reducing the hydrocarbon fuels consumption (i.e. diesel fuel and natural gas), it is considered that natural gas is substituted by pure hydrogen or Syngas (i.e. synthesis gas consisting of hydrogen and carbon monoxide) and also, diesel fuel is substituted by pure hydrogen, based on the difference between their lower heating values. Moreover, due to the challenge of the higher level of NOx emission related to the use of hydrogen as a fuel in an engine, the use of nitrogen as an air-fuel diluent and also EGR (i.e. carbon dioxide) for reducing the in-cylinder temperature is proposed. It is assumed that hydrogen or Syngas as an additive, nitrogen, and carbon dioxide as representative of EGR are injected into the engine intake port with methane during the engine intake stroke. Of course, it is expected that with reducing the hydrocarbon fuel consumption and the NOx emission level, the engine power to be maintained at 9.4bar gross IMEP and the engine operating under the RCCI combustion strategy to be without diesel knock.

For leading to the optimization purpose, at first; based on the engine operating conditions and the present authors' earlier work (Mabadi Rahimi, Jazayeri, & Ebrahimi, 2020), five levels of variation was chosen for each mentioned input parameter as presented in Table 4. Then, based on the DOE concept-Factorial method, the performance of the RCCI engine under investigation was assessed according to randomized treatment combinations of the mentioned input parameters.

Table 4: Five levels of variation for six selected input parameters based on the RCCI engine operating conditions

	Level of variations				
Selected parameter	0	1	2	3	4
SOI timing (° ATDC)	-45	-35	-55	-65	-75
Mass ratio of H2 to methane (mg/mg)	0.0/76.0	3.16/68.4	7.24/58.6	10.9/49.8	14.8/40.6
Mass ratio of H2 to diesel fuel (mg/mg)	0.0/13.0	1.0/10.31	2.0/7.62	3.0/4.93	4.0/2.25
EGR (%)	0	5	8	10	14
Volumetric ratio of CO to H2 (%)	0	25	50	100	200
Volumetric ratio of N2 to H2 (%)	0	25	50	100	200

After gathering the required data by the RCCI engine simulation through the DOE concept-Factorial method, an artificial neural network was used to directly identify the RCCI combustion mathematical model, according to the presented schematic in Fig. 4.

For the used artificial neural network (Fig. 4), two active layers include one hidden layer and one output layer was considered. The six selected engine input parameters were directly given to the artificial neural network as the input signals (Fig. 5).

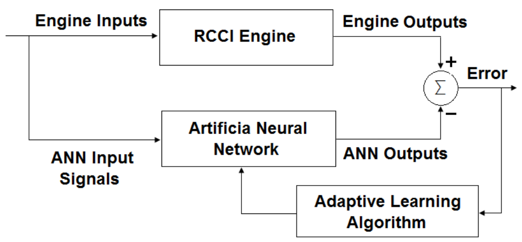


Figure 4: Direct identification of the RCCI combustion mathematical model through an ANN

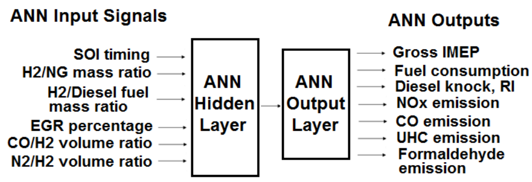


Figure 5: The used ANN active layers: a hidden layer and an output layer

According to the schematic shown in Fig. 4, the used ANN with the important parameters presented in Table 5 is trained through comparing its outputs with the engine outputs as response variables and minimizing the error between them. A second-order adaptive learning algorithm named the Levenberg-Marquardt algorithm is employed in the used ANN. As depicted in Fig. 5, in the current optimization study, seven engine outputs as response variables are selected include the gross IMEP, the amount of fuel consumption, the RI criteria as representative of the diesel knock occurrence, the NOx emission level, the CO emission level, the UHC emission level, and the formaldehyde emission level.

It should be noted that, based on the results of the work done by Eng (Eng, 2002), RI as criteria for detecting the diesel knock which is resulting from the excessive PPRR due to the faster HRR in an engine combustion chamber can be determined as:

$$RI = \frac{1}{2\gamma}\frac{\left(0.05\ (dP/dt)_{max}\right)^2}{P_{max}}\sqrt{\gamma\ R\ T_{max}} \quad (1)$$

In a heavy-duty diesel engine, for avoiding the diesel knock occurrence, the RI value should be below 5MW/m² (Eng, 2002).

After training the used artificial neural network and its ability to identify the RCCI combustion mathematical model at 9.4bar gross IMEP, the required initial population for optimization algorithms can be provided.

Table 5: The used ANN important parameters in the RCCI combustion mathematical model identification process

The number of the RCCI combustion simulation results which randomly used for training the ANN	80 %
The number of the RCCI combustion simulation results which randomly used for testing the ANN performance in its training process	20 %
The neuron activation function in the ANN hidden layer	Bipolar Sigmoid Function (Nonlinear)
The neuron activation function in the ANN output layer	Linear Function
The ANN allowable training epochs	1000

The focus of this optimization study is to maintain the RCCI engine power output, reduce the hydrocarbon fuel consumption, reduce the engine emissions (NOx, CO, UHC, and formaldehyde), and have lower combustion noise at 9.4bar gross IMEP. Thus, to achieve the mentioned goals, GA and PSO algorithms were used. The required initial population/swarm of these optimization algorithms is provided through the trained ANN governing equations. In Table 6, some important parameters for GA and PSO algorithms are listed.

Table 6: Optimization algorithms parameters

Initial population for GA/ PSO algorithms	5000 (chromosomes or particles)
Number of generation	100
GA parameters	
Selection method	Roulette wheel
Crossover rate	0.8
Mutation rate	0.2
Selection pressure	10
PSO algorithm parameters	
Inertia weight	1
Inertia weight damping ratio	0.99
Personal learning coefficient	0.5
Global learning coefficient	0.5

For each generated chromosome for genetic algorithm or particle for particle swarm optimization algorithm by the trained ANN, the following second-order cost (or fitness) function is used:

$$Cost\ \ Function = \sum_{i=1}^{7} \alpha_i \cdot \left[ANNOutput(i) - IdealValue(i)\right]^2 \quad (2)$$

It should be noted that, for seven selected engine outputs, the relation between the weight coefficients is:

$$\sum_{i=1}^{7} \alpha_i = 1 \quad (3)$$

Moreover, based on the engine operation under the RCCI combustion strategy, the ideal values which are favorable for each of seven selected engine outputs in the optimization process are presented in Table 7.

Table 7: Ideal values for each of the RCCI engine outputs

RCCI engine output	Ideal value
Gross IMEP (bar) (Walker, Wissink, DelVescovo, & Reitz, 2015)	> 9.4
Reduction in fuel consumption (Desirable in this study)	>50%
Ringing intensity (MW/m²) (Eng, 2002)	≤ 5
NOx emission (g/kWh)	0.4 (EURO VI level)
CO emission (g/kWh)	1.5 (EURO VI level)
UHC emission (g/kWh)	0.13 (EURO VI level)
Formaldehyde emission (g/kWh)	0.012 (EPA 2007 level)

5. Results and Discussions

To provide the initial population/swarm for two mentioned optimization algorithms; based on the range of variation of the engine input parameters are shown in Table 4, five thousand input parameters as the ANN input signals were generated in a randomized manner. According to considering different weight coefficients in Equation 2, as listed in Table 8, after about twenty generations in the optimization process (Fig. 6), four items for six input parameters as the optimal suggestions were proposed by GA and PSO algorithms which leads to the considered goals.

Table 8: Four proposed items for six selected input parameters by GA and PSO algorithms

Input Parameter (or Input Signal)	Proposed Items			
	GA#1	GA#2	PSO#1	PSO#2
SOI timing (° ATDC)	-35.0	-70.63	-71.4	-35.0
H2/NG mass ratio	0.364	0.364	0.364	0.364
H2/Diesel fuel mass ratio	0	0.024	0	0
EGR (%)	0	5.74	5.88	6.5
CO/H2 volume ratio	0	0	0	0
N2/H2 volume ratio	0.97	2.0	2.0	0.362

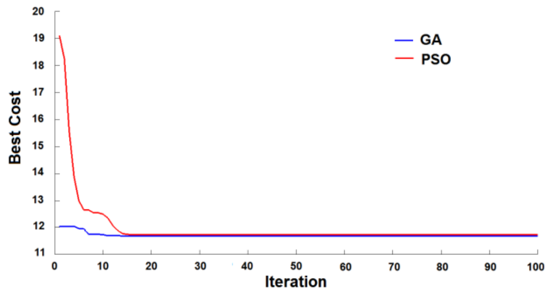


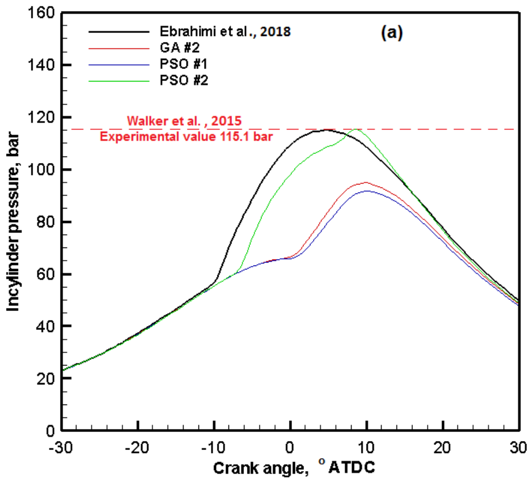
Figure 6: Optimization algorithms performance

In the final step of the optimization process, the proposed items by two algorithms are evaluated by the RCCI combustion simulation through the AVL FIRE CFD tool coupled with the CHEMKIN chemistry tool. Thus, the relevant value of all input parameters in four suggested items was used in the RCCI combustion simulation fueled with diesel fuel/ natural gas enriched with hydrogen. The obtained results from the RCCI combustion simulation are listed in Table 8 and compared with the outputs which resulted from two optimization algorithms. For the item of GA#1, the RCCI combustion simulation results shown that the maximum in-cylinder temperature is above 1900K. Thus, the low-temperature combustion concept is not met and the relevant results from the RCCI combustion simulation for this item (i.e. GA#1) were not presented in Table 9.

Table 9: Comparison between the outputs resulted from two optimization algorithms and the RCCI combustion simulation.

Output (Response) Parameter	Proposed Items			
	GA#1/RCCI	GA#2/RCCI	PSO#1/RCCI	PSO#2/RCCI
Gross IMEP (bar) Ideal value: 9.4bar	8.95/--	8.79/8.999	8.86/8.696	9.22/9.33
Fuel consumption (mg)	49.2/--	50.59/53.57	50.69/53.58	50.52/53.58
RI (MW/m2) Ideal value:RI < 5 MW/m2	2.91/--	3.37/0.92	3.59/0.94	1.63/2.67
NOx (g/kWh)EURO VI value: 0.4 g/kWh	0.540/--	0.847/0.085	0.912/0.065	0.810/2.363
CO (g/kWh)EURO VI value: 1.5 g/kWh	7.100/--	2.712/0.64	2.210/0.852	3.170/9.2E-5
UHC (g/kWh)EURO VI value: 0.13 g/kWh	-2.340/--	0.362/0.774	0.238/1.876	-1.930/8.3E-12
Formaldehyde (g/kWh)EPA 2007 value: 0.012 g/kWh	-0.060/--	0.064/0.046	0.070/0.086	0.013/1.4E-11

For items, GA#2, PSO#1, and PSO#2, the in-cylinder pressure and heat release rate resulted from the RCCI combustion simulation are depicted in Fig. 7 and compared with the experimental data (Walker, Wissink, DelVescovo, & Reitz, 2015) and Ebrahimi et al. simulation work (Ebrahimi, Najafi, Jazayeri, & Mohammadzadeh, 2018).



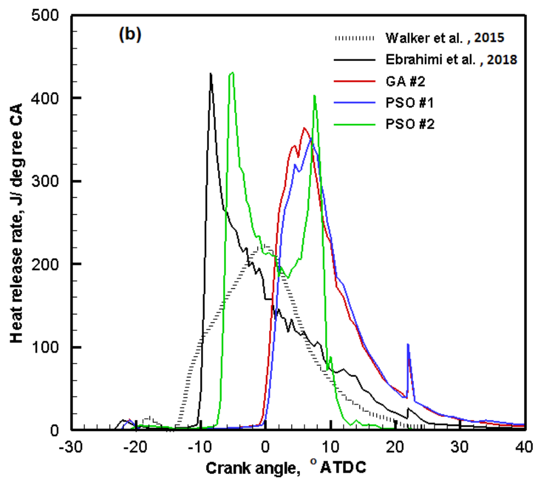


Figure 7: (a) In-cylinder pressure (b) Heat release rate for proposed items by the optimization algorithms

As shown in Fig. 7, the natural gas enrichment with hydrogen along with the use of EGR and nitrogen addition as intake charge diluents cause to delay the start of combustion. Thus, the overall combustion shifts to the engine expansion stroke. It causes that the in-cylinder pressure is affected by the expansion work and decreased. However, as shown in Fig. 8, losses in the RCCI engine output power (i.e. gross IMEP) are insignificant (about 8%) and the RCCI engine under investigation is not exposed to diesel knock because the RI value is below 5MW/m² (Eng, 2002).

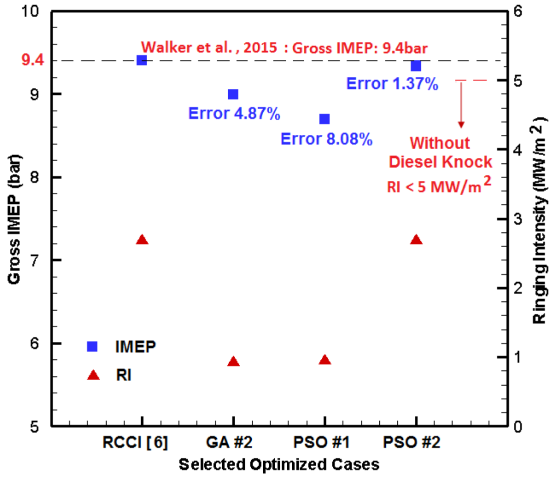


Figure 8: Gross IMEP and RI for proposed items by the optimization algorithms

In Table 10, based on the proposed items by the optimization algorithms, some RCCI combustion characteristics are listed. The higher hydrogen flame velocity causes to release of the fuel energy faster, increases the in-cylinder temperature, increases the peak pressure rise rate, and reduces the combustion duration. But, based on the proposed items resulted from the optimization algorithms, the RCCI combustion simulation results show that when natural gas is enriched with hydrogen, by advancing the diesel fuel injection as high reactive fuel (i.e. the case Nos. of GA#2 and PSO#1) along with the use of the appropriate amount of EGR and nitrogen as diluents, the combustion duration would be increased compared to the experimental data (i.e. 25° CA) (Walker, Wissink, DelVescovo, & Reitz, 2015). Moreover, it causes to shift the overall combustion process to the engine expansion stroke that causes to shift the CA50 location to after TDC point further. Therefore, the negative work resulted from the release of more percentage of the fuel energy in the engine compression stroke is reduced. However, the effect of the expansion work reduces the in-cylinder peak pressure up to 20.55% compared to the experimental results (i.e. 115.1bar) (Walker, Wissink, DelVescovo, & Reitz, 2015).

By comparing the obtained results, among the proposed items from the optimization process, in terms of minimum losses in the engine power, the gross indicated efficiency above 50%, reduction in hydrocarbon fuel consumption about 40%, without the exposure to diesel knock, and overcoming the NOx emission challenge as the main challenge of the use of hydrogen as a sole fuel or an additive in an engine, the item GA#2 is able to meet the desired conditions. However, although the case of GA#2 has also the potential to meet the EURO VI level of CO emission, , the penalty is that the EURO VI level of UHC emission and EPA (2007) level of formaldehyde emission could not be met. Hence, since the main object of this study is to overcome the NOx emission challenge when hydrogen is used as an additive to hydrocarbon fuel in RCCI combustion, the item GA#2 conditions can be selected as an optimal item resulted from the optimization process.

Table 10: Some RCCI combustion characteristics for proposed items by the optimization algorithms

RCCI Combustion Characteristic	Proposed Items		
	GA#2	PSO#1	PSO#2
Max. in-cylinder pressure (bar)	94.9	91.44	115.34
Max. in-cylinder temperature (K)	1693.3	1658.5	1892.0
Peak pressure rise rate (bar/°)	4.33	3.75	7.92
Gross indicated efficiency (%)	50.2	48.5	52.0
CA50 (° ATDC)	7.50	8.25	1.00
Combustion duration (CA90-CA10) (° CA)	33	35	20.3
Combustion delay (CA /µSec)	9.5/1218	10/1282	3.5/448.7

6. Conclusions

This study aims to implement the optimization of a RCCI engine performance fueled with diesel fuel and natural gas enriched with hydrogen at 9.4 bar gross indicated mean effective pressure (Mid-Load). In this study, a single-cylinder heavy-duty diesel engine with bathtub piston bowl geometry was used to assess the effects of six engine input parameters on seven of the engine outputs. By identifying the RCCI combustion mathematical model through an artificial neural network coupled with the design of the experiment concept, the required population for two optimization algorithms, namely, genetic algorithm and particle swarm optimization algorithm were provided. Thus, in this optimization study, aiming to overcome the main challenge of the use of hydrogen as an additive to hydrocarbon fuel (i.e. NOx emission); the following results can be derived:

1) In order to optimize engine performance, an artificial neural network coupled with the design of the experiment-factorial method has the potential to provide the required initial population for optimization algorithms.

2) Despite this matter that in a RCCI engine fueled with diesel oil and natural gas, by enrichment of the natural gas with hydrogen, the EURO VI level of NOx emission could not be achieved [11], the results from the optimization process illustrated that by advancing the diesel fuel injection up to -71° ATDC along with the appropriate amount of EGR and the use of nitrogen as diluents, the level of EURO VI for NOx emission can be achievable. Moreover, the EURO VI level of CO emission can be met at the same time. But, the EURO VI level of UHC emission and the EPA (2007) level of formaldehyde cannot be met along with the overcome the NOx challenge.

3) Although, due to the higher flame velocity of hydrogen, the fuel energy is released faster in the

RCCI engine's combustion chamber and the combustion duration would be shorter, but, by advancing the diesel fuel injection along with the appropriate amount of EGR and the use of nitrogen as diluents, longer combustion duration compared to the case of without the use of hydrogen can be achievable.

4) In RCCI combustion, when hydrogen is added to hydrocarbon fuels, the CA50 shifts to before the TDC (i.e. compression stroke). But, the RCCI engine operation under the suggested optimal conditions leads to shifting the CA50 to after the TDC (i.e. expansion stroke) and the negative work resulted from the heat releasing in the compression stroke would be reduced. Also, the losses in the engine output power would be less than 5%, the hydrocarbon fuels would be reduced by about 40%, and the gross indicated efficiency over 50% can be achievable.

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