



Investigating the effects of fuel injection strategies in a dual-fuel diesel-H₂ compression ignition engine

A. Shaafi^a, M. J. Noroozi^{a,*}, V. Manshaei^a

^a Department of Mechanical Engineering, Ayatollah Boroujerdi University, Boroujerd, P.O. Box: 69199-69411, Iran

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Abstract

In this computational research, the separate and simultaneous impacts of diesel direct injection timing, fuel spraying cone angle, and hydrogen gas addition on combustion characteristics, output emissions, and performance in a single-cylinder direct injection diesel engine was studied. In order to conduct the simulations, valid and reliable models for combustion, break-up, and for turbulence was used. The effects of fifteen fuel injection strategies based on characteristics such as time of fuel spraying (-15, -10 CA BTDC, and TDC) and nozzle cone angle (105, 115, 125, 145, and 160 degrees) under neat diesel combustion and diesel-hydrogen combustion engine operations conditions were explored. The obtained results indicated that the addition of H₂ due to significant heating value has increased indicated power and improved indicated specific energy consumption at the expense of NO_x emissions but considerably decreased CO and soot emissions simultaneously. By advancing injection timing, maximum pressure peak point, maximum temperature peak point, and maximum heat release rate peak point have increased and caused lower indicated specific energy consumption. However, using a wide spray angle (e.g., 160 cone degrees), resulted in lower indicated power and higher indicated specific energy consumption due to more fuel could spray in regions with lower oxygen concentrations compared to baseline operation case.

Nomenclature

BDC	Bottom dead center
BTDC	Before top dead center
CA	Crank angle
CFD	Computational fluid dynamic
CO	Carbon monoxide
DHC	Diesel hydrogen combustion
DI	Direct injection
EVO	Exhaust valve opening
HRR	Heat release rate
HSDI	High speed direct injection

ID	Ignition delay
IMAP	Intake manifold air pressure
IMAT	Intake manifold air temperature
IMEP	Indicated mean effective Pressure
IP	Indicated power
ISEC	Indicated specific energy consumption
IT	Injection timing
IVC	Intake valve closing
MHRRPPP	Max. heat release rate peak

*Corresponding author

Email address: Mo.j.noroozi@gmail.com; m.j.noroozi@abru.ac.ir

	point
MPPP	Max. pressure peak point
MTPP	Max. temperature peak point
NDC	Neat diesel combustion
NOx	Nitrogen oxides
SOI	Start of injection
TDC	Top dead center

1. Introduction

Due to lower energy consumption, higher thermal efficiency, and less CO and CO₂ emissions compared to spark ignition and gas engines, compression ignition known as diesel engines are widely used in transportation, agriculture, and also powering stationary/mobile equipment [1-2]. However, because of the type of combustion, they produce a high level of NO_x and PM emissions. To reduce pollutant emissions and meet stringent emission regulations, extensive researches and investigations have been conducted by many researchers [3-10]. Kim et al. [11] have investigated the effects of nozzle cone angle and time of fuel spraying on the combustion and emissions in a HSDI compression ignition engine. The engine they have used for their study is a single-cylinder equipped with Bosch common rail direct injection system. Their results showed that, spraying fuel by 60 degrees cone angle accompanied by higher MPPP, MHRRPPP, and shorter ignition delay period compared to 156 degrees. In the case of emissions formation, they indicated that using narrow spray angle simultaneous with early injection timing resulted in low UHC, CO, and NO_x emissions. Also, IMEP for a narrow nozzle cone angle is higher than 156 degrees cone angle.

Benajes et al. [12] have explored the influences of blending ratio and fuel spray timing. Their case study was RCCI combustion in a single-cylinder diesel engine. Their results showed that retarding the combustion phasing near TDC point have promoted an increase in NO_x emissions. Furthermore, advancing diesel direct injection timing has led to diminish soot at low load. They also reported that by retarding the injection timing amounts of CO, UHC, and soot emissions considerably have increased.

The clean combustion of hydrogen which produces zero CO₂, CO, UHC, and PM emissions attracted lots of attention to use H₂

gas as a clean fuel for internal combustion engines, especially diesel engines. For years, lots of researches have done in order to explore the possibility and impacts of using H₂ gas on the combustion process, emissions formation, and performance in diesel engines [13-15]. In their paper, Christodoulou and Megaritis [16] have examined the effects of hydrogen gas addition on the pollutant emissions and combustion of a DI diesel engine. The engine which they used for their study was a four-cylinder, HSDI compression ignition. Their results showed that hydrogen gas addition had decreased PM and CO, but NO_x emissions considerably have increased. Also, increasing hydrogen concentration has reduced CO emissions since mixtures carbon/hydrogen ratio has decreased.

This numerical research aims to explore the influences of using H₂ addition and diesel direct injection strategies in a heavy-duty diesel engine. This study divided into three sections; the first part discusses the effects of hydrogen gas addition and fuel direct injection characteristics such as fuel spray timing and nozzle cone angle on in-cylinder pressure, temperature, and heat release rate. In the second and third part, the effects of study strategies on emissions formation (such as NO_x, soot, and CO) and engine performance will be discussed respectively.

2. Model description

AVL ESE Fire code and its tools were used to numerically predict Diesel-H₂ dual-fuel combustion and also, creating computational grid [17]. Due to symmetrical shape of combustion chamber and using six-holes nozzle, computations conducted on 60 degrees segment. Table 1 shows some of the computational grid specifications. Fig. 1 shows the computational grid at TDC.

Table 1. Computational grid specifications.

Number of boundary layers (-)	2
Thickness of boundary layer (mm)	0.2
Average cell area size (mm)	1.2
Number of cells at IVC event (-)	77650
Number of cells at TDC (-)	31300

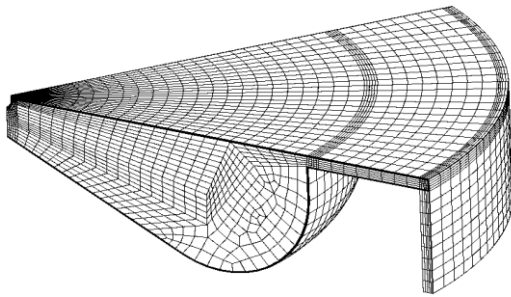


Fig. 1. The computational grid at TDC.

Extended Coherent Flame Model 3 Zone (ECFM-3Z) was used for simulating premixed and diffusive combustion [17]. In order to take auto-ignition and flame propagation into account, this model temporarily combines fuel components to a fuel mixture during calculations [18-19]. Also, transport equations of ECFM-3Z able to solve the averaged quantities of species such as N, N₂, O, O₂, CO, CO₂, H, H₂, OH, H₂O, and NO [17].

K-Zeta-F model was applied for simulating the turbulence flow inside the combustion chamber. This model was developed in 2004 by Hanjalic, Popovac, and Hadziabdic [20]. In order to enhance the stability of the v²-f model, the authors introduced a form of an eddy viscosity based on Durbin's elliptic relaxation concept [17]. Also, they provided a merging formula for the quantities determined at the cells near the wall as:

$$\varphi_p = \varphi_v e^{-\Gamma} + \varphi_t e^{-1/\Gamma} \quad (1)$$

Where v: viscous, t: the fully turbulent value of the wall shear stress, production, and dissipation of the turbulent kinetic energy [17]. Dukowicz model [21] used to predict the fuel parcels evaporation process. In order to model the first and second breakup of fuel sprayed particles, Kelvin-Helmholtz coupled with Rayleigh-Taylor mechanism was used [22]. The Kelvin-Helmholtz mechanism is responsible for high velocities. Furthermore, the Rayleigh-Taylor mechanism is able to predict the time and length of the second breakup of the injected fuel parcels [17]. Also, Nordin collision model was used for takes fuel particles

interactions into account [23]. Along with other sub-models, Naber, and Reitz method [24] was applied for simulating the fuel particles and wall interactions.

Finally, Extended Zeldovich + Prompt + Fuel and Hiroyasu/Nagle/Strickland-Constable models were used for calculating the exhaust gas NO_x and soot emissions formation, respectively [17].

3. Engine specifications, Experimental Setup, and Model Validation

A heavy-duty single-cylinder turbocharged DI diesel engine known as caterpillar 3401, was used for this numerical research [27]. The engine and fuel injection system specifications are presented in Table 2 and Table 3, respectively [27].

Table 2. Engine specifications.

Engine type	Heavy-duty turbo-charged diesel engine
Bore (mm) x stroke (mm)	137.16 x 165.1
Geometric compression ratio	16.1:1
Displacement volume (L)	2.44
Connecting rod length (mm)	261.6
TDC clearance gap (mm)	1.97
Engine speed (rpm)	1208
Bowl volume (cc)	110.8
IVC (CA BTDC)	143
EVO (CA BTDC)	-130
IMAP (bar)	2.0
IMAT (K)	313

Table 3. Fuel injection system specifications.

Injector holder	Bosch CRIN 2
Number of injector holes	6
Spray angle (degree)	145
Nozzle hole diameter (mm)	0.25
Injection pressure (bar)	755

Total fuel per cycle (mg)	172.2
Fuel injection timing (CA BTDC)	10
Fuel injection duration (CA)	16.8

Table 4 and Table 5 show the Diesel and H₂ fuels specifications respectively.

Table 4. Diesel fuel specifications [27].

Specific gravity @ 15.5 C (-)	0.856
Viscosity @ 40 C (cSt)	2.71
Lower heating value (MJ/Kg)	42.526
Cetane number	46.1

Table 5. Hydrogen gas specifications [28].

Property	Unit	Values
Adiabatic flame temperature ($\phi = 1$)	[K]	2480
Auto ignition temperature in air	[K]	858
Density	[kg/m ³]	0.0824
Flame velocity ($\phi = 1$)	[ms ⁻¹]	1.85
Lower heating value	[MJ/kg]	119.7

The experimental in-cylinder pressure and HRR trends were averaged from 499 working cycles [27]. The results obtained from the calculations are based on the assumption of a uniform wall temperature of 520 K for the cylinder head and the piston top and 420 K for the cylinder wall. Fig. 2 reports the comparison of measured and calculated in-cylinder pressure and HRR results [27]. As indicated in Fig. 2, the in-cylinder mean pressure and HRR modeled by the Fire code is reasonably close to measured results. However, there are some discrepancies as reported in Fig. 2 that could be linked to experimental uncertainties such as IMAT, duration of injection, and or exact SOI.

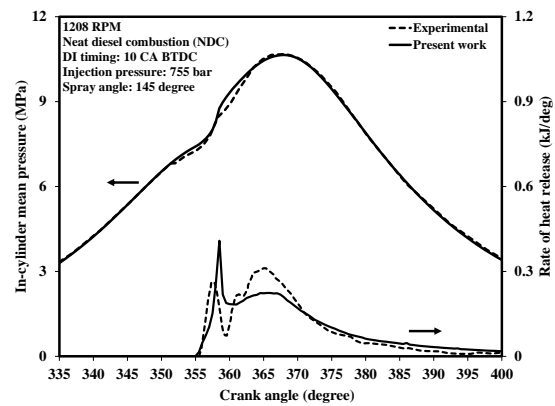


Fig. 2. Comparison of measured and calculated results of in-cylinder mean pressure and rate of heat release under baseline condition [27].

Table 6 shows the comparison of measured and calculated engine output emissions under the baseline operation condition. As reported in Table 6, emissions formation are well simulated by the CFD Fire code compared with experimental results.

Table 6. Comparison of numerical and experimental results of output pollutant emissions under the baseline operation condition [27]

Emissions (g/kg. fuel)	NOx	CO	Soot
Current research	52.91	2.75	0.27
Experimental	49.8	3.1	0.31

4. Modeling methodology

This study aims to examine the impacts of fuel injection strategies on the combustion process of heavy-duty dual-fuel compression ignition engine. Direct diesel injection timing and nozzle cone angle are the two variables that their effects are the primary purpose of this numerical study. In addition to baseline operation case, 15 fuel spraying strategies based on the fuel DI characteristics such as spray timing (-15, -10 CA BTDC, and TDC) and nozzle cone angle (105, 115, 125, 145, and 160 degrees) have been considered and their influences on the combustion specifications (in-cylinder mean temperature, pressure, and HRR), emissions formation (NOx, soot, and CO), and engine performance (ISEC and IP) under NDC and DHC (80-20% energy fraction)

engine operations conditions were investigated. Finally, the obtained results of this computational research have been presented in detail in the form of charts and Fig.s.

5. Results and discussion

5.1. Influence of study strategies on the combustion specifications

Fig. 3 shows the effects of hydrogen addition on in-cylinder pressure, temperature, and HRR.

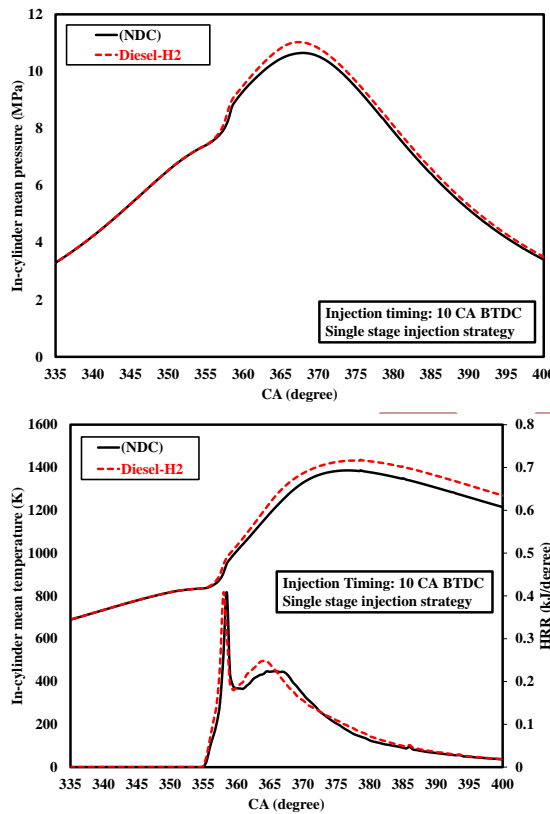


Fig. 3. Impacts of hydrogen addition on combustion specifications.

As can be seen in Fig. 3, using of H₂ gas led to increasing the in-cylinder MPPP, MTPP, and MHRRPP. High heating value and fast combustion rate of H₂ gas led to improve the air-fuel mixture oxidation process for DHC case compared to NDC mode. Fig. 4 shows the influences of spray timing on in-cylinder mean pressure, temperature, and HRR. As illustrated in Fig. 4, advancing direct injection timing has

increased MPPP, MTPP, and MHRRPP. While retarding the injection timing has opposite effects.

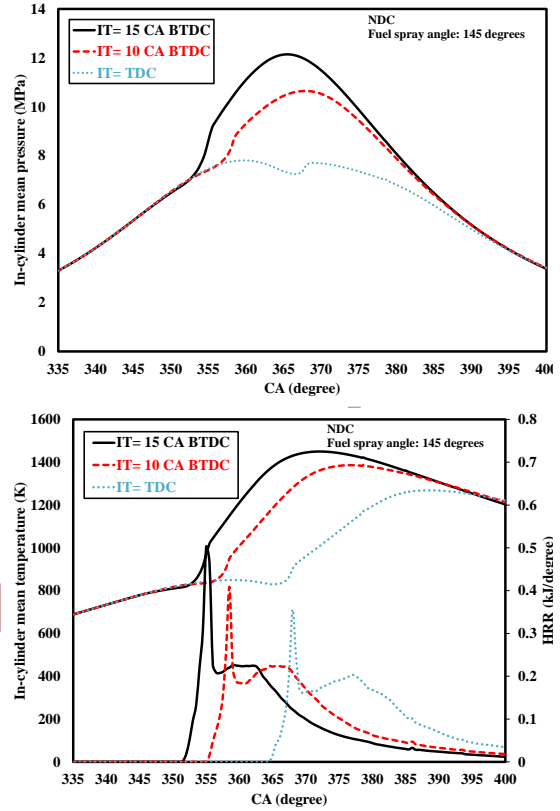


Fig. 4. Impacts of fuel spray timing on combustion specifications.

In direct injection compression ignition engines, the heat release process consists of premixed and diffusive combustion [29]. Initially, combustion occurs in the premixed burning mode until the air-fuel mixture which formed during the ignition delay period is ready to ignition; then, the rest of the evaporated air-fuel mixture will burn in diffusive combustion mode and this continues until the end of the heat release period. By advancing direct spray timing, due to lower in-cylinder pressure and temperature compared to baseline operation case, ID period has been extended. More extended ID period leads more fuel to be evaporated and accumulated and burn in premixed combustion mode. Due to the high rate of premixed combustion, pressure and temperature rise rate for advanced ITs could be

increased and as illustrated in Fig. 4, for 15 CA BTDC IT, the MPPP, MTPP, and MHRRPP compared to baseline case have increased. However, by retarding the fuel spray timing due to higher in-cylinder pressure and temperature compared to the baseline case, ID period could be shortened, and most of the evaporated fuel burns in diffusive combustion mode. In addition to that, diffusive combustion leads to lower pressure and temperature rise rate and as can be seen in Fig. 4, TDC IT has decreased MPPP, MTPP, and MHRRPP compared to baseline operation case.

Fig. 5 shows the influences of fuel spraying angle on in-cylinder mean pressure, temperature, and HRR. As illustrated in Fig. 5, by increasing fuel spray angle MPPP, MTPP, and MHRRPP have increased. Proper fuel spray angle causes the fuel to be sprayed in regions with higher oxygen concentrations that lead to improvement of the mixture oxidation process, and as can be seen in Fig. 5, MPPP, MTPP, and MHRRPP have increased.

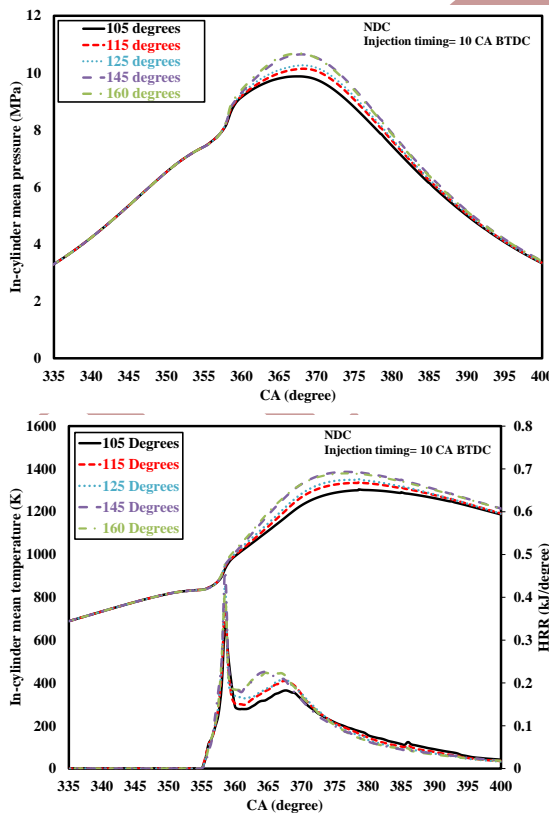


Fig. 5. Effects of study strategies on combustion characteristics.

5.2. Effects of study strategies on the emissions formation

Fig. 6 shows the impacts of fuel spray timing, fuel spraying angle, and H₂ gas addition on NO_x and soot emission. As illustrated in Fig. 6, the use of hydrogen gas considerably has decreased soot emission for all injection timings and fuel spraying angles at the expense of NO_x emissions. Induction of H₂ gas and participating in the combustion process due to higher heating value compared to diesel fuel led to higher MPPP, MTPP, and MHRRPP. As a result, air-fuel mixture oxidation has improved and led to higher NO_x and lower soot emissions compared to NDC mode.

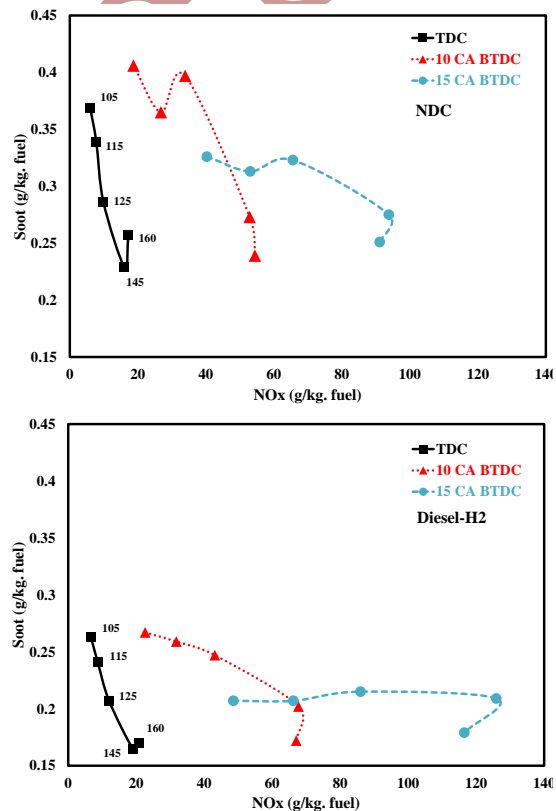


Fig. 6. Effects of study strategies on the soot-NO_x trade-off.

As illustrated in Fig. 6, by advancing the direct injection timing, the amount of NO_x emissions have increased. Advanced ITs led to more evaporated fuel burns in premixed combustion

that could increase pressure and temperature rise rate of compression ignition combustion, and as reported in Fig. 6, the amounts of NOx emissions increased. Furthermore, increasing the fuel spraying angle due to a better air-fuel mixture formation led to decrease the soot emission considerably. It must be mentioned that for TDC IT, injecting fuel with 160 degrees as spraying cone angle led to increasing soot emission that must be due to more fuel sprayed in a region with low oxygen concentration.

Fig. 7 shows the influences of fuel spray timing, fuel spraying angle, and H₂ gas addition on NOx and CO emission. As indicated in Fig. 7, by the addition of H₂ into the combustion chamber the amount of CO emission has decreased considerably. In other words, by replacing part of the diesel fuel with H₂ gas, the amount of fuel carbon species that participates in combustion has decreased, and as a result, CO emission has diminished compared to NDC mode. Furthermore, retarding the injection timing due to lower MPPP, MTPP, and MHRPP caused by more evaporated fuel, which burned in diffusive combustion mode, led to higher CO emission. As presented in Fig. 7, a wider spray cone angle led to lower CO emission due to better air-fuel mixing that has improved fuel oxidation process.

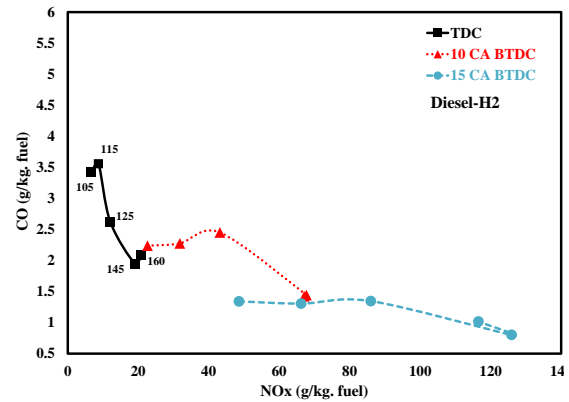
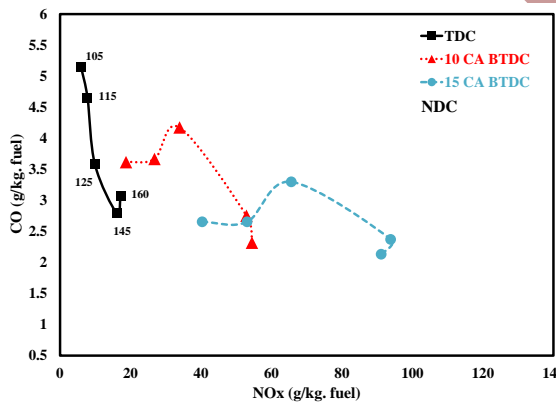


Fig. 7. Impacts of study strategies on the CO-NOx trade-off.

5.3. Effects of study strategies on engine performance

Fig. 8 reports the effects of fuel spray timing, fuel spraying angle, and H₂ gas addition on IP and ISEC. As illustrated in Fig. 8, the use of H₂ has increased IP and improved ISEC simultaneously. In other words, the addition of hydrogen gas due to high heating value led to increasing the MPPP, MTPP, and MHRPP that resulted in the improved fuel oxidation process. Better air-fuel mixture oxidation could improve engine performance, especially lower ISEC compared to NDC mode. Advancing the direct injection timing has increased the IP and decreased ISEC simultaneously. For advanced ITs, more evaporated fuel could burn in premixed combustion that led to higher pressure and temperature rise rate. As a result, MPPP, MTPP, and MHRPP have increased, and engine performance has improved. Furthermore, increasing the fuel spray cone angle due to better air-fuel mixing and improved fuel oxidation has increased the IP and improved the ISEC. However, 160 degrees cone angle has decreased engine performance due to more fuel could be sprayed in regions with lower oxygen level that led to lean mixture formation and oxidation.

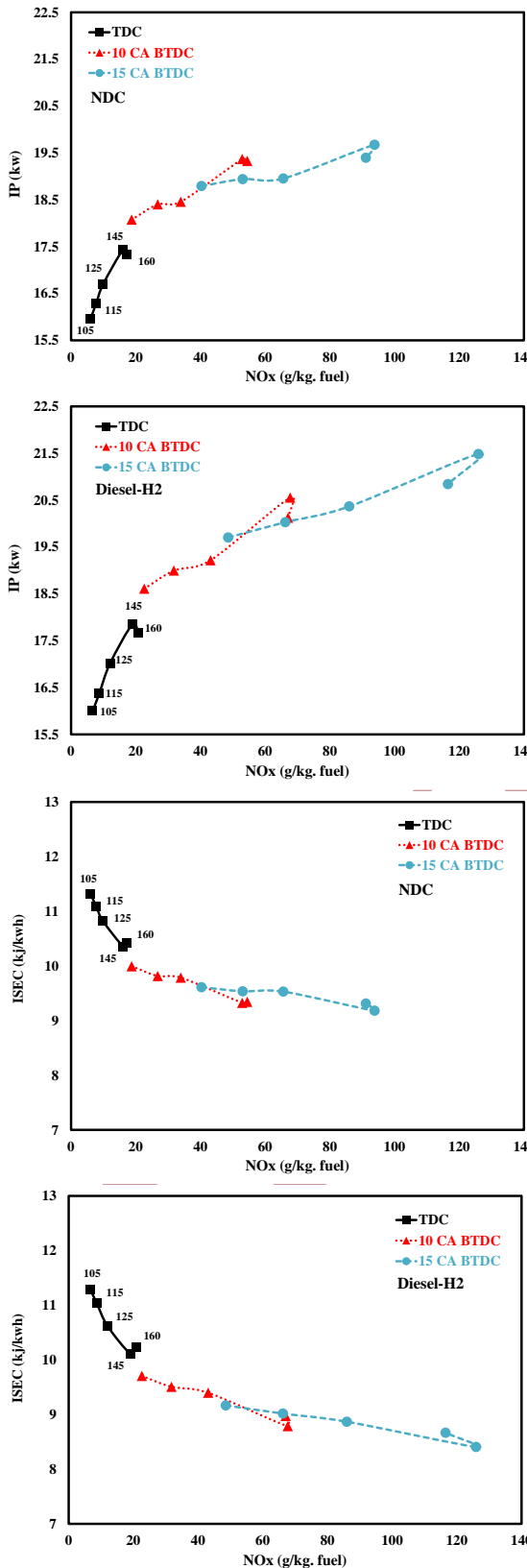


Fig. 8. Effects of study strategies on the IP-NOx and the ISEC-NOx trade-off.

6. Conclusion

In present study, the separate and simultaneous effects of diesel fuel spray timing, nozzle cone angle and addition of H₂ gas on combustion characteristics, output pollutant emissions, and performance of a single-cylinder heavy-duty compression ignition engine have been examined. Obtained results revealed that:

- Induction of H₂ gas into the engine cylinder has increased MPPP, MTPP, and MHRPP compared to NDC mode. Also, higher combustion temperature has improved mixture oxidation, and as a result, soot and CO emissions significantly have decreased. However, because of the high heating value of H₂ gas and higher combustion temperature of H₂-Diesel compared to NDC mode, NOx emissions have increased.
- Advancing fuel DI timing led to longer ID period. More extended ID accompanied by more evaporated fuel to ignite in premixed combustion, which resulted in higher pressure and temperature rise rate that could increase MPPP, MTPP, and MHRPP. As a result, the air-fuel mixture formation has improved, and following that, soot and CO emissions have diminished.
- Simultaneous addition of H₂ gas and advancing the fuel DI timing led to the improvement of ISEC and increasing IP at the expense of high NOx emissions.
- Wide fuel spray cone angle (e.g., 160 degrees) led to more fuel to spray in regions with lower oxygen concentrations that could decrease IP and increase ISEC simultaneously.

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