

Influence of Intake Charge Temperature and EGR Rate on the Combustion and Emission Characteristics of Ammonia/Diesel Dual-Fuel Engine

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Abstract

Ammonia has emerged as a promising carbon-free alternative fuel for internal combustion engines (ICE), particularly in large-bore engine applications. However, integrating ammonia into conventional engines presents challenges, prompting the exploration of innovative combustion strategies like dual-fuel combustion. Nitrous oxide (N₂O) emissions have emerged as a significant obstacle to the widespread adoption of ammonia in ICE. Various studies suggest that combining exhaust gas recirculation (EGR) with adjustments in inlet temperature and diesel injection timing can effectively mitigate nitrogen oxides (NO_x) emissions across diverse operating conditions in dual-fuel diesel engines. This study conducts a numerical investigation into the impact of varying inlet charge temperatures (330K, 360K, and 390K) and EGR rates (0%, 10%, and 20%) on the combustion and emission characteristics of an ammonia/diesel dual-fuel engine operating under high-load conditions, while considering different shares of ammonia energy. Computational fluid dynamics (CFD) simulations are executed using Converge software. Subsequently, multi-linear regression models are developed, utilizing ammonia share, inlet charge temperature, and EGR rate as independent variables, and emission parameters as dependent variables. The best-fitted regression model can be employed to analyze the response surface of performance parameters. The findings indicate that EGR rate and inlet charge temperature significantly impact N₂O and other emission parameters. However, the extent of this influence and the optimal percentage of each parameter may vary across different engine operating conditions, particularly concerning the ammonia share in a dual-fuel ammonia-diesel engine.

1.Introduction

Compression ignition diesel engines are frequently found in heavy-duty transportation, power production, and maritime vehicles because of their effectiveness and long-term operability. However, they release significant amounts of NO_x, soot as well as CO₂ due to their combustion characteristics. A wide range of technologies such as exhaust gas recirculation (EGR), exhaust after-treatment devices, time injection management, engine geometry modification, and dual fuel mode using alternative fuels are practical in reduction these emissions [1-3]. For diesel combustion systems to reduce CO₂ emissions, carbon-free fuels must be introduced. In compression ignition engines, dual-fuel mode provides flexibility for the fuel and the possibility of clean, efficient combustion. Natural gas is becoming more popular as a dual-fuel alternative due to its low

reactivity. Premixed natural gas can now be used in certain diesel engines thanks to modifications [4-5]. Due to the usage of natural gas, dual-fuel engines have reduced soot emissions, but their NO_x emissions can be on par with diesel engines. When it comes to reducing NO_x in dual-fuel engines, exhaust gas recirculation (EGR) works incredibly well [6-7]. With EGR, certain exhaust gases are sent back into the engine's inlet system, where they partially replace nitrogen and oxygen with exhaust constituents. Because there is less oxygen present during combustion, this method lowers the temperature of the gas, which lowers flame temperature and prevents the generation of NO_x. There are two primary forms of EGR used: cold EGR lowers NO_x emissions while hot EGR increases thermal efficiency. Therefore, temperature can have a major impact on EGR performance [8].

Furthermore, reducing NO_x and glasshouse gas emissions from dual-fuel diesel engines can be achieved by the use of cleaner fuels and increasing fuel efficiency. One carbon-free energy source that has promise for heavy-duty transportation is hydrogen (H₂). But infrastructure, distribution, and storage issues prevent its full implementation [9]. Ammonia (NH₃), a hydrogen carrier, is becoming another popular as a potential hydrocarbon fuel substitute because of its high energy density, carbon-free status, and adaptable infrastructure, all of which serve to mitigate hydrogen's drawbacks [10]. Similar to hydrogen, burning ammonia produces no CO₂. It reduces its carbon footprint because it is made from renewable resources ("green ammonia") [11]. It is thought to be feasible to partially substitute dimethyl ether, biodiesel, or diesel in dual-fuel compression ignition. Ammonia's carbon-free nature, high H₂ density, and ease of storage and transportation make it appealing for significant greenhouse gas reductions, even though its combustion characteristics may not surpass those of methanol, ethanol, or methane. A premixed ammonia-air mixture is injected into the cylinder during intake, compressed, and ignited by diesel injection in ammonia-diesel dual-fuel combustion. High auto-ignition temperature, sluggish flame speed, and limited flammability range are problems for pure ammonia in CI engines [12-14]. Additionally, compared to diesel-only mode, ammonia combustion in dual-fuel systems might result in higher NO_x emissions and the powerful greenhouse gas N₂O. For ammonia to be a viable carbon-free fuel source, advanced combustion techniques are required to reduce N₂O emissions in ammonia-diesel dual-fuel combustion [15].

The use of ammonia in CI engines with ammonia diesel dual fuel (ADDF) combustion was first introduced by Bro et al 1977's [16] study. Reiter et al. [17-18] (2008, 2011) reported that ADDF engines have reduced CO₂ and equivalent output. Increased ammonia proportion was observed to decrease fuel efficiency and increase N₂O emissions by Niki et al. [19] (2018). By modifying the timing of

diesel injection, N₂O issues were alleviated and GHG emissions were reduced by 30.6 percent at a 40 percent NH₃ energy fraction. Yousefi et al. [15] investigated the effects of diesel injection time and ammonia fraction and found that while N₂O emissions were higher, Green House Gases (GHG) emissions were up to 12% lower when only diesel was used. Studies on NH₃ addition to different fuels to reduce emissions have been conducted. In general, a review of the literature shows that no study so far has performed on the analyzing and modeling the performance of an ammonia-diesel dual-fuel engine working at different intake temperature and EGR percentage while as it mentioned these can have a remarkable effect on the performance of dual-fuel CI engine.

The material mentioned above demonstrates the growing interest in using ammonia in CI engines to lower greenhouse gas emissions. This study thoroughly examines how an ADDF engine's combustion performance and emissions are affected by the inlet charge temperature and EGR percentage. Using CONVERGE 2.4 software, a computational fluid dynamics (CFD) model is created to simulate ADDF combustion and examine how exhaust emissions are affected by EGR and inlet charge temperature. To comprehend fundamental phenomena, the model looks at engine-out emissions and cylinder pressure.

2. Material and method

2.1. Numerical model

The commercial CFD software, CONVERGE v3.0, was used to simulate a close cycle (i.e., IVC to EVO) of the investigated engine. The engine specification is reported in table 1 and a brief summary of the numerical method and important models is described in this section. With CONVERGE, the true boundary shape is accurately represented without requiring the computational grid to be molded with the geometry of interest thanks to a modified cut-cell cartesian approach. This method fully automates the mesh generation process and permits the usage of straightforward orthogonal grids. The cylinder geometry and meshes are displayed in Figure 1.

Table 1: Engine specification

Engine model	Caterpillar 3401
Number of cylinders	1
Bore*stroke (mm*mm)	137.2*165.1
Connecting rod length(mm)	261.62
Compression ratio	16.25
Displacement(L)	2.44
Intake valve opening (IVO)	-.358.3°ATDC
Intake valve closing (IVC)	-.169.7°ATDC
Exhaust valve opening (EVO)	-.145.3°ATDC
Exhaust valve closing (EVC)	-.348.3°ATDC

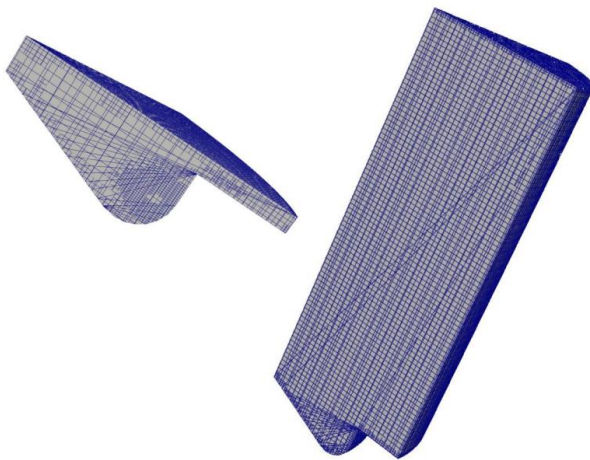


Figure 1: The cylinder geometry and the meshes of Caterpillar 3401

A comprehensive transient chemical kinetics solver called SAGE was used to simulate the combustion process [20]. The SAGE solver solved new species mass fractions right before the transport equation in each time step and cell. The pressure implicit with splitting of operator approach was utilized to solve the transport equations. 388 reactions and 69 species made up the chemical kinetic mechanism used in this simulation. Figure 2 shows the effect of fuel chemistry on the solution at the beginning of each time scale of the software, which is introduced to each computational cell by the single-region zero-dimensional model. Entering the information of chemical equations and reaction coefficients into the software is based on a text file in auxiliary format, which includes stoichiometric reactions and kinetic coefficients [21-22]. In the simulation of the present work, the perfect gas assumption was used to estimate the thermodynamic behavior of the gas mixture.

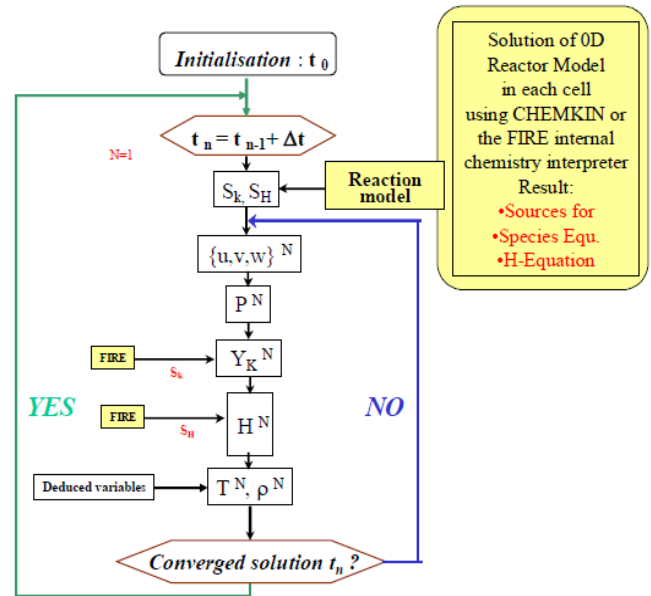


Figure 2: The process of solving the combination of multi-dimensional computational fluid dynamics model with fuel chemical kinetics.

The diesel injection pressure and time in the simulation were in line with the measured data, and the injector had six holes. The "DIESEL2" fuel surrogate, which is provided in the CONVERGE library for the spray and mixing process, was used to mimic the physical characteristics of diesel fuel [23]. Table 2. presents specifics of a few adopted spray models. Also, turbulence in the combustion chamber flow field was simulated using a re-normalization group (RNG) k- ϵ model based on the Reynolds Averaged Navier-Stokes (RANS) [24]. A grid size of 0.25 mm was produced with the aid of adaptive mesh refinement, which was anticipated to precisely resolve the features in the turbulent flame front [25].

Table 2: summary of key spray processes used for the spray model

Physical process	model
Liquid injection	Blob injection model
Spray breakup	KH-RT model
evaporation	Frossling model
Droplet collision	NTC model
Drop drag	Dynamic drag model
Drop turbulent dispersion	O'Rourke model
Drop/wall interaction	Rebound/slide model

The input for the simulation was the three minutes of engine steady state settings, averaged different condition of intake air temperature (IAT), exhaust gas recirculation (EGR), and diesel, ammonia, and air flow rates, which address in Table 3. To get the simulations' intake pressure closer to the experimental pressure during the compression stroke and the mass flow rates of ammonia and air, 5 kPa was changed. It was believed that the inflow consisted of a uniform mixture of air and ammonia. Given that the experiment's ammonia port fuel injector is situated a considerable distance from the engine block's inlet, this assumption seems probable.

Table 3: Simulation conditions.

NH3 Energy Fraction (%)	IAT (K)	EGR %	Diesel (kg/h)	NH3 (kg/h)	Air (kg/h)
0	330-360-390	0	3.38	0	83.26
20%	330-360-390	0	2.73	1.56	80.64
		10	2.73	1.56	76.60
		20	2.73	1.56	74.02
40%	330-360-390	0	2.08	3.18	77.92
		10	2.08	3.18	72.58
		20	2.08	3.18	70.13

2.2. Model validation

The ADDF engine's measured and calculated cylinder pressures at commencement of injection at -14.2°ATDC and with varying ammonia energy percentages are compared in Figure 3. Additionally, a comparison will be made between the calculated and experimental combustion characteristics and emissions (NH3, NO, N2O, and CO2). The outcomes are contrasted with the diesel and ammonia-diesel dual-fuel combustion outcomes of reference [13]. In their research a Caterpillar 3401 diesel engine with the specification reported in table 1, modified for ammonia/diesel dual-fuel combustion was used for the experiments. It is evident that the peak cylinder pressure, initiation of combustion, and numerical cylinder pressure correspond well with the experimental data. Overall, the validation results demonstrate the current numerical simulation's capacity to qualitatively replicate the ADDF engine's emissions and combustion characteristics.

2.3. Optimization and statistical analysis

In this section, a mathematical model that could forecast engine performance and ideal conditions was created using statistical approaches. Initially, the multiple linear regression models were used to the simulation data from the preceding section in order to characterize the behavior of the system and connect engine performance with operating factors. Numerous fields have effectively employed this technique [26-28]. The following is an expression for MLR models [29]:

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \sum_{j=i+1}^k \beta_{ij} x_i x_j + \sum_{i=1}^k \beta_{ii} x_i^2 + \varepsilon$$

where the dependent variable is called y , the independent variables are called x_i and x_j , and they range in length from 1 to k . The intercept coefficient is denoted by β_0 , and the regression coefficients of the linear, quadratic, and second-order terms are represented by β_i , β_{ii} , and β_{ij} , respectively. The number of independent parameters in this work is 2, and the regression error is called ε . Using linear, quadratic, reduced quadratic, and two-factor interaction (2FI) models to analyses the experimental data, the optimum regression equations were identified for this investigation.

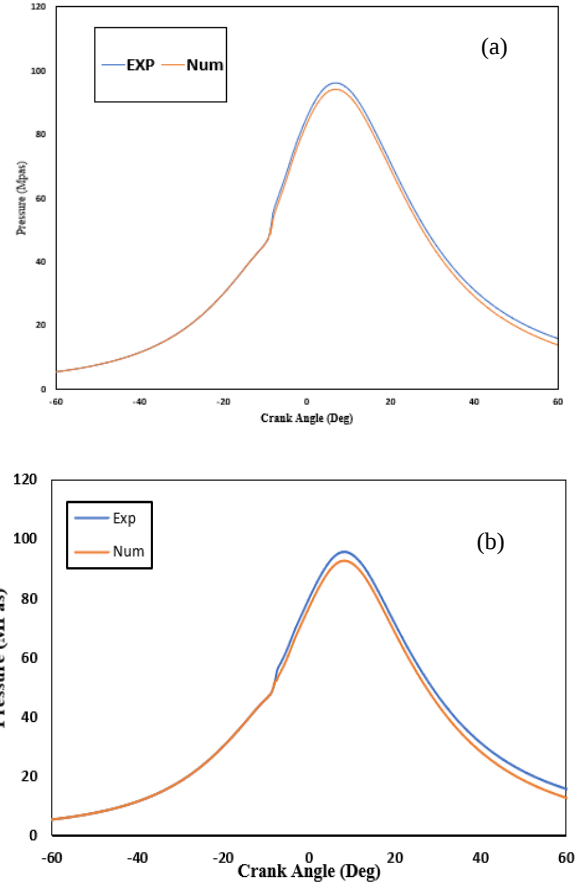


Figure 3: Comparison of measured and calculated cylinder pressure combustion for pure diesel (a) and 20% NH3 (b).

4. Results and discussion

This part presents and discusses the numerical results for intake charge temperature (330K, 360K, and 390K) and EGR (0, 10%, 20%, and 30%) on the cylinder pressure, heat release rate, and emission exhaust of the studied dual-fuel engine. Examining different percentages can assist in achieving emissions-based operating conditions that are optimum. Additionally, the net diesel engine would be compared to the effects of these parameters in two dual-fuel scenarios (20 percent and 40 percent ammonia). The emission in this study is determined using the following equation 2 to the stated particular values of ISCO2, ISN2O, ISNO, ISNO2, and ISNH3. Where m_{ex} and m_{fuel} are the amount of each species and consumed fuel, respectively, m_{fuel} is the mass flow rate of fuel and IP is the indicated power.

$$ISex \left(\frac{gr}{kw.h} \right) = \frac{m_{ex}(kg)}{m_{fuel}(kg)} * \dot{m}_{fuel} \left(\frac{kg}{h} \right) * \frac{1}{IP(kW)}$$

4.1. cylinder pressure and heat release rate

The computed cylinder pressure and HRR of the diesel and ADDF engine during running conditions with a 20 percent and 40 percent ammonia energy fraction, respectively, as shown in Figures 4 and 5. Because the difference between the three temperatures was nearly equal, the outcome is only visible at the mild temperature of 360K.

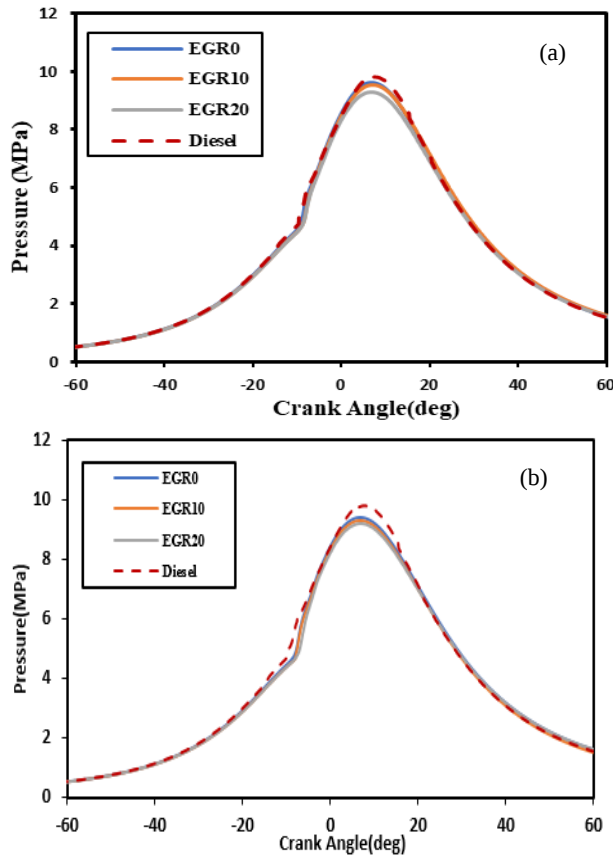


Figure 4. Comparison of calculated cylinder pressure of diesel and ADDF combustion mode with different EGR ratio for a) 20% ammonia b) 40% ammonia energy fractions

It is clear that when ammonia replaces diesel fuel, the ignition delay and peak cylinder pressure decrease proportionately. The increased ignition delay can be explained by two main explanations. First, by using less diesel fuel spray, the fuel momentum required for effective atomization and mixing is reduced, which leads to ignite. Secondly, the use of ammonia in replace of some diesel makes it more difficult for ignition to occur due to its strong resistance to autoignition [11 and 13]. Furthermore, at higher ammonia fueling conditions, the comparison of the two different dual modes, EGR0 at Figures 4a and 4b, shows that the maximum pressure was 9.61 MPa and 9.39 MPa at 6.83 ATDC and 6.21 ATDC, respectively.

The heat release rate statistics in Figures 5a and 5b demonstrate that the energy scenario utilizing only diesel fuel exhibits diffusion burns and discrete premixed burns, which are features of ordinary diesel combustion. These characteristics are still present for diesel fuel energy percentages of 20 and 40 percent. When the energy level of the diesel fuel is reduced to 80% (EGR0 at figure. 5a), there is a slight decrease in the premixed phases; however, a more notable reduction occurs when the ammonia content is 40% (EGR0 at figure. 5b). It is clear that the extended ignition delay resulted in a large premixed combustion for diesel fuel with a rather high peak heat release rate. The combustion begins at -15.3°ATDC rather than -15.1 when the ammonia energy percentage is raised from 20 to 40%.

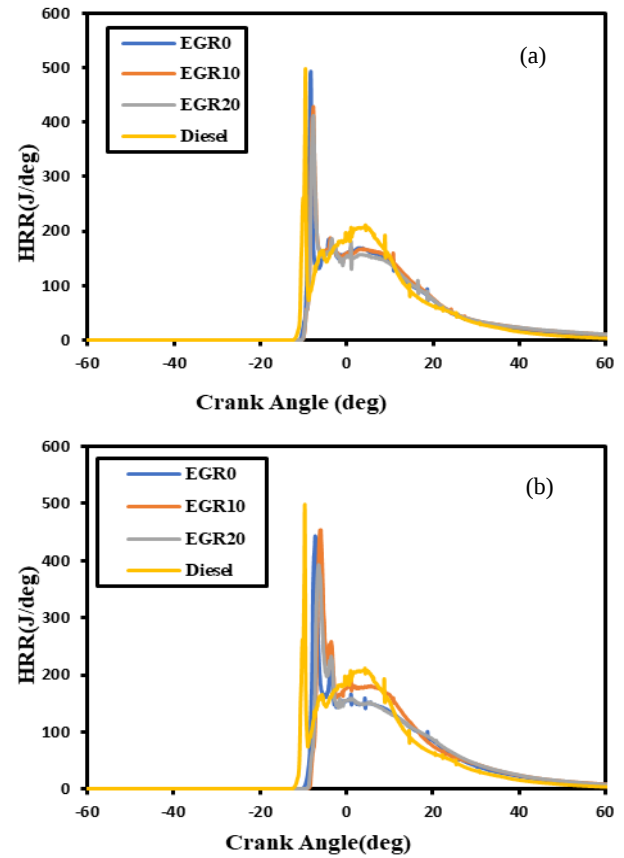


Figure 5. Comparison of calculated HRR of diesel and ADDF combustion mode with different EGR ratio for a) 20% ammonia b) 40% ammonia energy fractions

Moreover, Figures 4 and 5 show the in-cylinder pressure and heat release rate for the ammonia-diesel dual fuel at 360K intake charge temperature for EGR rates ranging from 0 to 20 percent. It is clear that the application of EGR decreased the rate of heat release and the in-cylinder pressure in dual-fuel scenarios; however, this reduction was negligible in dual-fuel cases with 40% ammonia. Both a decrease in oxygen availability and a drop in the rate of fuel burning during the diffusion phase could be the cause of this decline [30]. It is important to note that at various temperatures, the trends for pressure and heat release rate were constant.

The ignition delay in the dual-fuel operation mode was generally investigated. The ignition delay increases with increasing EGR rate. In order to account for the reason behind the extended ignition delay with increasing EGR rate, the oxygen molar concentration at the injection timing decreased as the EGR rate grew because the volume percent of oxygen in the intake mixture decreased. The temperature of the unburned mixture decreased as the EGR rate increased because specific heat increased at fixed volume. Because of the decline in the unburned mixture's temperature and the drop in the oxygen molar concentration at injection timing, the ignition delay increased as the EGR rate increased [30]. However, a comparison of Figures 5a and 5b shows that the ignition delay under dual fuel operation was not the same under ammonia injection of different volumes. In dual-fuel modes, it turned out that the effect of EGR on the higher (40 percent) ammonia level was less pronounced than it was on the lower premixed fuel percentage.

4.2. Indicated Specific Emission Exhaust

4.2.1. ISCO₂

Figure 6 depicts the CO₂ emissions from a diesel engine running on ammonia and diesel. As can be shown, the net diesel fuel is compared to three distinct intake charge temperatures in two distinct dual-fuel cases, with 20% and 40% of the ammonia energy fraction and varying EGR percentages. As seen in Figure 6, adding varying amounts of EGR would result in increased CO₂ emission for dual-fuel instances, even though employing ammonia as both 20 percent and 40 percent energy fraction reduces the CO₂ emission at different temperature when comparing EGR0 with diesel.

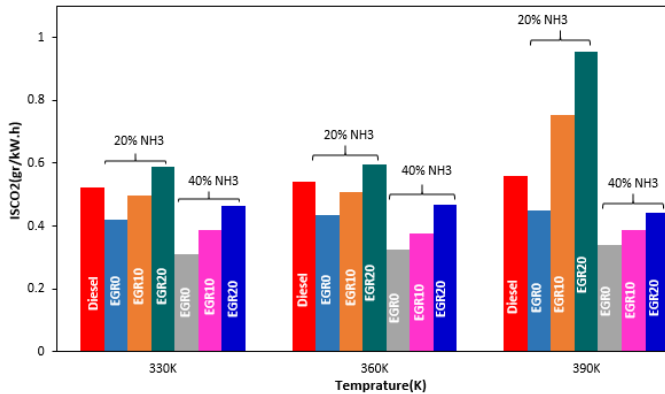


Figure 6. Effect of EGR on ISCO₂ emission of engine fueled by two ammonia fractions worked at different charge temperature.

Since ammonia is a carbon-free alternative fuel that replaces more diesel fuel, the decrease in CO₂ with dual fuel cases was predicted. Furthermore, recirculating some of an engine's exhaust gas (including CO, CO₂,...) back into the engine cylinders may be the cause of the increased CO₂ emission for dual-fuel situations with EGR. Nonetheless, it is evident that the cases with 40% ammonia and two distinct fractions of EGR (pink and blue columns) would have lower CO₂ emissions than the net diesel cases (red column). This could be because ammonia is a carbon-free fuel that replaces a larger proportion of diesel. Thus, while the CO₂ emissions of the ADDF combustion mode can be further increased by adopting the EGR method in comparison to the diesel injection strategy, the CO₂ emissions of stops with a greater ammonia percentage (40 percent) would still be lower than those of diesel. Furthermore, in general, all cases especially those with lower ammonia percentages produce more CO₂ emissions at higher temperatures. The outcomes may demonstrate improved fuel combustion brought on by a greater temperature.

4.2.2. ISNH₃

Figure 7 illustrates how two ammonia energy fractions and three distinct input temperatures affect the indicated specific NH₃ emissions when using with EGR. The amount of NH₃ is anticipated to rise in comparison to all dual fuel cases with the net diesel fuel because ammonia is added as a premixed fuel [31]. Additionally, Figure 7 shows that there is an increase in unburned ammonia emissions when the ammonia energy portion rises. The primary cause of this is the premixed ammonia-air mixture's ineffective flame propagation [19]. When using EGR10, a reduction in the NH₃ emission was seen. There is an exception for EGR10 of 20 percent ammonia at 390K when compared to EGR0 for both 20 and 40 percent ammonia. It is clear that the reduction for 40% ammonia is

more noteworthy. This decrease may be explained by the way NH₃ reacts with the types of exhaust gases that are recirculated in the intake manifold; nonetheless, a higher EGR percentage usually results in a higher amount of unburned NH₃, particularly for 20 percent ammonia 330K, because of a lower combustion temperature. Even so, the amount of unburned ammonia remains smaller in larger percentage ammonia at higher temperatures than in circumstances without an EGR (comparing dark blue column with grey one at 360 and 390K). Since greater combustion temperatures may overcome the higher auto-ignition temperature of ammonia as a premixed fuel, higher input temperatures generally resulted in fewer unburned NH₃ for various instances.

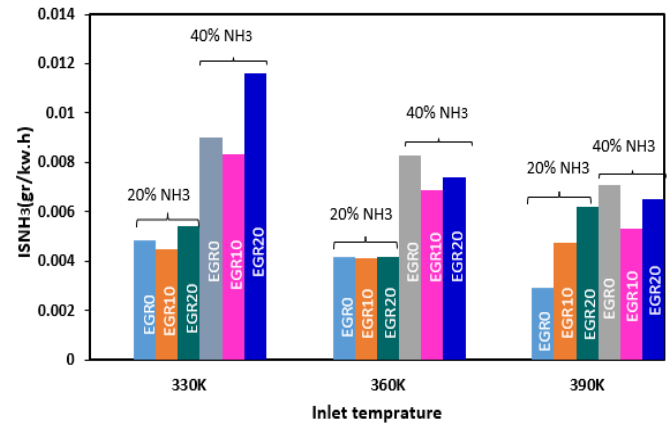
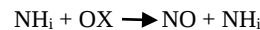


Figure 7. Effect of EGR on ISNH₃ emission of engine fueled by two ammonia fractions worked at different charge temperature.

4.2.3. ISNO

The indicated specific NO (ISNO) emissions for two ammonia energy fractions at various EGR percentages and inlet charge temperatures are displayed in Figure 8 shows that at different temperatures, dual fuel situations (EGR0 for both ammonia energy fraction, light blue and grey column compared with red column) can reduce ISNO emissions more than 70%. The primary cause of NO creation in CI engines is the lower combustion temperature in ADDF mode, which tends to generate less NO via the thermal-NO formation route. Furthermore, the formation of fuel-NO via reaction (6), in which nitrogenous radicals (primarily NH and NH₂) react with oxygenated species (primarily O and O₂) at high combustion temperatures (i.e., T > 1400 K) to form NO, is primarily responsible for the higher amount of NO for dual-fuel cases at higher temperatures.



Using EGR would also significantly reduce the ISNO emission at the same time. The examples with the greater ammonia and EGR percentages (dark blue column) have the lowest NO emission levels at varying temperatures. Generally speaking, the ADDF mode's lower combustion temperature tends to produce less NO through the thermal-NO production route. Furthermore, lowering the oxygen concentration in the combustion chamber and increasing heat absorption from a rise in the specific heating capacity of the premixed mixture in the intake manifold result in a decrease in the quantity of NO_x produced by using and increasing the EGR percentage. Furthermore, the increased level of NO in exhaust emissions is a predicted consequence of the greater inlet charge temperature. Regarding all of cases in this investigation, 40-EGR20 at 330K yielded the lowest unburned ammonia emissions of 0.0046 g/kW.h, while the net diesel at 390K produced the highest emissions

at 0.0014 g/kW.h. In comparison to the lowest unburned ammonia emissions in ADDF mode with a single diesel injection technique, they are reduced by approximately 64 percent and 76 percent, respectively.

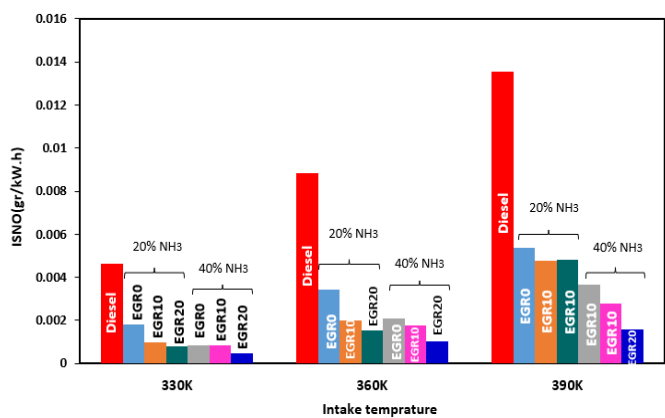


Figure.8. Effect of EGR on ISNO emission of engine fueled by two ammonia fractions worked at different charge temperature.

4.2.4. ISNO2

When the NO2 emissions from the dual fuel instances are compared to the net diesel in Figure 9, it can be seen that while the cases with 40% ammonia, both with and without EGR, emit less NO2, the cases with 20% ammonia exhibit a different pattern. This indicates that NO2 emissions were higher than the net diesel in the cases with 20% ammonia and no EGR (light blue column); however, the cases with EGR (20-EGR10 and 20-EGR20) exhibit lower NO2 exhaust emissions than the net diesel, with the exception of 390K. The larger increase in NOx-thermal production at the study's greatest temperature may be the source of the divergent results. Put another way, a greater combustion temperature, particularly for a smaller ammonia proportion, may be the cause of the increase in this particular sort of nitrogen oxides at higher temperatures. This indicates that at different temperatures, the cases containing 40 percent ammonia and 10–20 percent EGR produce the least amount of NO2, whereas the instances containing 20 percent ammonia with and without EGR show the largest quantity of NO2. Thus, in general, higher ammonia fraction and EGR percentages were associated with the lowest amount of NO2 (dark blue column 40-EGR10).

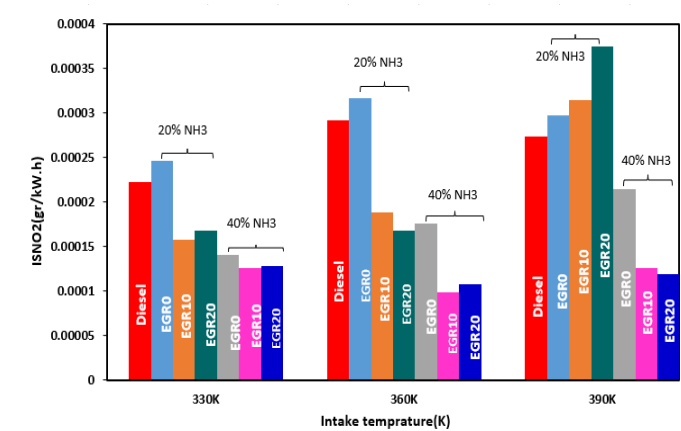


Figure.9. Effect of EGR on ISNO2 emission of engine fueled by two ammonia fractions worked at different charge temperature.

4.2.5. ISN2O

Figure 10 shows that at all temperatures tested, the diesel combustion mode emits very little N2O. Nonetheless, since the greenhouse gas impact of N2O is around 300 times greater than that of CO2 over a 100-year period, N2O emissions are one of the primary issues associated with ammonia combustion [32]. Nitrous oxide is formed when nitrogenous radicals, primarily NH and NH2, react with NO and NO2 at temperatures lower than 1400K to generate nitrous oxide. Numerous investigations have documented these reactions as the primary mechanisms of N2O generation [15, 33-34].

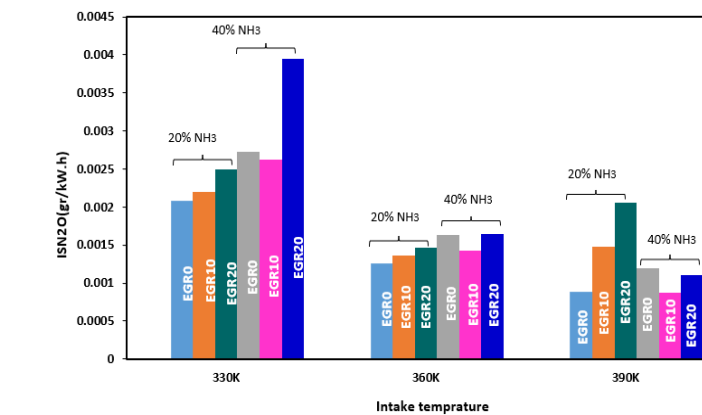


Figure.10. Effect of EGR on ISN2O emission of engine fueled by two ammonia fractions worked at different charge temperature.

A higher inlet temperature would result in less N2O being released into the exhaust, even though using EGR would somewhat increase ISN2O emissions. Consequently, dual fuel cases with a smaller ammonia proportion and no EGR at a higher temperature would produce the least quantity of N2O. (20-EGR0 light blue column). The reaction described above and a lower temperature in the ammonia-diesel dual-fuel combustion process are likely connected to increasing N2O with EGR. Furthermore, a higher ammonia fraction was found to increase the amount of N2O (comparing 20 percent and 40 percent) at 330 and 360K, but a higher ammonia fraction at 390K produced the opposite result, indicating that the cases with 40 percent ammonia and EGR emit less N2O than the cases with 20 percent ammonia dual fuel and EGR.

4.3. Multiple linear regression model for predicting engine performance parameter

As it explained in section 2.3, in this study two independent factors (x_i and x_j) were the EGR ratio (0, 10 and 20) and the temperature of inlet charge (330, 360 and 390). The dependent variables (y) were ISCO2, ISNO, ISNO2, ISN2O, and ISNH3. As previously noted, in order to identify the best-fitting models, four regression models have been created to predict eight engine performance metrics. Two metrics were used to assess the quality of fitted models: the coefficient of determination (R^2) value and the adjusted R^2_{adj} . To put it another way, these two coefficients are used to determine whether an MLR model is compatible. Based on the results shown in Table 4. the reduced quadratic model, with the highest value of determination coefficient, is determined to be best-fitted model for most of emission parameter all cases at two different ammonia fractions. The best fitted model for each species is shown bold style in table.

Table 4. R₂ and adjusted R₂ coefficients of four different MLR models for five engine emission parameters while consuming biodiesel produced using Conv., Micro and Ultra. heating system.

Model	ISCO ₂			
	20% NH ₃		40% NH ₃	
	R ²	R ² _{adj}	R ²	R ² _{adj}
linear	0.998	0.997	0.985	0.982
2FI	0.998	0.998	0.989	0.986
Red.Quad	0.999	0.999	0.996	0.994
Quad.	0.998	0.997	0.988	0.983
ISNH ₃				
linear	0.887	0.868	0.470	0.381
2FI	0.927	0.907	0.684	0.598
Red.Quad	0.934	0.898	0.808	0.701
Quad.	0.898	0.857	0.549	0.369
ISNO				
linear	0.850	0.825	0.804	0.595
2FI	0.944	0.929	0.804	0.695
Red.Quad	0.989	0.983	0.764	0.663
Quad.	0.856	0.798	0.699	0.579
ISNO ₂				
linear	0.770	0.732	0.520	0.440
2FI	0.824	0.776	0.766	0.702
Red.Quad	0.894	0.835	0.899	0.842
Quad.	0.792	0.709	0.584	0.418
ISN ₂ O				
linear	0.911	0.896	0.610	0.545
2FI	0.930	0.911	0.727	0.652
Red.Quad	0.993	0.989	0.804	0.695
Quad.	0.979	0.971	0.681	0.553

In the cases with the coefficient about 0.99, this means that the model can estimate the emission very well. Therefore, the obtained equation for each parameter would be helpful to analysis the response of emission exhaust running at different EGR ratio and inlet temperature. Moreover, this can be practical to achieve the optimum amount of EGR and temperature for dual-fuel cases via optimization algorithm.

5. Conclusion

In this study, CFD methods are used to investigate the emission parameter of an ammonia-diesel dual-fuel engine when it is fueled with two different ammonia (20% and 40% ammonia) and working with different EGR ratio (0, 10, 20) at different inlet charge temperature (330, 360 and 390). In general, in-cylinder and heat release rate of dual-fuel cases decrease in comparison with diesel mode, and the amount of ISCO₂, ISNO for dual-fuel cases were lower than diesel one while ISNH₃, ISNO₂ and ISN₂O with ammonia-diesel dual-fuel cases increase generally. Comparison dual-fuel cases with EGR also, show that using EGR increase ISCO₂ while it was more significant for lower percentage of ammonia, but ISNH₃ for lower percentage of ammonia with EGR generally increase while for cases with higher ammonia percentage and low percentage of EGR this can be lower. Moreover, for dual-fuel cases with EGR the amount of ISNO and ISNO₂ decrease. while, lower amount of these nitrogen oxides would be for the cases with higher ammonia fraction and EGR ratio. Regarding ISN₂O as an important species for dual-fuel cases represent that the use of low level of EGR for higher fraction of ammonia can decrease this emission exhaust at all of investigated temperature. finally, applying regression model shows that the amount of emission parameter would be predictable with some multi-linear regression that would be helpful to find the optimum amount of EGR and intake temperature for dual-fuel cases.

References

- Sharma, Vipin, Yogesh Dewang, Supriya Jain, Sachin Jat, and Mukesh Singh Baghel. "Strategies for Reduction of Harmful Emissions from Diesel Engines." In IOP Conference Series: Earth and Environmental Science, vol. 795, no. 1, p. 012027. IOP Publishing, 2021. doi:10.1088/1755-1315/795/1/012027
- Senecal, P. K., and Felix Leach. "Diversity in transportation: Why a mix of propulsion technologies is the way forward for the future fleet." Results in Engineering 4 (2019): 100060. doi.org/10.1016/j.rineng.2019.100060
- Tonetti, Marco, Giorgio Rustici, Massimo Buscema, and Luca Ferraris. Diesel engine technologies evolution for future challenges. No. 2017-24-0179. SAE Technical Paper, 2017. doi.org/10.4271/2017-24-0179.
- Muralidharan, M., Ajay Srivastava, and M. Subramanian. "A technical review on performance and emissions of compressed natural gas-diesel dual fuel engine." (2019). doi.org/10.4271/2019-28-2390
- Yousefi, Amin, Hongsheng Guo, Shouvik Dev, Brian Liko, and Simon Lafrance. "Effect of pre-main-post diesel injection strategy on greenhouse gas and nitrogen oxide emissions of natural gas/diesel dual-fuel engine at high load conditions." Fuel 302 (2021): 121110. doi.org/10.1016/j.fuel.2021.121110
- Kumar, Parvesh, and Naveen Kumar. "Effect of EGR on performance and emission characteristics of a dual fuel engine fuelled with CNG and JOME." Biofuels 7, no. 6 (2016): 743-751. doi.org/10.1080/17597269.2016.1193838
- .Andwari, Amin Mahmoudzadeh, Azhar Abdul Aziz, Mohd Farid Muhamad Said, and Zulkarnain Abdul Latiff. "Experimental investigation of the influence of internal and external EGR on the combustion characteristics of a controlled auto-ignition two-stroke cycle engine." Applied Energy 134 (2014): 1-10. doi.org/10.1016/j.apenergy.2014.08.006
- Kumaraswamy, A., and B. Durga Prasad. "Performance analysis of a dual fuel engine using LPG and diesel with EGR system." Procedia engineering 38 (2012): 2784-2792. doi.org/10.1016/j.proeng.2012.06.326
- Vavra, Jiri, Ivan Bortel, and Michal Takats. A dual fuel hydrogen-diesel compression ignition engine and its potential application in road transport. No. 2019-01-0564. SAE Technical Paper, 2019. doi.org/10.4271/2019-01-0564
- Untheim, Thomas, Fabian Großmann, Paul Tatucu-Ertel, Marius Jochem, Peter Weigand, and Georgios Bikas. Experimental Study on Ammonia/OME Combustion in a Dual-Fuel Engine with Emphasis on Highly Diluted Intake Air Conditions. No. 2023-01-0283. SAE Technical Paper, 2023. doi.org/10.4271/2023-01-0283
- Dimitriou, Pavlos, and Rahat Javaid. "A review of ammonia as a compression ignition engine fuel." International Journal of Hydrogen Energy 45, no. 11 (2020): 7098-7118. doi.org/10.1016/j.ijhydene.2019.12.209
- Xu, Leilei, Shijie Xu, Xue-Song Bai, Juho Aleks Repo, Saana Hautala, and Jari Hyvönen. "Performance and emission characteristics of an ammonia/diesel dual-fuel marine engine." Renewable and Sustainable Energy Reviews 185 (2023): 113631. doi.org/10.1016/j.rser.2023.113631
- Yousefi, Amin, Hongsheng Guo, Shouvik Dev, Brian Liko, and Simon Lafrance. "Effects of ammonia energy fraction and diesel injection timing on combustion and emissions of an ammonia/diesel dual-fuel engine." Fuel 314 (2022): 122723. doi.org/10.1016/j.fuel.2021.122723

14. Nadimi, Ebrahim, Grzegorz Przybyła, Michał T. Lewandowski, and Wojciech Adamczyk. "Effects of ammonia on combustion, emissions, and performance of the ammonia/diesel dual-fuel compression ignition engine." *Journal of the Energy Institute* 107 (2023): 101158. doi.org/10.1016/j.joei.2022.101158
15. Yousefi, A., Guo, H., Dev, S., Lafrance, S., & Liko, B. (2022). A study on split diesel injection on thermal efficiency and emissions of an ammonia/diesel dual-fuel engine. *Fuel*, 316, 123412. doi.org/10.1016/j.fuel.2022.123412
16. Bro, Klaus, and Peter Sunn Pedersen. Alternative diesel engine fuels: An experimental investigation of methanol, ethanol, methane and ammonia in a DI diesel engine with pilot injection. No. 770794. SAE technical paper, 1977. doi.org/10.4271/770794
17. Reiter, Aaron J., and Song-Chang Kong. "Combustion and emissions characteristics of compression-ignition engine using dual ammonia-diesel fuel." *Fuel* 90, no. 1 (2011): 87-97. doi.org/10.1016/j.fuel.2010.07.055
18. Reiter, Aaron J., and Song-Chang Kong. "Demonstration of compression-ignition engine combustion using ammonia in reducing greenhouse gas emissions." *Energy & Fuels* 22, no. 5 (2008): 2963-2971. doi.org/10.1021/ef800140f
19. Niki, Yoichi, Yoshifuru Nitta, Hidenori Sekiguchi, and Koichi Hirata. "Emission and combustion characteristics of diesel engine fumigated with ammonia." In *Internal Combustion Engine Division Fall Technical Conference*, vol. 51982, p. V001T03A016. American Society of Mechanical Engineers, 2018. doi.org/10.1115/ICEF2018-9634
20. Richards K.J. SPK and PE. Converge Manual. Converge (Version 24) Manual, Converge Sci Inc, Madison, Wisconsin, USA, 2017.
21. Fakhari, Amir Hossein, Ayat Gharehghani, Mohammad Mahdi Salahi, and Amin Mahmoudzadeh Andwari. "RCCI combustion of ammonia in dual fuel engine with early injection of diesel fuel." *Fuel* 365 (2024): 131182. doi.org/10.1016/j.fuel.2024.131182
22. Salahi, Mohammad Mahdi, Vahid Esfahanian, Ayatallah Gharehghani, and Mostafa Mirsalim. "Investigating the reactivity-controlled compression ignition (RCCI) combustion strategy in a natural gas/diesel fueled engine with a pre-chamber." *Energy Conversion and Management* 132 (2017): 40-53. doi.org/10.1016/j.enconman.2016.11.019
23. Amsden, A. A. "A computer program for chemically reactive flows with sprays." Los Alamos National Laboratory Report LA-11560-MS (1989).
24. Yakhot, V. S. A. S. T. B. C. G., S. A. Orszag, Siva Thangam, T. B. Gatski, and CG1167781 Speziale. "Development of turbulence models for shear flows by a double expansion technique." *Physics of Fluids A: Fluid Dynamics* 4, no. 7 (1992): 1510-1520. doi.org/10.1063/1.858424
25. Senecal, P. K., K. J. Richards, E. Pomraning, T. Yang, M. Z. Dai, R. M. McDavid, M. A. Patterson, S. Hou, and T. Shethaji. A new parallel cut-cell Cartesian CFD code for rapid grid generation applied to in-cylinder diesel engine simulations. No. 2007-01-0159. SAE Technical Paper, 2007. doi.org/10.4271/2007-01-0159
26. Zareei, Javad, Abbas Rohani, and Wan Mohd Faizal Wan Mahmood. "Simulation of a hydrogen/natural gas engine and modelling of engine operating parameters." *International Journal of Hydrogen Energy* 43, no. 25 (2018): 11639-11651. doi.org/10.1016/j.ijhydene.2018.02.047
27. Siavash, Nemat Keramat, Barat Ghobadian, Gholamhassan Najafi, Abbas Rohani, Teymur Tavakoli, Esmail Mahmoodi, and Rizalman Mamat. "Prediction of power generation and rotor angular speed of a small wind turbine equipped to a controllable duct using artificial neural network and multiple linear regression." *Environmental research* 196 (2021): 110434. doi.org/10.1016/j.envres.2020.110434
28. Ashtiani, Seyed-Hassan Miraei, Abbas Rohani, and Mohammad Hossein Aghkhani. "Soft computing-based method for estimation of almond kernel mass from its shell features." *Scientia Horticulturae* 262 (2020): 109071. doi.org/10.1016/j.scienta.2019.109071
29. Allami, Hassanian Abdolkarim, Mohammad Tabasizadeh, Abbas Rohani, Hamed Nayebezhadeh, Abdolali Farzad, and Marziyeh Hoseinpour. "Modeling and optimization of performance and emission parameters of a diesel engine: A comparative evaluation between date seed oil biodiesel produced via three different heating systems." *Energy Conversion and Management* 283 (2023): 116909. doi.org/10.1016/j.enconman.2023.116909
30. Zareei, Javad, Abbas Rohani, and José Ricardo Nunez Alvarez. "The effect of EGR and hydrogen addition to natural gas on performance and exhaust emissions in a diesel engine by AVL fire multi-domain simulation, GPR model, and multi-objective genetic algorithm." *International Journal of Hydrogen Energy* 47, no. 50 (2022): 21565-21581. doi.org/10.1016/j.ijhydene.2022.04.294
31. Tomita, Eiji, Yuji Harada, Nobuyuki Kawahara, and Atsushi Sakane. Effect of EGR on combustion and exhaust emissions in supercharged dual-fuel natural gas engine ignited with diesel fuel. No. 2009-01-1832. SAE Technical Paper, 2009. doi.org/10.4271/2009-01-1832
32. <https://www.epa.gov/ghgemissions/understanding-global-warming-potentials> Accessed 2017;1-5.
33. Mathieu, Olivier, and Eric L. Petersen. "Experimental and modeling study on the high-temperature oxidation of Ammonia and related NOx chemistry." *Combustion and flame* 162, no. 3 (2015): 554-570. doi.org/10.1016/j.combustflame.2014.08.022
34. Nakamura, Hisashi, Susumu Hasegawa, and Takuya Tezuka. "Kinetic modeling of ammonia/air weak flames in a micro flow reactor with a controlled temperature profile." *Combustion and Flame* 185 (2017): 16-27. doi.org/10.1016/j.combustflame.2017.06.021
35. Gopal, Rajendiran, Mayilsamy Kavandappa-Goundar, Subramanian Ramasamy, Nedunchezian Natarajan, and Venkatachalam Ramasamy. "Experimental and regression analysis for multi cylinder diesel engine operated with hybrid fuel blends." *Thermal Science* 18, no. 1 (2014): 193-203. doi.org/10.2298/TSCI130130127G
36. Tosun, Erdi, Kadir Aydin, and Mehmet Bilgili. "Comparison of linear regression and artificial neural network model of a diesel engine fueled with biodiesel-alcohol mixtures." *Alexandria Engineering Journal* 55, no. 4 (2016): 3081-3089. doi.org/10.1016/j.aej.2016.08.011

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