Investigation of Combustion and Emission Performance in Ammonia-Diesel Dual-Fuel Engines

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***Abstract*--The growing interest in ammonia as a zero-carbon fuel for internal combustion engines has highlighted its potential, particularly in large-displacement engines. Despite its environmental advantages, the use of ammonia introduces considerable challenges in terms of combustion dynamics and pollutant formation. This research uses computational fluid dynamics (CFD) modeling through CONVERGE software to evaluate how varying the share of ammonia, diesel injection duration, and injection timing affects engine behavior under high-load conditions. The findings reveal that introducing a 10% ammonia blend results in peak pressures surpassing those of conventional diesel combustion. While ammonia tends to delay ignition and reduce the heat release rate, optimizing injection timing and shortening injection duration improves premixed combustion characteristics. Notably, nitrogen oxide (NO) emissions are substantially decreased by as much as 92%, with higher ammonia content, likely due to thermal DeNOx reactions. However, shortening injection at higher ammonia levels elevates NO output, and advancing injection timing has limited impact on this trend.**

Keywords: Ammonia Combustion; CFD Simulation; Dual-Fuel Engine; Injection Strategy; Emissions

I. Introduction

Ammonia (NH_3) has emerged as a promising alternative fuel due to its favorable properties in terms of environmental sustainability, storage, and distribution [1, 2]. Unlike conventional carbon-based fuels, ammonia combustion does not emit carbon dioxide or sulfur oxides, contributing to cleaner air and reduced greenhouse gas emissions. Its high-octane number (above 130) also makes it highly resistant to engine knock, which enhances combustion stability, particularly in engines operating at high compression ratios. Furthermore, ammonia's relatively low liquefaction temperature (−33.34 °C) compared to hydrogen makes it easier and safer to store and transport. In addition, it possesses good resistance to auto-ignition [3, 4].

Despite these advantages, ammonia is not without challenges when considered for direct use in internal combustion engines. Its low flame speed and slow ignition characteristics often lead to delayed combustion, reducing thermal efficiency. Moreover, the long quenching distance during ammonia combustion may leave pockets of unburned fuel in the combustion chamber, further limiting performance. However, ammonia's high latent heat of vaporization can help reduce peak temperatures in the combustion chamber, potentially benefiting emissions control and combustion regulation [5]. Nonetheless, ammonia's weak chemical reactivity and slow flame propagation have hindered its application in compression ignition engines [6, 7].

To address these limitations, researchers have proposed blending ammonia with diesel fuel, forming what is known as an ammonia-diesel dual-fuel (ADDF) system. Liu et al. [8] showed that using diesel as a pilot fuel could significantly lower the compression ratio required for ammonia ignition. Similarly, Pearsall et al. [2] examined how fuels with varying cetane numbers influenced ignition delay and overall engine efficiency. Studies have shown that ADDF engines can generate power levels comparable to traditional engines while reducing CO_2 emissions. However, they often exhibit increased emissions of carbon monoxide and unburned hydrocarbons due to incomplete combustion. When the ammonia energy share remains below 40%, nitrogen oxide (NO_x) emissions can be minimized, but unburned ammonia in the exhaust becomes a concern [9, 10]. Niki et al. [11] conducted experiments under varying load conditions and observed that increasing the ammonia ratio from 0% to 30% resulted in higher emissions of ammonia and nitrous oxide (N_2O). Yet, technical limitations in the ammonia supply system restricted the achievable ammonia energy ratio to 30% [11]. Yousefi et al. [12] investigated the combined effects of ammonia blending and diesel injection timing in a CI engine. They found that advancing the diesel injection timing could reduce greenhouse gas and N_2O emissions by approximately 12%.

In summary, ammonia holds considerable promise in decarbonizing internal combustion engines and contributing to long-term carbon neutrality goals. Yet, key technical hurdles, particularly those related to low thermal efficiency and high emissions at higher ammonia ratios, remain unresolved. Further experimental and modeling efforts are needed to optimize fuel injection strategies and better understand combustion behavior in ADDF engines.

To facilitate ADDF combustion, this study employs a reconfigured diesel engine setup. It aims to comprehensively evaluate the effects of three critical factors, ammonia blending ratio (ABR), injection duration (DOI), and start of injection timing (SOI), on the combustion process and emission profile of an ADDF engine. Initially, the influence of varying ammonia content on pollutant formation and combustion stability was analyzed. Following this, the impact of different injection durations was studied under several ammonia blending conditions. Finally, the start of injection was varied to explore its effect on fuel efficiency, combustion behavior, and exhaust emissions.

A detailed computational fluid dynamics (CFD) model was developed using the CONVERGE software platform to simulate the ADDF combustion process. The model captures key in-cylinder phenomena such as pressure evolution and emission formation, providing insights into how injection parameters and ammonia blending influence engine performance.

II. MATERIAL AND METHOD

A. *Numerical model*

In this study, engine simulations were performed using Converge CFD version 3.0, a commercial computational fluid dynamics software, to model a full closed cycle, from the intake valve closure (IVC) to the exhaust valve opening (EVO). The engine's key specifications are outlined in Table 1, and this section briefly outlines the main numerical techniques and modeling strategies adopted.

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

To enhance mesh resolution in areas requiring higher accuracy, the Adaptive Mesh Refinement (AMR) technique was employed. This method dynamically adjusts the cell sizes based on the complexity of the local flow features. A base cell size of 0.002 meters was defined, with the ability to generate finer mesh resolutions, especially near turbulent flame fronts, to capture detailed combustion dynamics. Figure 1 illustrates the three-dimensional computational domain of the engine cylinder at two critical crank angles: top dead center (TDC) and bottom dead center (BDC). These views are shown on the left and right sides of the figure, respectively. In addition to geometry, the associated computational grid structure is also visible in the illustrations.

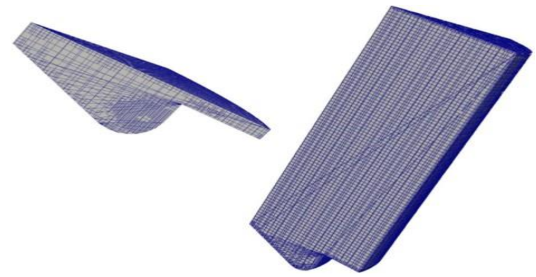

Figure 1: Caterpillar 3401 – cylinder geometry and meshing.

To accurately capture the auto-ignition characteristics in the simulation, the SAGE detailed chemical kinetics solver was employed to model the combustion process. This solver updates the mass fractions of chemical species in each computational cell and time step prior to solving the transport equations. The Pressure Implicit with Splitting of Operators (PISO) algorithm was utilized to resolve the transport phenomena during the simulation. A chemical reaction mechanism developed by Xu et al. [13] was implemented to represent the combustion chemistry of ammonia and n-heptane, the latter acting as a surrogate for conventional diesel fuel [13]. This mechanism comprises 69 chemical species and a total of 389 elementary reactions, allowing for detailed modeling of fuel oxidation and intermediate species formation [14-16]. Figure 2 presents a schematic representation of the workflow used for integrating chemical reaction mechanisms within the multi-dimensional CFD environment.

The injection pressure and timing of the diesel fuel in the simulation were aligned with experimentally measured values, and the fuel injector was equipped with six orifices. To replicate the physical properties of diesel during the spray and mixing phases, the "DIESEL2" surrogate fuel from the Converge CFD database was utilized [17]. Key parameters for several spray modeling techniques are summarized in Table 2. Turbulence within the combustion chamber flow was modeled using the Reynolds-Averaged Navier-Stokes approach, specifically employing the Re-Normalization Group (RNG) k-ε turbulence model [18-20]. An adaptive mesh refinement strategy was implemented to generate a computational grid with a base cell size of 0.25 mm, ensuring sufficient resolution of the turbulent flame front structures [17, 21].

TABLE 2: KEY SPRAY PROCESSES UTILIZED IN THE SPRAY MODELING

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 interation	Rebound/slide model

The simulation inputs consisted of averaged values representing various conditions of injection duration (DOI), start of injection (SOI), and flow rates of diesel, ammonia, and air, as detailed in Table 3. All cases were conducted under a constant brake which mean effective pressure (BMEP) of 8.1 bar and an engine speed of 910 rpm.

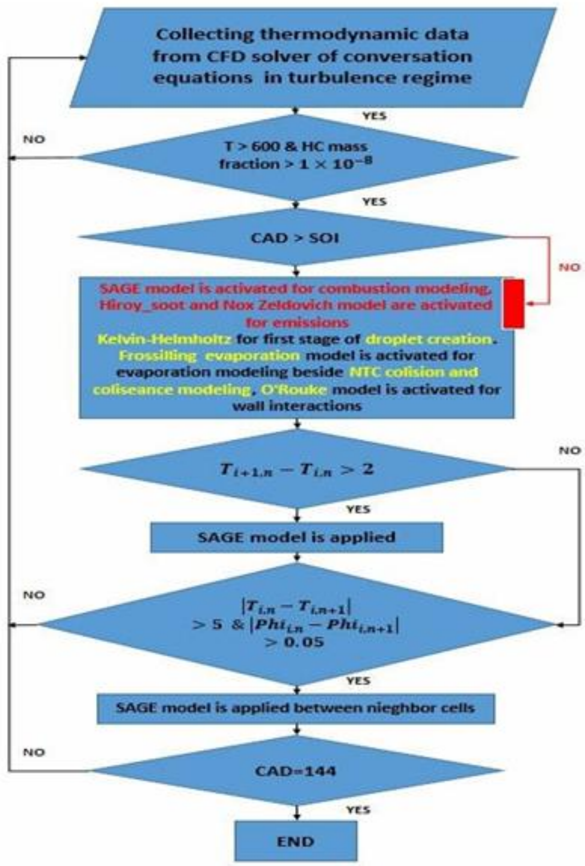

Figure 2: CFD simulation process using chemical kinetics [22].

The engine load was maintained at 50% of the maximum capacity. To ensure closer alignment between the modeled and experimental intake manifold pressures during the compression phase, and to adjust the mass flow rates of ammonia and air with greater accuracy, a pressure offset of 5 kPa was introduced.

TABLE 3: SIMULATION CONDITIONS

case	Am (%)	DOI	SOI	Diesel (kg/h)	NH3 (kg/h)
Diesel	0	16.48	-14.2	3.38	0
N10	10	16.48	-14.2	3.042	0.79
N20	20	16.48	-14.2	2.73	1.56
N30	30	16.48	-14.2	2.38	2.37
N40	40	16.48	-14.2	2.08	3.18
N10/Du1	10	15.31	-14.2	3.042	0.79
N20/Du2	20	14.31	-14.2	2.73	1.56
N30/Du3	30	13.31	-14.2	2.38	2.37
N40/Du4	40	12.02	-14.2	2.08	3.18
N10/Du1/Ad2°	10	15.31	-16.2	3.042	0.79
N20/Du2/Ad2°	20	14.31	-16.2	2.73	1.56
N30/Du3/Ad2°	30	13.31	-16.2	2.38	2.37
N40/Du4/Ad2°	40	12.02	-16.2	2.08	3.18

B. *Model validation*

Figure 3 presents a comparison between the experimentally measured and numerically predicted in-cylinder pressures for the ammonia-diesel dual-fuel (ADDF) engine, with the injection start timing set at −14.2° ATDC, for ammonia energy shares of 0% and 20%. The experimental data were sourced from reference [12], where a Caterpillar 3401 diesel engine, whose specifications are listed in Table 1, was modified to operate on an ammonia-diesel dual-fuel system. The comparison shows a strong agreement between the peak cylinder pressures, the onset of combustion, and the simulated pressure traces with the experimental observations.

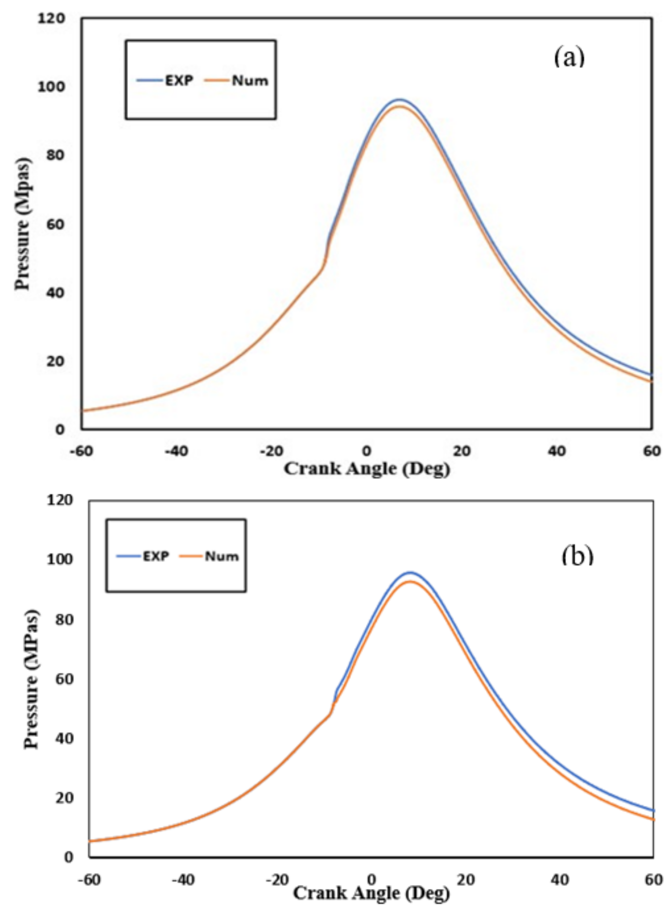

Figure. 3: Measured vs. simulated cylinder pressure for 0% NH_3 (a) and 20% NH_3 (b).

III. RESULT AND DISCUTION

A comparison of Figures 4a to 4c reveals that although the in-cylinder pressure in ammonia-diesel dual-fuel mode is lower than that of pure diesel across all substitution ratios (10% to 40%), where pure diesel reaches a peak pressure of approximately 9.8 MPa, while in all dual-fuel cases, the pressure remains below 9 MPa, the reduction in injection duration shown in Figure 4b can compensate for this pressure drop. Specifically, in the 10% ammonia case, the peak pressure exceeds that of pure diesel, and in other dual-fuel modes, the pressure increases significantly. According to the findings of Yousefi et al. [12], increasing the ammonia energy share from 0% to 40% leads to a reduction in peak cylinder pressure, dropping from 85.4 bar to 80.8 bar.

Furthermore, an analysis of different conditions in Figure 4c demonstrates that advancing the injection timing by 2 degrees along with shortening the diesel injection duration leads to an increase in in-cylinder pressure, this can be because of the low flame speed of ammonia [12]. As a result, at 10% ammonia substitution, the pressure is notably higher than that of pure diesel, while at 20% and 40% substitutions, the pressure remains nearly equivalent to that of pure diesel. Moreover, the heat release rate (HRR) in Figures 5a, 5b, and 5c indicates that while the use of ammonia in dual-fuel mode reduces the heat release rate and delays the start of combustion (Figure 5a), shortening the injection duration (Figure 5b) and advancing the injection timing (Figure 5c) can enhance the heat release rate, particularly in the premixed combustion phase. Additionally, combustion initiation occurs earlier, resulting in an advanced start of combustion.

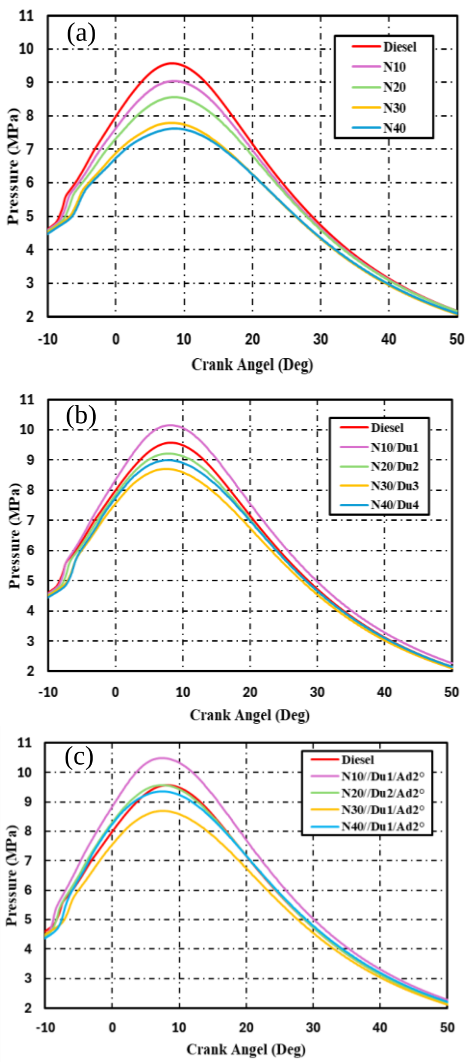

Figure. 4: In-cylinder pressure of dual-fuel engine at a) different percentage of NH_3 b) different injection duration c) advanced start of injection.

A comparison of carbon dioxide levels in the exhaust gases, as shown in Figure 6, indicates that using different ammonia blends, as a carbon free fuel, leads to a significant reduction in this pollutant, up to 42% for the 40% ammonia case. However, shortening the injection duration in dual-fuel mode with 10% ammonia resulted in an increase in carbon dioxide emissions, whereas this reduction in injection duration had no notable effect on other ammonia concentrations. Furthermore, as illustrated in Figure 6, advancing the fuel injection timing in the final case had no impact on the level of this pollutant, yielding results like those of the dual-fuel mode with reduced injection duration.

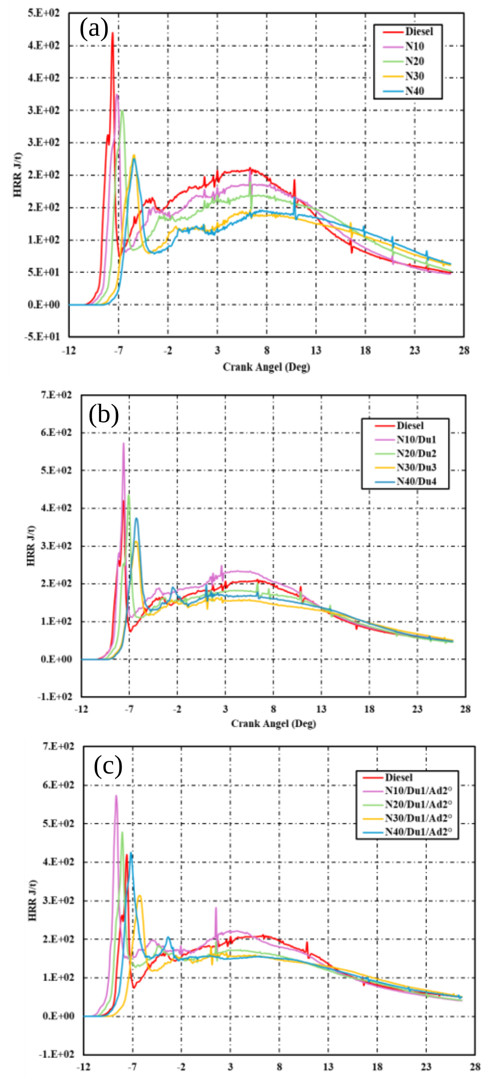

Figure. 5: Heat release rate of dual-fuel engine at a) different percentage of NH_3 b) different injection duration c) advanced start of injection.

The NO pollutant levels in Figure 7 also demonstrate that using different ammonia blends significantly reduces this emission in exhaust gases. The reductions of 10%, 20%, 30%, and 40% ammonia were 42%, 70%, 92% and 90%, respectively. This effect is likely caused by the thermal DeNOx mechanism [23, 24], which starts when ammonia (NH_3) reacts with hydroxyl radicals (OH) and oxygen atoms, producing amidogen (NH_2) radicals. Additionally, shortening the diesel injection duration in dual-fuel mode at 10%, 20%, and 40% ammonia) increased NO levels significantly. Like carbon dioxide emissions, advancing the injection timing in this case had no notable effect on NO levels, with results comparable to those of the dual-fuel mode with reduced injection duration.

A comparison of N_2O emission levels in Figure 8 reveals that while this pollutant was negligible in pure diesel mode, the use of ammonia fuel at all blend ratios resulted in significant N_2O formation and increased emissions. From the discussion above, the rise in N_2O emissions diminishes the advantage gained from the reduced CO_2 emissions in the ADDF combustion mode. However, reducing the injection duration substantially decreased N_2O levels, with reductions of 44%, 20%, 40%, and 61% for 10%, 20%, 30%, and 40% ammonia blends, respectively. Furthermore, advancing the injection timing was found to increase NO levels compared to dual-fuel operation with reduced injection duration, except in the 30% ammonia case.

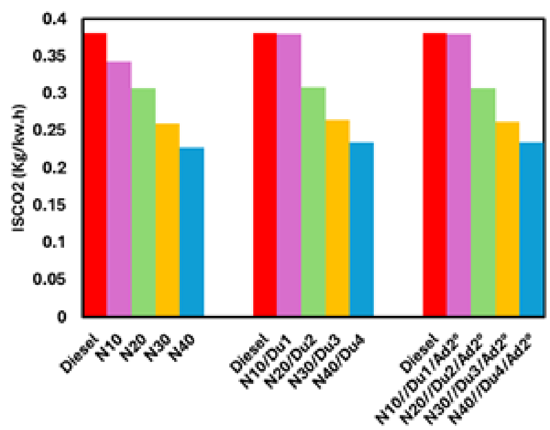

Figure. 6: In-cylinder CO_2 of dual-fuel engine at a) different percentage of NH3 b) different injection duration c) advanced start of injection.

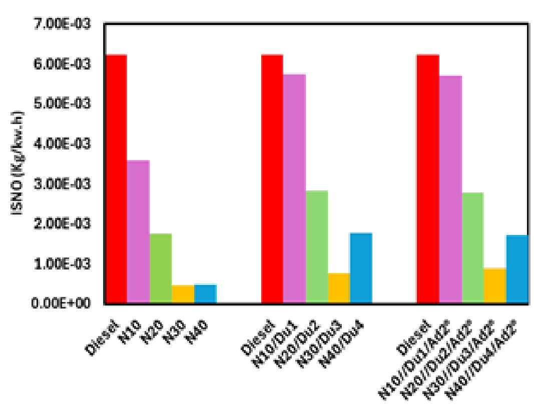

Figure. 7: In-cylinder NO of dual-fuel engine at a) different percentage of NH_3 b) different injection duration c) advanced start of injection.

Figure 9 demonstrates that all ammonia-diesel dual-fuel modes produced lower NO_2 levels compared to pure diesel operation, with higher ammonia blends yielding progressively greater reductions. Analysis of injection duration effects (comparing the first two bar groups in the chart) reveals that shortened injection increased NO_2 emissions by approximately 2.5%, 23%, and 32% for 10%, 20%, and 40% ammonia blends respectively, relative to standard dual-fuel operation. The 30% ammonia blend showed a reduced injection duration which slightly decreases emission. Furthermore, combining advanced injection timing with shorter injection duration elevated NO_2 concentrations, resulting in emissions 5% and 10% higher than pure diesel for 10% and 20% ammonia blends respectively

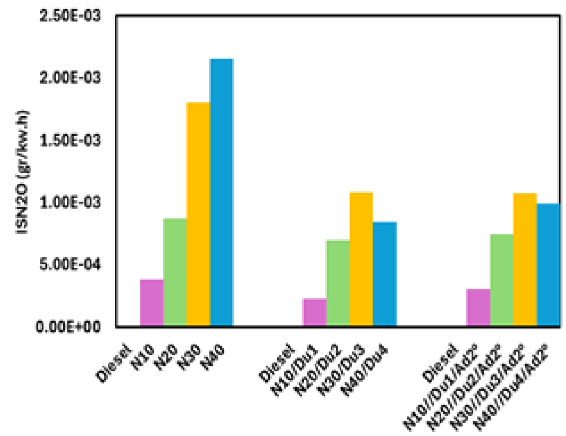

Figure. 8: In-cylinder N_2O of dual-fuel engine at a) different percentage of NH_3 b) different injection duration c) advanced start of injection.

The exhaust ammonia concentration analysis in figure 10 revealed significant unburned ammonia emissions in all dual-fuel modes, with levels escalating sharply at higher ammonia blends. However, implementing both reduced injection duration and advanced injection timing could effectively mitigate this slip - achieving up to 50% reduction for the 30% ammonia blend with shortened injection duration.

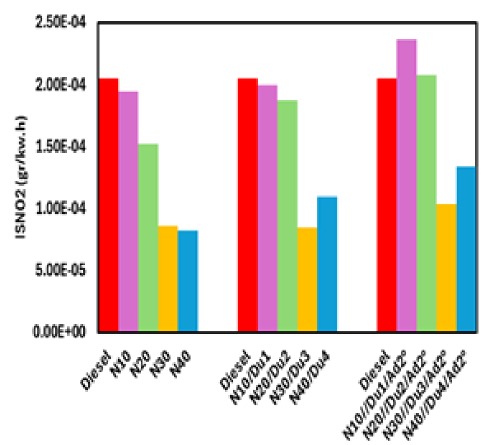

Figure. 9: In-cylinder NO_2 of dual-fuel engine at a) different percentage of NH_3 b) different injection duration c) advanced start of injection.

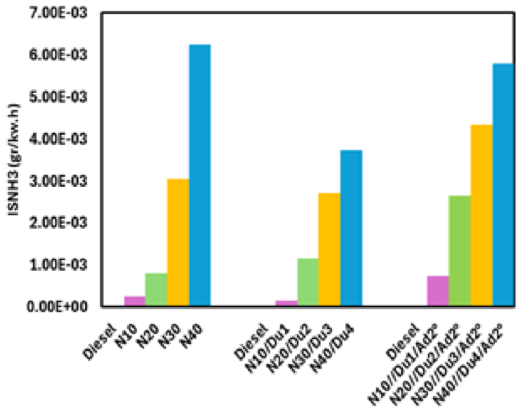

Figure. 10: In-cylinder NH3 of dual-fuel engine at a) different percentage of NH_3 b) different injection duration c) advanced start of injection

IV. CONCLUSION

In the present study, the effects of different ammonia injection ratios, along with reducing the injection duration and advancing the diesel injection angle, were investigated. The obtained results indicate that although the use of ammonia fuel and increasing its substitute percentage in diesel engines lead to a reduction in in-cylinder pressure and heat release rate, these can be compensated by shortening the diesel injection duration and advancing the injection angle, thereby improving engine performance. Additionally, while the use of ammonia can reduce the levels of CO_2, NO, and NO_2 in the exhaust gases, the N_2O emission level increases significantly. However, this negative effect can be mitigated by reducing the injection duration and advancing the injection angle. Therefore, optimizing the injection duration and injection angle in an ammonia-diesel dual-fuel engine can be crucial for improving performance and reducing emissions.

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