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DME – Combustion Enhancer for Ammonia Engines

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ABSTRACT

Due to the combustion properties of ammonia, ammonia engines have a limited operating window at low load, low, and high engine speed conditions. Therefore, a suitable combustion enhancer is needed to sustain ignition and improve stability. Recently, DME has been identified as a promising combustion enhancer because of its high reactivity, low carbon content, and soot-free combustion. This study explores the potential of dimethyl ether (DME) as a combustion enhancer in ammonia engines operating under both traditional and advanced combustion modes with small DME additions, by conducting chemical kinetics simulations and engine experiments.

1. Introduction

Ammonia (NH₃), a zero-carbon fuel and potential hydrogen energy carrier, is seen as a game changer in the hydrogen economy. At low loads, ammonia requires a combustion enhancer to overcome its long ignition delay, low laminar flame speed, and combustion stability. The combustion enhancer investigated so far in the case of Spark Ignition (SI) engine are highly reactive molecules such as hydrogen, gasoline, methane or alcohols, especially at low load [1]. For advanced combustion modes such as Homogeneous Charge Compression Ignition (HCCI) or Dual Fuel (DF) Combustion, NH₃-H₂ blends [2, 3], and NH₃/Diesel ones [4, 5] present notable improvements in combustion performance and emissions. However, as for SI engines, poor at low load and low and high-speed conditions.

DME (C₂H₆O) is a low-carbon, high-reactivity biofuel that can balance the ammonia's slow combustion dynamics and improve combustion performance as a combustion enhancer. Dai et al. [6] developed and validated a new kinetic mechanism, revealing early DME oxidation as the trigger for NH₃ ignition via radical generation. The key finding is that even minimal DME addition enables practical NH₃ ignition by reducing ignition delay time (IDT) at temperatures ~250 K lower than those of pure ammonia. Issayev et al. [7] measured laminar flame speed (LFS) of NH₃/DME/air mixtures at elevated pressures and temperatures. While Dai et al. emphasize ignition feasibility, Issayev et al. target flame stability and kinetics. Both underscored DME's strong promoting effect on NH₃ reactivity. The key inference is that DME enhances both ignition and flame propagation of NH₃ with small amounts. The experimental study by Tutak et al. [8] on a single-cylinder SI engine of 10 Compression Ratio (CR) at 600 rpm, demonstrated that adding 8% DME by energy to NH₃ significantly improves combustion stability and engine performance. The addition of 18% DME by energy resulted in an efficiency of around 30%, marking optimal combustion conditions by reducing drastically the ignition delay from the spark and the combustion development duration with an optimum phasing of the overall combustion. DME also ensured stable operation with a covariance of Indicated

Mean Effective Pressure (CoV_{IMEP}) lower than 5%. These literature outcomes motivated this study: to explore DME as a combustion enhancer for ammonia engines by combining both kinetic and experimental investigations to understand its efficacy in promoting the ignition of ammonia in both conventional and advanced combustion modes.

2. Effect of DME addition on IDT and LFS of ammonia/air Mixtures

To analyze the impact of small addition of DME on IDT and LFS of ammonia/air mixtures, an estimation of both parameters at different equivalence ratios as a function of DME volume fraction was conducted using a 0D-closed homogeneous reactor and a 1D model of a freely propagating premixed flame configuration with ANSYS-ChemkinPRO. The chemical reaction mechanism consisting of 176 species and 1,418 reactions, developed and validated by Issayev et al. [7], was used.

Fig. 1 (a) highlights that adding DME to NH₃-air mixtures significantly improve ignition delay even small DME volume fractions by considering an overall stoichiometric equivalence ratio at 50 bar of pressure in the reactor, pressure that can be reached in Compression – Ignition (CI) engine. This makes DME an effective ignition enhancer for ammonia-fueled combustion systems; for example, the lowest IDT is obtained at 1250 K for pure ammonia, same IDT is obtained for 1100 K when 2% of DME is added and 1000 K for 5% only. The IDT curves for 10% DME blends display a steeper decline in the low-temperature region compared to pure ammonia. This indicates enhanced reactivity at low temperatures, which is absent in pure NH₃. DME addition enables low-temperature ignition by introducing active radical chemistry [6]. This behavior is key for advanced combustion strategies such as HCCI mode, where autoignition at lower temperatures is important. It also explains why DME is an effective combustion enhancer for fuels with poor combustion properties, such as NH₃. In Fig. 1 (b), an example of improvement of LFS by the addition of DME is shown at the in-cylinder pressure and temperature data (~7.2 bar, 515 K at 1000 rpm and 7.8 bar, 535 K at 2000 rpm) at the SIT of -36 CAD aTDC.

This is due to its higher intrinsic flame speed, enhanced radical chemistry [7], and favorable thermal characteristics. This can make the mixture more reactive and better suited for stable, high-speed flame propagation in SI or premixed combustion systems. Fig. 1. (c) shows the rate of production (ROP) -

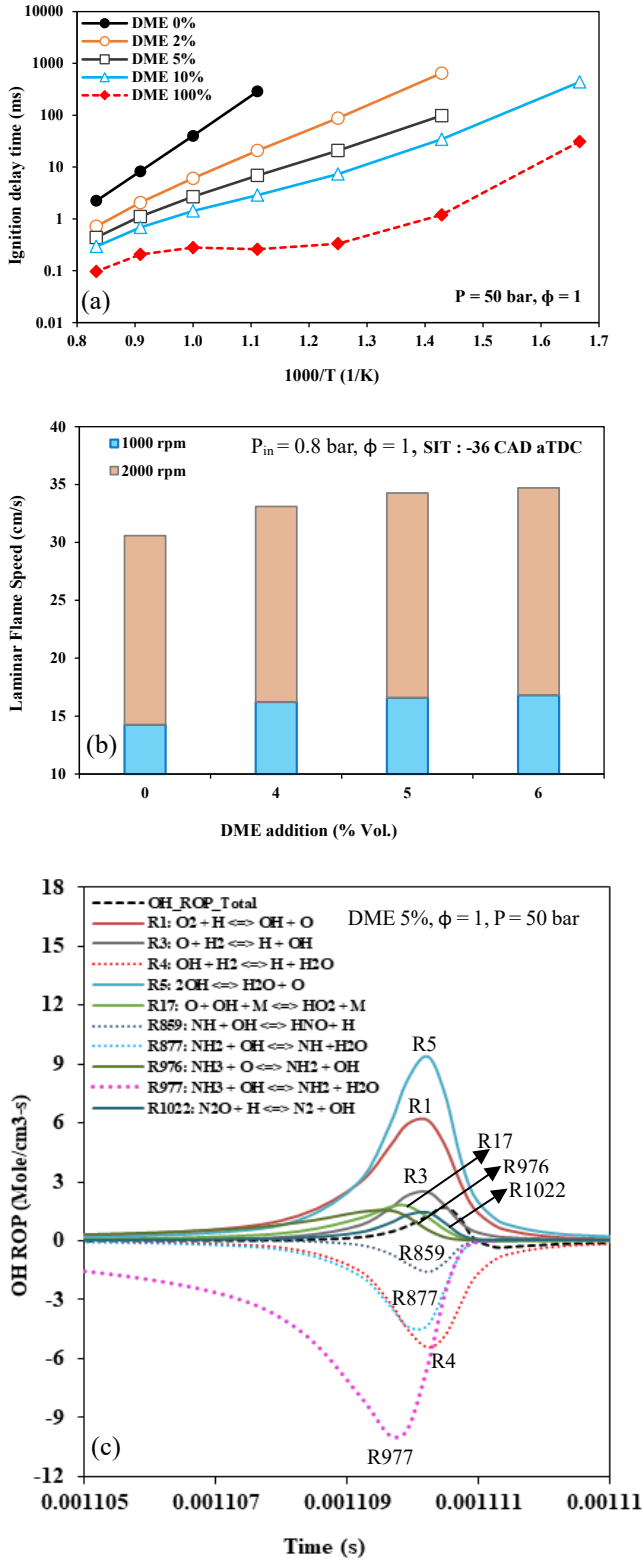


Fig. 1 Influence of DME addition on (a) IDT, (b) LFS,

and (c) OH ROP of NH₃/air mixtures -of hydroxyl radicals (OH) as a function of time for a 95% NH₃-5% DME blend at $\phi = 1$ and 50 bar pressure. In ammonia combustion, DME plays a critical role in initiating and sustaining the reaction by enhancing key radical-generating pathways. DME decomposition [6] produces hydrogen and reactive radicals (H, CH₃, CH₃O), which significantly promote chain-branching reactions such as $O_2 + H \rightleftharpoons OH + O$ (R1) and $2OH \rightleftharpoons H_2O + O$ (R5), both of which accelerate OH radical formation. Additionally, DME oxidation leads to the formation of intermediates like N₂O, activating high-temperature reactions such as $N_2O + H \rightleftharpoons N_2 + OH$ (R1022), further boosting OH levels. These reactions effectively compensate for ammonia's dominant OH-consuming pathway $NH_3 + OH \rightleftharpoons NH_2 + H_2O$ (R977), allowing the overall radical pool to grow, thereby sustaining stable and complete combustion even at low DME concentrations.

3. DME as a combustion enhancer in ammonia fuelled SI, HCCI, and DF combustion engines

Each possible combustion mode presents unique challenges for NH₃, due to its poor ignitability and slow flame speed. DME's high chemical reactivity, strong low-temperature oxidation chemistry, and fast flame speed are the main reasons for using DME as a combustion enhancer in ammonia-fueled engines. Engine experiments were conducted on an ammonia-fueled engine operating at 1000 rpm under SI, HCCI, and CI by a small amount of DME added. The in-cylinder pressure and Heat Release Rate (HRR) evolution are presented in Fig.2.

3.1. Role of DME in premixed Ammonia SI combustion

Fig. 2 (a) illustrates NH₃ combustion in an SI engine with varying DME volume fractions (0%, 2%, 5%, 10%) at $\phi = 0.8$, intake pressure (P_{in}) of 1 bar. DME addition significantly induces less advanced spark-ignition timing and reduces the delay until the flame-kernel is self-developed, compared to neat ammonia (i.e., DME 0%). This is evident as the pressure rise shifts earlier, and peak in-cylinder pressure increases with increasing DME. The HRR peaks are sharper and earlier with higher DME volume fractions. At 10% DME, the HRR peak occurs just after TDC and is significantly higher in magnitude, indicating enhanced and faster combustion.

In contrast, neat ammonia shows a broader and delayed HRR curve due to ammonia's slow reactivity. DME addition increases peak in-cylinder pressure from around 34 bar to 67 bar. This reflects more complete and rapid combustion due to the synergy between DME's fast ignition and ammonia's energy density. At $\phi = 0.8$, neat ammonia struggles to ignite and sustain combustion reliably as shown in Fig. 2 (a). DME addition increases HRR magnitude and pressure, indicating faster combustion starting from lower temperatures and pressures. Even though spark ignition timing (SIT) is retarded from -40 to -32 CAD aTDC, combustion starts

earlier with more DME. This strongly suggests that DME lowers the ignition energy requirement and enhances pre-flame chemistry. This is reflected in the shorter delay between spark timing and HRR rise, and the faster pressure and heat release buildup, especially at higher DME concentrations. Adding 2-10% DME by volume to premixed NH₃-air mixtures in an SI engine significantly enhances combustion quality, allowing for higher peak pressures, faster HRR, and improved timing control – even with lean mixtures and retarded spark ignition timings. DME serves as a powerful combustion enhancer, enabling efficient and stable ammonia combustion in practical engine conditions.

3.2. Role of DME in Ammonia HCCI combustion

Fig. 2 (b) shows the in-cylinder pressure and HRR evolution during premixed HCCI combustion of NH₃-DME/air mixtures in a 16.4 CR engine operating at a P_{in} of 1.2 bar and an engine speed of 1000 rpm. DME fraction and Intake Temperature (T_{in}) are adjusted to achieve stable engine operation, defined by parameters $COV_{IMEP} \leq 5\%$ and ringing intensity (RI) ≤ 5 MW/m². From Fig. 2 (b), it is evident that as the DME volume fraction increases from 7% to 10%, the peaks in HRR and pressure occur earlier in CAD, despite lower temperatures. The notable decrease in T_{in} , even with a small 1% volumetric increase in DME, highlights DME's strong ignition-promoting properties. At a low ϕ of 0.5, ammonia struggles to auto-ignite because of its high autoignition temperature and low reactivity. DME, being highly reactive and oxygenated, supports low-temperature oxidation and radical formation [6, 7], allowing ammonia to ignite with appropriate T_{in} . Interestingly, the T_{in} needed for NH₃-DME/air HCCI combustion is lower than for NH₃-H₂/air HCCI mode [2]. As the DME fraction rises, the required T_{in} for stable operation drops sharply, improving thermal efficiency. This reduction in intake heating also enhances the practical viability of ammonia-DME HCCI combustion.

Fig. 2 (b) presents a typical two-stage HCCI combustion, i.e., low temperature heat release (LTHR) followed by high temperature heat release (HTHR) phases. The single-stage premixed combustion characteristics of ammonia shift to a two-stage heat release profile due to the small addition of DME in ammonia. The LTHR phase acts as a precursor to the main combustion, helping synchronize combustion phasing. With increased DME, this phase becomes more prominent, enabling better control over ignition delay and combustion stability. A visible LTHR peak appears before HTHR, indicating preparatory low-temperature chemistry activity that assists transition to the main combustion phase. Therefore, DME facilitates low temperature reaction (LTR), reduces ignition delay, enhances HRR, and ensures earlier complete combustion. This improves the practicality of ammonia-fuelled HCCI engines by broadening the autoignition window and reducing thermal energy input requirements. The described effects collectively enable more stable and efficient HCCI combustion of ammonia,

making DME a viable combustion enhancer in ammonia-fueled engines.

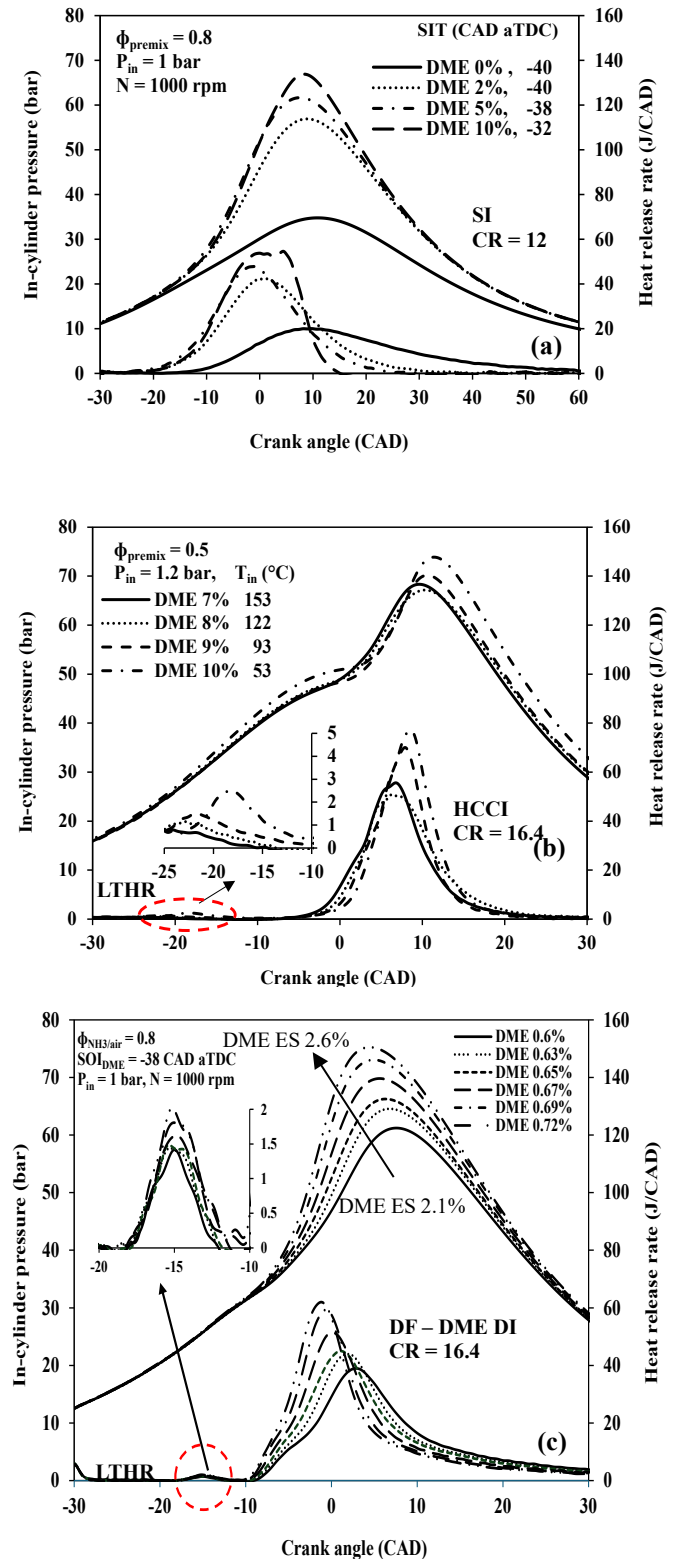


Fig. 2. Effect of DME addition on NH₃ in (a) SI, (b) HCCI, and (c) DF combustion modes

3.3 Role of DME in ammonia compression ignition combustion

In this investigation, DME was injected directly in liquid phase using a GDI injector at the average pressure of 130-

135 bar on a premixed heated NH_3/air mixture between -26 and -38 CAD aTDC. Fig. 2. (c) shows that even at very low DME energy shares (2.1% to 2.6%) which corresponds to 0.6% to 0.72% by volume only, DME significantly improves the autoignition and combustion quality of NH_3 in a compression ignition engine. As highlighted in the magnified inset it promotes low-temperature reactions, enables two-stage combustion, and supports stable operation ($\text{COV}_{\text{IMEP}} \leq 5\%$) at an intake pressure of 1 bar. LTHR becomes more intense and broader as DME ES increases, suggesting enhanced low-temperature chemistry, crucial for triggering ammonia ignition. Two distinct peaks were observed in HRR, the first stage initiated by DME oxidation [6], and the second stage wherein NH_3 combustion is triggered by radicals generated in LTHR. This behavior is like classic low-temperature/high-temperature reaction sequences in dual-fuel HCCI/PCCI combustion modes. Both in-cylinder pressure and HRR peaks occur earlier as a function of DME amount, showing an earlier start of combustion. As shown in Fig. 3, for a constant start of DME injection, as DME ES increases, the ignition delay (CA10-SOI) and the combustion duration (CA90-CA10) decrease while the combustion is better phased (CA50). Advancing combustion timing with an increase in DME ES helps to improve IMEP and indicated thermal efficiency (ITE).

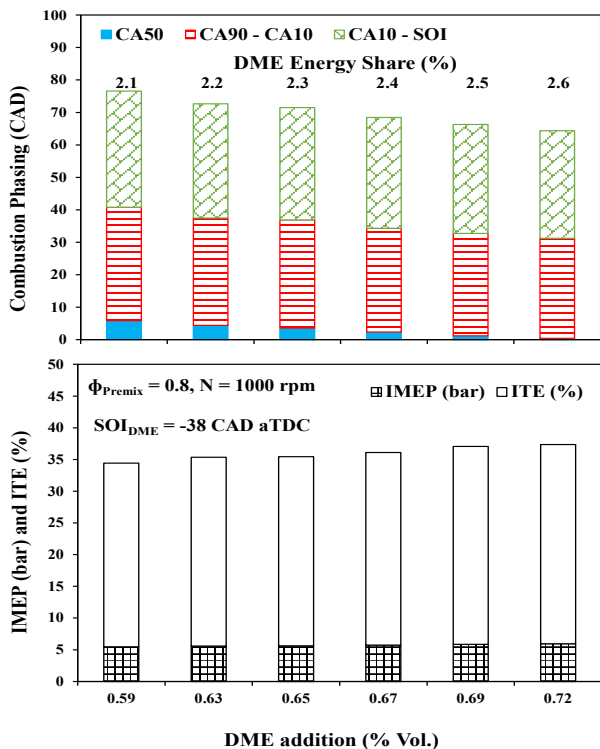


Fig.3. Effect of DME ES on combustion performance of dual-fuel mode

4. Conclusion

Across all modes, DME is a key enabler for practical ammonia combustion. It triggers ignition where ammonia alone fails and modifies combustion kinetics to improve performance and stability. While SI relies on DME for flame speed enhancement, HCCI exploits its autoignition capability, and Compression Ignition with DME Direct

injection leverages both its ignition quality and injection flexibility to achieve efficient, lean, and controlled combustion with minimal DME supplementation. DME is an effective combustion enhancer for ammonia engines such as:

1. Promotes the ignition even with low concentration
2. Triggers low-temperature reactions
3. Lowers the intake temperature required in HCCI
4. Enhances combustion phasing control and efficiency
5. It is versatile across combustion modes

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