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COMBUSTION AND EMISSIONS OF POLYOXYMETHYLENE DIMETHYL ETHER 3 BLENDED WITH DIESEL AND GASOLINE IN A HOMOGENEOUS CHARGE COMPRESSION IGNITION ENGINE: A NUMERICAL STUDY

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ABSTRACT

With high oxygen content and cetane number, polyoxymethylene dimethyl ether 3 ($PODE_3$) is favorable as a fuel to be used in internal combustion engines. In this study, $PODE_3$/diesel/gasoline blends in a homogeneous charge compression ignition engine are numerically studied for the first time. The effects of fuel blend ratio as well as equivalence ratio (ER) are investigated. It is noticed that high temperature heat release depends largely on blend ratio. Furthermore, indicated thermal efficiency is observed to be better with higher ER and is generally higher with increased $PODE_3$. As for emissions, higher ERs show trends of less CO and more NOx. Moreover, similar trends are seen when diesel addition to $PODE_3$ is made comparison with gasoline addition to $PODE_3$, potentially putting CO and NOx in a trade-off relationship.

Keywords: PODE3, polyoxymethylene dimethyl ether, homogeneous charge compression ignition, internal combustion engine, oxygenated fuel, renewable fuel

NOMENCLATURE

Abbreviations	
CAD	Crank Angle Degree
CFD	Computational Fluid Dynamics
CO	Carbon Monoxide
CO_2	Carbon Dioxide
CA50	Crank angle at which 50 percent of heat is released
ER	Equivalence Ratio
HCCI	Homogeneous Charge Compression Ignition
HRR	Heat Release Rate
HTHR	High Temperature Heat Release
ITE	Indicated Thermal Efficiency
LTHR	Low Temperature Heat Release
NOx	Oxides of Nitrogen
PAH	Polycyclic Aromatic Hydrocarbon
PODE	Polyoxymethylene Dimethyl Ether
$PODE_3$	Polyoxymethylene Dimethyl Ether 3
PRF	Primary Reference Fuel

1. INTRODUCTION

Apart from being renewable and sustainable, many oxygenated fuels are known to reduce soot emissions from internal combustion engines. One of them is PODE [1] which has gained recent popularity within the research community. Not only does PODE contain a significantly high amount of oxygen at 45.3% by weight, but it also has a lack of C-C bonds which creates difficulty for the formation of PAH, a known precursor of soot. Moreover, this fuel can be produced at a rate of 30,000 ton/year with prices matching that of diesel [2]. Furthermore, PODE can be synthesized using methanol [3], mitigating the depletion of fossil fuels. On top of that, the high energetic efficiency [4] of its production demonstrates PODE as a desirable alternative fuel. Among the various PODE oligomers, $PODE_3$ has the most ideal characteristics for use in engines after taking physical properties into consideration [3].

As highlighted by Wang et al. [5], fundamental studies in HCCI combustion using PODE is helpful in understanding PODE blend fuel combustion. They [5] had successfully proven the feasibility of PODE combustion in

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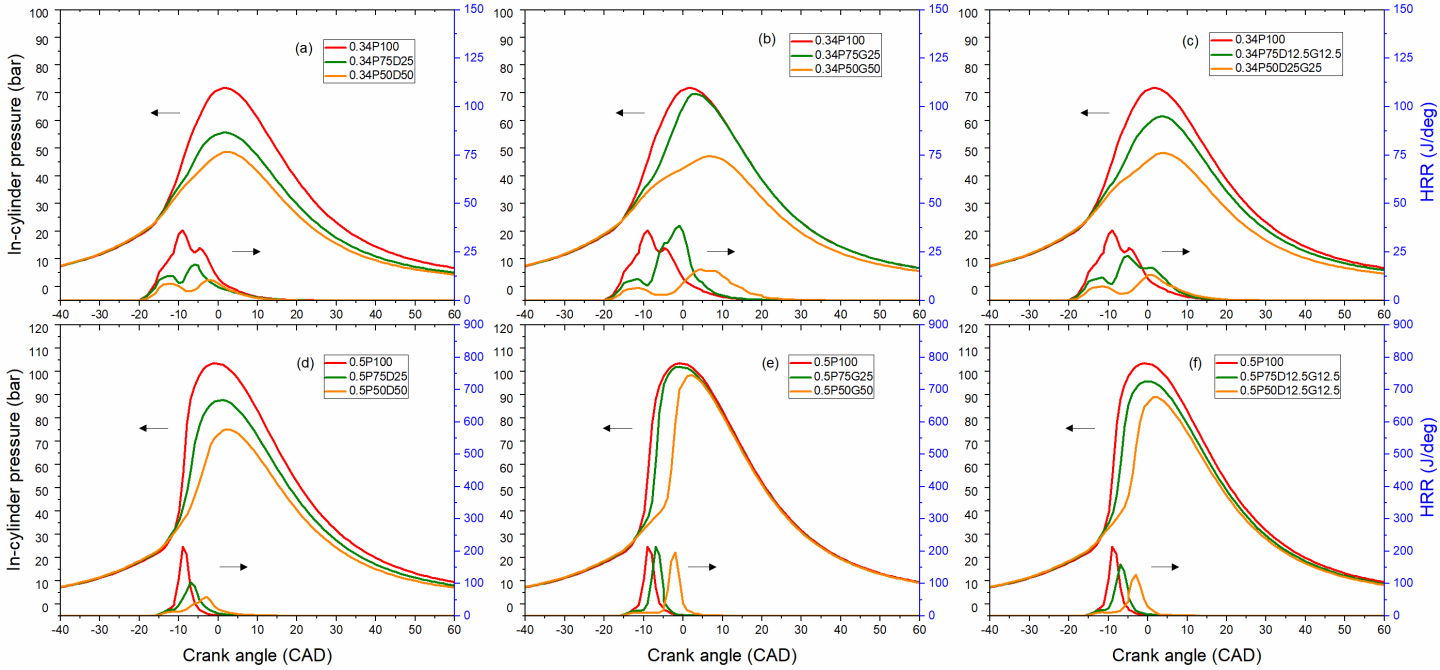

Figure 1 In-cylinder pressures and HRRs for (a) $PODE_3$/diesel blends at 0.34 ER, (b) $PODE_3$/gasoline blends at 0.34 ER, (c) $PODE_3$/diesel/gasoline blends at 0.34 ER, (d) $PODE_3$/diesel blends at 0.5 ER, (e) $PODE_3$/gasoline blends at 0.5 ER and (f) $PODE_3$/diesel/gasoline blends at 0.5 ER.

HCCI engines. However, no other studies have been conducted regarding PODE combustion under HCCI mode. Considering that PODE has a high likelihood to be used in conjunction with diesel and gasoline [1], this work aims to extend the fundamental PODE HCCI study to include blends with these fuels, allowing better understanding of the blends especially in terms of auto-ignition properties. Hence, the objective of this work is to investigate the combustion and emission characteristics of $PODE_3$/diesel/gasoline blends in a HCCI engine, varying fuel blend ratio and ER.

Cases are denoted by "aPxDyGz". ER is represented by "a", with cases at 0.34 and 0.5. "x", "y" and "z" represent mass percentages of PODE3, diesel and gasoline respectively. Here, cases are at either 100%, 75% or 50% $PODE_3$ with the remaining as either diesel, gasoline or diesel/gasoline added in equal amounts.

2. METHODOLOGY

In this work, a combined PRF-$PODE_3$ reaction mechanism developed by Lin et al. [3] was used. A PRF mechanism consists of n-heptane and iso-octane sub-mechanisms which are commonly utilized to represent diesel and gasoline combustion respectively. The PRF-$PODE_3$ mechanism was well validated in terms of ignition delay times, laminar flame speeds and flame species concentrations. Containing only 61 species and 190 reactions, the PRF-$PODE_3$ mechanism is robust yet sufficiently compact for parametric studies. Furthermore, validation was completed for the mechanism in terms of PODE HCCI combustion at 0.34 ER which was used as the base case for this investigation. More details on the mechanism and validations can be found in Lin et al.'s [3] work. In this study, simulations were conducted using the KIVA4 CFD code [6] integrated with CHEMKIN-II [7]. The fuels were assumed to be entirely premixed prior to combustion.

3. RESULTS AND DISCUSSION

The combustion and emission characteristics of $PODE_3$/diesel/gasoline blends under HCCI mode will be discussed in this section.

3.1 In-cylinder pressure and HRR

Figure 1 shows the in-cylinder pressures and HRRs for $PODE_3$/diesel blends, $PODE_3$/gasoline blends and $PODE_3$/diesel/gasoline blends under ERs of 0.34 and 0.5. From the HRR plots, it can be observed that all cases display a LTHR regime as well as a HTHR regime, typical of HCCI combustions [8]. Although all blends with the same ER seem to have LTHRs occurring at the same time, the HTHRs take place at different crank angles. The HTHR is retarded when diesel or gasoline is added to $PODE_3$, with gasoline addition showing more significant difference. Consequently, the respective in-cylinder pressures have peaks which are delayed. This is due to

the very low cetane number of gasoline at only 15.1 [9], as compared to that of diesel at 56.5 and $PODE_3$ at 78 [1], which results in a longer ignition delay for gasoline exhibited via the HTHRs. This postulates that the high temperature kinetic reactions are dependent on the cetane number of the fuel blend. Furthermore, comparing across the two ERs of 0.34 and 0.5, the start of combustion occurs earlier for 0.34 ER at -20 CAD as opposed to -15 CAD. At 0.34 ER with a leaner mixture, there is more air during compression, leading to higher temperature rise rate of the mixture. As a result, the auto-ignition temperature of the fuel blend is achieved earlier which sets off the combustion.

3.2 CA50 and ITE

Figure 2 describes the CA50 of all cases with respect to the mass percentage of $PODE_3$. Here, it can be noticed that cases at 0.34 ER have their CA50s occurring later than the respective counterparts at 0.5 ER in spite of having earlier start of combustions. With a leaner mixture that contains less fuel, there is lower as well as delayed HTHR, leading to delayed occurrences of CA50. Besides, it can be observed that the addition of gasoline at 0.34 ER has a more significant effect on CA50 than that at 0.5 ER. From this, the higher sensitivity of CA50 towards the cetane number of the fuel blend in a leaner mixture is manifested.

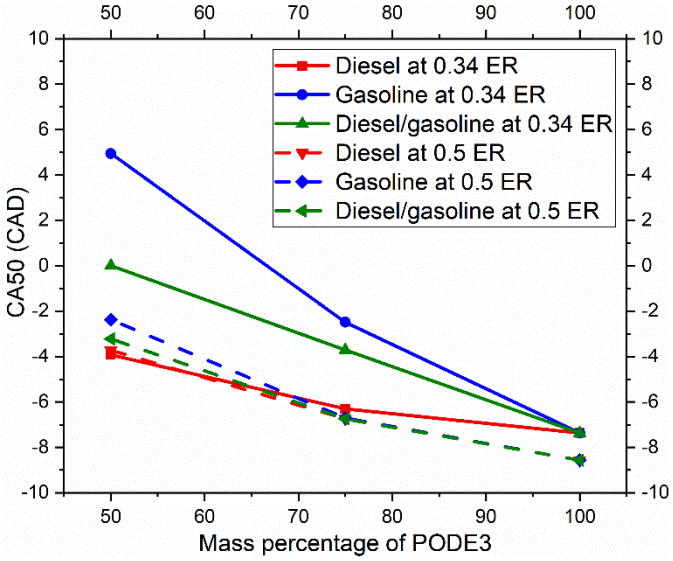

Figure 2 CA50 against mass percentage of $PODE_3$ for all cases.

Figure 3 illustrates the normalized ITE of all fuel blends at both ERs of 0.34 and 0.5, against the base case of pure $PODE_3$ at 0.34 ER. Overall, combustion at a higher ER proves higher efficiency, which is due to higher HRR and consequently higher temperatures in the combustion chamber. Moreover, it can be observed that ITE is generally higher with higher mass percentage of $PODE_3$. This could be attributed to $PODE_3$ having high oxygen content which promotes the oxidation processes throughout, leading to improved combustion. However, it is interesting to note that the effects of gasoline addition to $PODE_3$ on ITE display an opposite trend. In particular, the ITE of 0.34P100 is lower than that of 0.34P75G25 because the CA50 occurs too early at -7.37 CAD where work is done against the compression stroke. The same can be explained for the discrepancy in the case of 0.5P50G50.

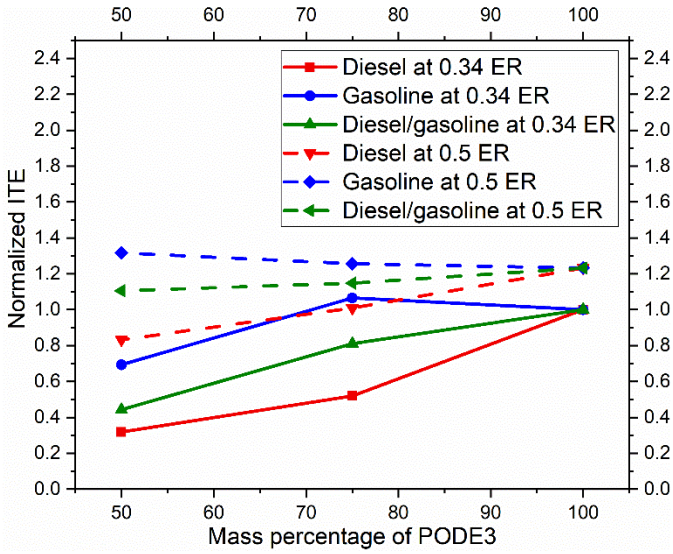

Figure 3 Normalized ITE against mass percentage of $PODE_3$ for all cases.

3.3 Emissions

Figure 4 shows the mass of CO, CO_2 and NOx emissions for all cases with respect to the mass percentage of $PODE_3$. Generally, it can be observed that cases at 0.5 ER emit less CO as compared to those at 0.34 ER. Such an advantage comes from better combustion where higher HRR can be observed. This is in tandem with the fact that cases at 0.5 ER possess higher ITEs as shown in Figure 3. Furthermore, respective levels of CO_2 are higher which implies that CO is oxidized to CO_2. On the other hand, combustions at 0.5 ERs can be seen to release more NOx. This is due to higher HRRs which increase in-cylinder temperatures, ultimately favoring the formation of NOx.

At 0.5 ER, it is noteworthy that the increment of CO with gasoline addition is negligible. Here, comparing CO levels of diesel addition to that of gasoline, it is evident that diesel encourages more CO formation. Similarly, this is due to lower in-cylinder temperatures which consequently result in lower NOx formation when diesel is added. As one might have expected, the addition of

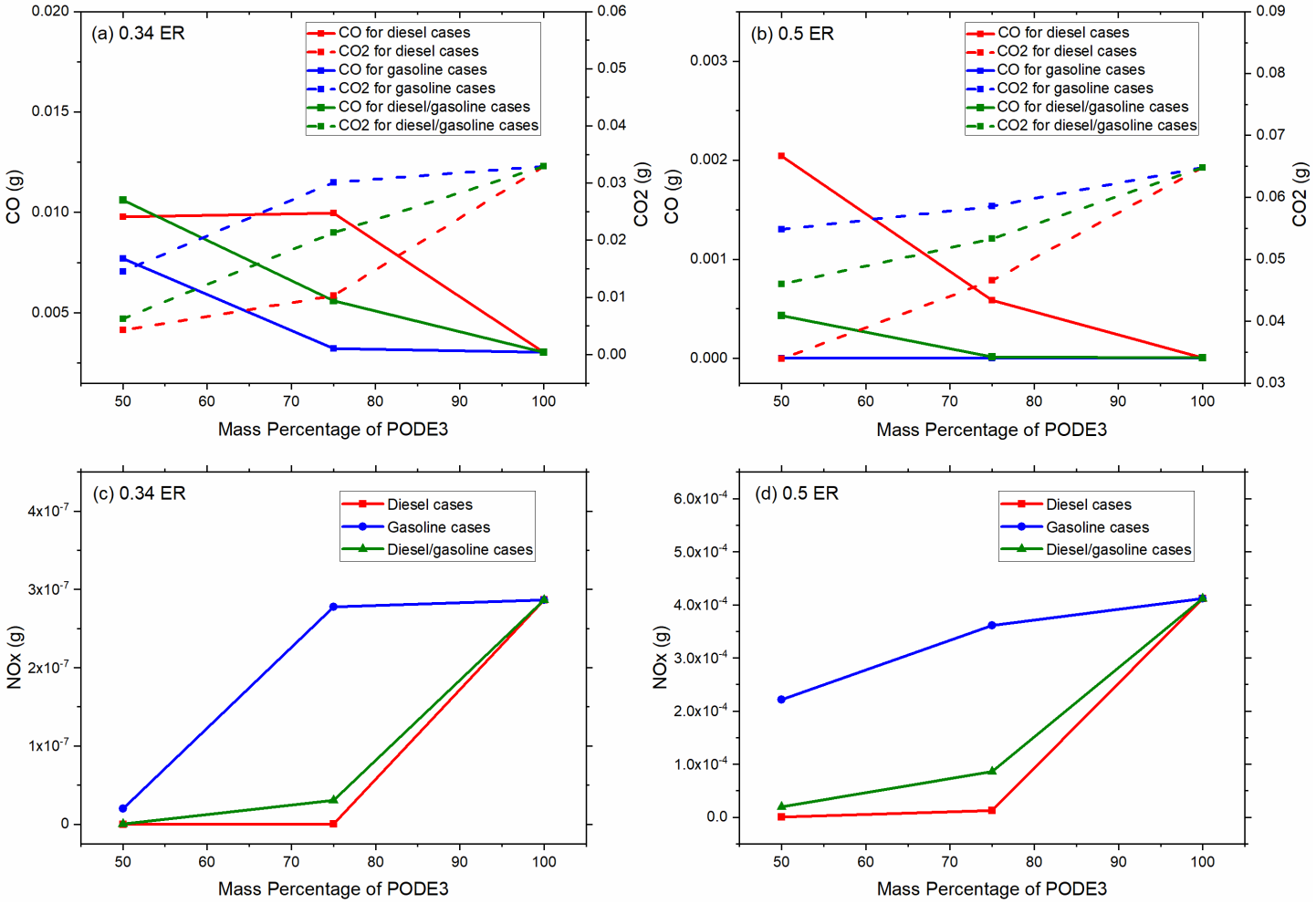

Figure 4 Emissions against mass percentage of $PODE_3$ of (a) CO and CO_2 at 0.34 ER, (b) CO and CO_2 at 0.5 ER, (c) NOx at 0.34 ER and (d) NOx at 0.5 ER.

diesel/gasoline has CO, CO_2 and NOx trends which fall in between those of neat diesel or gasoline addition. Also, it is worth noting that at case 0.5P75D12.5G12.5, the CO levels remain near zero when diesel/gasoline blend is added, while NOx decreases significantly, potentially making this blend the most optimal in this scope of study.

4. CONCLUSION

In summary, the effects of blend ratio and ER on the combustion and emission characteristics of $PODE_3$/diesel/gasoline blends have been numerically investigated in HCCI engine for the first time. It is noticed that HTHR is highly dependent on cetane number which is affected by blend ratio. Furthermore, CA50 shows higher sensitivity towards blend ratio in a leaner mixture. Moreover, ITE is observed to be better with higher ER and is generally higher with more $PODE_3$ in the blend. As for emissions, cases with higher ER show trends of less CO and more NOx. Besides, similar trends are seen when diesel addition is made comparison with gasoline addition, seemingly putting CO and NOx in a trade-off relationship.

ACKNOWLEDGEMENT

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