

Investigation of biogas composition effects on combustion characteristics of an RCCI engine

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Abstract: Fuel reactivity controlled compression ignition (RCCI) engines are promising approaches to achieve high efficiency and clean combustion. Using biogas as a primary fuel in the engines causes better control of the combustion process due to its reactivity gradient with diesel fuel. In this study, biogas is inducted into the engine through an inlet port, and diesel as a high reactivity fuel is injected into the engine. At a constant engine speed of 1300 rpm and a fixed amount of diesel mass, a broad range of indicated mean effective pressure from 5.6 to 13.5 is studied. Also, the effects of different compositions of biogas and biogas to diesel ratio on combustion characteristics and emission levels are studied. Results show that changes in the amount of CO₂ in biogas composition lead to drastic changes in maximum pressure, temperature, and emission levels. In other words, increasing the amount of CO₂ in biogas and also the ratio of biogas to diesel both significantly decrease maximum pressure, temperature, and NO_x emission.

keywords: Reactivity controlled compression ignition; biogas; diesel engine; emission.

1. Introduction

Recently, CI engines are getting more attention thanks to having higher fuel efficiency compared to SI engines. Controlling the emission of NO_x and soot is one of the most problematic issues in CI engines. Thus, much research has been carried out to reduce the NO_x emission and to keep the high efficiency of the diesel engine simultaneously through advanced combustion strategies. These strategies are usually based on retarding the long ignition to create a better homogeneous mixture before the combustion starts, which prevents the fuel-rich areas in the combustion chamber; as a result, soot formation is decreased.

The most top-notch low-temperature combustion strategy is reactivity controlled compression ignition (RCCI). In RCCI engines, two fuels with different auto-ignition characteristics are used to achieve an in-cylinder air-fuel blend with a fuel reactivity gradient (Kokjohn, Hanson, Splitter, & Reitz, 2011). Kokjohn et al. (2011) introduced an RCCI engine that can operate over a wide range of engine loads with near-zero levels of NO_x and soot, with acceptable pressure rise rate and ringing intensity, and with high indicated efficiency. They simulated the single-cylinder test engine (SCOTE) of the Caterpillar engine to compare RCCI combustion with

conventional diesel combustion (CDC). The comparison resulted in NO_x reduction by three orders of magnitude, soot reduction by a factor of six, and 16.4 percent gross indicated efficiency increase.

Splitter et al. (2014) studied the effects of intake pressure and temperature, premixed, and global equivalence ratio on gross thermal efficiency in an RCCI engine. The experiments were conducted on a heavy-duty, single-cylinder engine at constant indicated mean effective pressure (IMEP) of 8.45 bar, 1300 rev/min engine speed, with 0% EGR, and crank angle of 50% fuel burned (CA₅₀) of 0.5° crank angle (CA) after top dead center. The results showed that the premixed equivalence ratio approached the global equivalence ratio at higher intake temperature; also, increasing intake temperature resulted in higher combustion efficiency.

Meanwhile, there have been lots of researches on using alternative fuels in RCCI engines. Gasoline and diesel are the initial options as low and high reactivity fuel, respectively (R. Hanson et al., 2012; R. M. Hanson, Kokjohn, Splitter, & Reitz, 2010; Kokjohn et al., 2011; Splitter et al., 2010). In recent studies, diesel is injected as high reactivity fuel directly into the combustion chamber, but natural gas (J. Li, Yang, Goh, An, & Maghbouli, 2014; Nieman, Dempsey, &

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Reitz, 2012; Ryan Walker, Wissink, DeVescovo, & Reitz, 2015) and alcoholic fuels, such as methanol (Y. Li, Jia, Liu, & Xie, 2013; Zang & Yao, 2015), ethanol (Dempsey, Adhikary, Viswanathan, & Reitz, 2011; Han, Divekar, Reader, Zheng, & Tjong, 2015) as low reactivity fuel are injected into the inlet manifold as an alternative to gasoline. Petroleum-based fuels not only contain aromatics that result in soot formation but also face an energy shortage issue. In contrast, biogas is free of aromatics and widely available and has a higher octane number than gasoline, which provides a larger reactivity difference in the cylinder; as a result, it causes more efficient and controllable combustion in RCCI engines.

Nieman et al. (2012) numerically investigated the effect of using methane and diesel in RCCI combustion to achieve efficient combustion in a wide range of operations. Walker et al. (2015) carried out experimental research on an RCCI engine operating with methane, as a natural gas surrogate fuel, and diesel to investigate the characteristics of the combustion process in different operating loads. They used methane that represents natural gas in both experimental and numerical research. It was proved that using methane rather than gasoline in an RCCI engine could extend operating loads.

Few studies have been devoted to an RCCI engine fueled with biogas and diesel. So far, only experimental studies on the engine fueled have been reported. The ability to predict the effects of various parameters on RCCI engines running on biogas and diesel has not been feasible due to the lack of simulation models of the engine. Thus, the objective of the current study is to investigate the effects of using biogas as a low-reactivity in an RCCI engine fueled with biogas and diesel. Also, the effects of biogas to diesel ratio on combustion characteristics such as engine efficiency and emission levels in the engine are studied.

Composition of biogas

Biogas is a mixture of several gases, CH₄, CO₂, and a small amount of H₂, N₂, O₂, and H₂S. Methane is the main component of biogas and exhibits greater resistance to the knock phenomenon due to its higher octane rating and auto-ignition temperature, making it a promising candidate for engines with high compression ratios.

Since H₂S causes corrosion of mechanical parts of the engine, biogas firstly is required to be upgraded through removing H₂S and water vapor, which can be done by the water scrubbing method.

After purifying the biogas, the main components are CH₄ (60-100%) and CO₂ (0-40%). The percentage of CH₄ and CO₂ depends on the source and the way distracted from it. In this paper, it is assumed that the biogas consists of 60% methane and 40% CO₂.

Model and validation

1- Model

To simulate the combustion, reduced primary reference fuel (PRF) mechanism consisting of 76

species and 464 reactions (Rahimi, Fatehifar, & Saray, 2010), standard wave model (Liu, Mather, & Reitz, 1993), wall jet model (Naber & Reitz, 1988), Duckowicz model (Dukowicz, 1979), diesel nozzle flow (von Kuensberg Sarre, Kong, & Reitz, 1999) and turbulent dispersion model (Gosman & Loannides, 1983) were employed. Soot is predicted by using a phenomenological soot model (Heywood, 1988) based on the approach of Hiroyasu. NO_x formation is modeled using an extended Zeldovich mechanism (Hiroyasu & Kadota, 1976).

Also, a 2.44 L Caterpillar 3401E (SCOTE) (Ryan Walker et al., 2015) as a heavy-duty diesel engine is simulated. The specifications of the engine and fuel injection system are listed in "Table 1".

Table1: engine geometry (Ryan Walker et al., 2015)

Caterpillar 3401E SCOTE	
Cylinders	Single
Compression ratio	14.88:1
Bore × Stroke	137.2mm × 165.1 mm
Connecting rod length	261.6
Intake valves	2
Exhaust valves	2
Intake valve closing (IVC)	-143 deg. ATDC
Exhaust valve opening (EVO)	130 deg. ATDC
Swirl ratio	0.7
Piston bowl type	Bathtub
Common rail diesel fuel injector	
Injector holes	6
Injector hole diameter	250µm
Included spray angle	145 deg.
Injection pressure	500 bar
Injection duration	15 crank angle degree
Biogas	Port injection
Computational grid	
Cells at BDC	11480
Average cell size	1.8 mm

In the RCCI combustion, the biogas as a less-reactive fuel with a lower heating value (LHV) of 30 MJ/kg and diesel as a high-reactive fuel with LHV of 45.1 MJ/kg are used. Diesel is injected in one stage and the amount of injected diesel fuel for each cycle is fixed at 13 mg/s. Combustion is investigated in a condition that the intake air temperature and engine speed are at 40°C and 1300 rpm respectively. To maintain the equivalence ratio at 0.3, air mass flow into the cylinder and engine load are increased through increasing the intake pressure and the amount of injected biogas into the inlet port, respectively.

Ring intensity (RI) is defined in eq. (1) as follow, which is proposed by Eng (Nieman et al., 2012)

$$RI = \frac{1}{2\gamma} \frac{(\beta (dp/dt)_{\max})^2}{P_{\max}} \sqrt{\gamma RT_{\max}} \quad (1)$$

where $(dp/dt)_{\max}$, P_{\max} , T_{\max} , γ and R , respectively, are the maximum pressure rise rate, peak pressure, in-cylinder peak temperature, Cp/ Cv ratio, and the gas constant. In a heavy-duty engine, the value of RI should be less than 5 MW/m² (Dec & Yang, 2010; Sjöberg, Dec, Babajimopoulos, & Assanis, 2004).

The gross indicated efficiency (GIE) is defined by the eq. (2)(Nieman et al., 2012) in which E_{in} , m_{fuel} , x_{biogas} , and x_{diesel} are the fuel energy introduced into the engine cylinder, a mass of the consumed fuel, mass fraction of the premixed methane, and n-heptane with lower heating values of LHV_{biogas} and LHV_{diesel} , respectively.

$$\eta = GIE = \frac{Work}{E_{in}} = \frac{\int_{-180}^{+180} P dV = V_{displacement} \cdot IMEP}{m_{fuel} (x_{biogas} \cdot LHV_{biogas} + x_{diesel} \cdot LHV_{diesel})} \quad (2)$$

2- Validation

To validate the model, the biogas is purified and upgraded up to 100% CH₄, then the results are compared with the experimental model of methane /diesel combustion presented by Walker et al. (2015) in “Table 2”. According to “Table 2”, the model simulates the experimental results quite accurately.

Table 2. Comparison of the model with experimental results

IMEP ₅₀ (bar)	Peak pressure (bar)		Start of combustion (deg. ATDC)		PPRR (bar/deg.)		CA50 (deg.ATDC)	
	Sim.	Exp.	Sim.	Exp.	Sim.	Exp.	Sim.	Exp.
5.6	68.5	68.8	-7	-10	6.9	4.4	2	0
6.3	77.5	77.6	-8	-11	6.7	3.9	1.5	0
7.7	93.3	94.9	-9	-12	7.7	4.2	1	0
9.4	114.8	115.1	-11	-14	8.1	5.0	0.8	0
11.5	141.7	140.9	-12	-15	8.6	6.4	-0.8	0
13.5	161.8	164.1	-13	-15	8.5	7.8	-1.2	0

Results

As can be seen in figure 1, using biogas (%60 methane and % CO₂) as a premixed low-reactivity fuel instead of pure methane leads to lower maximum cylinder pressure and temperature, mainly due to the existence of CO₂ as an inert gas that dilutes the

cylinder charge and reduces the heating value of the fuel. Thus, the more amount of CO₂ is available in biogas composition, the more gaseous fuel escapes from the combustion zone, resulting in oxygen concentration and temperature drops.

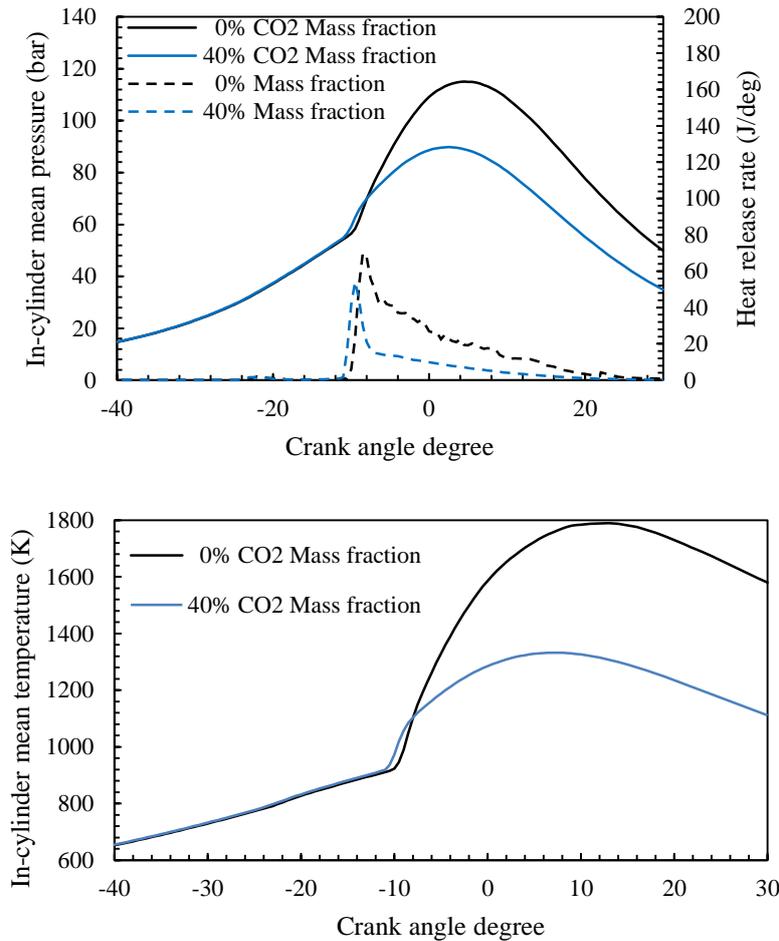


Figure 1. Pressure and temperature variations versus crank angle for different mixtures of biogas

Table 3. Comparison of maximum pressure and temperature in RCCI engine fueled with biogas/diesel against the one fueled with methane/diesel

IMEP _i (bar)	5.6	6.3	7.7	9.4	11.5	13.5
maximum pressure in model 1 (bar)	66.2	72.5	86.1	110.2	124.5	139.4
Maximum pressure in model 2(bar)	68.6	77.6	93.2	114.9	141.8	161.8
maximum Temperature in model 1 (K)	1475.2	1476.8	1510.6	1643.7	1682.1	1686.2
maximum Temperature in model 2 (K)	1546.78	1614.4	1677	1787	1930	1971.3
GIE in model 1 (%)	50.47	48.9	51.9	41.5	40.2	40.9
GIE in model 2(%)	50.88	50.65	50.99	52.33	52.12	55.05
RI in model 1 (MW/m ²)	3.03	2.83	2.79	2.6	2.33	2.13
RI in model 2 (MW/m ²)	3.27	2.71	2.94	2.74	2.59	2.24

Figure 1. Pressure and temperature variations versus crank angle for different mixtures of biogas In “Table 3”, the engine fueled with biogas/diesel (model 1) is compared with the one fueled with methane/diesel (model 2) in terms of GIE, RI, maximum pressure, and temperature for different loads.

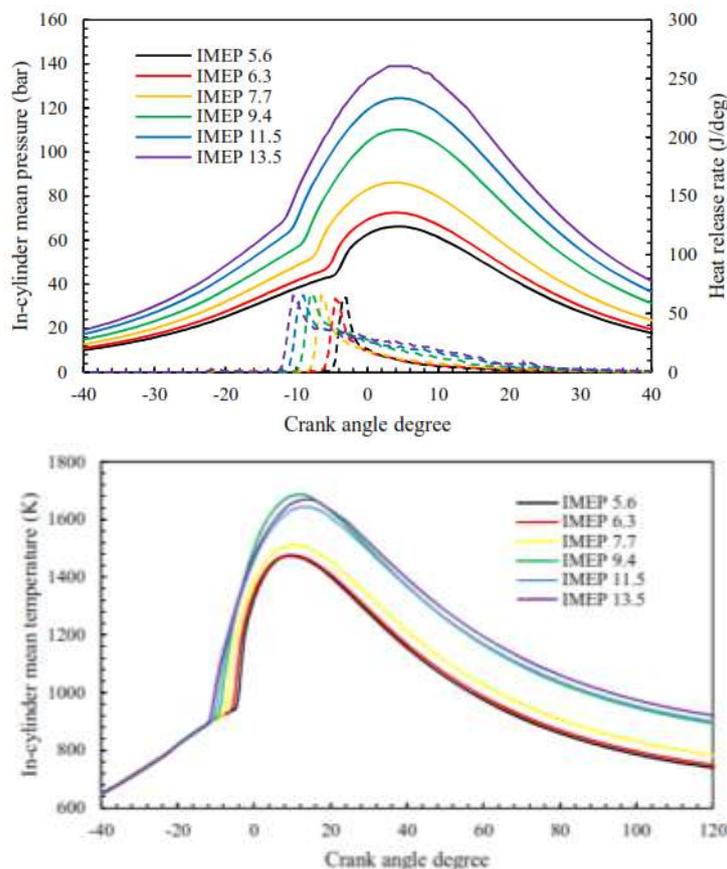
As can be seen, the temperature at IMEP= 11.5 bar in model 1 is lower by about 143°K than in model 2.

Increasing the amount of CO₂ in biogas means that more fuel is needed to generate the same power output. In other words, using biogas instead of methane as a low reactivity fuel in an RCCI engine reduces the power output and increases the fuel consumption to gain the same power output.

Also, using biogas instead of methane causes that the combustion lasts longer and consequently decreases the GIE and RI as well.

In this section, the effects of different parameters on the RCCI engine fueled with biogas and diesel are investigated. In this paper, biogas is considered to be a mixture of 40% CO₂ and 60% methane. For instance, at IMEP= 11.5 bar, GIE and RI are decreased by about 12% and 10% as biogas is used rather than pure methane in the engine.

In “Figure 2”, the in-cylinder pressure and temperature for different loads are demonstrated. As it is clear, by increasing the IMEP, the combustion starts sooner and pressure is increased. Also, the cool flame and the start of combustion locations are advanced by increasing the engine load.

**Figure 2. Emission, GIE, and RI variations versus CO₂ mass fractions**

In “Figure 3”, variations of CO and NO_x versus

IMEP are depicted. As it is known, NO_x directly

depends on temperature. Thus, NO_x emission is increased due to the temperature rise. Also, the higher amount of CO₂ in biogas results in more CO emissions.

Besides, the presence of a higher amount of CO₂ in the gaseous fuel causes a longer ignition delay, the

time interval between the start of injection and the start of combustion. As load is increased, engine efficiency is also increased, leading to better combustion, so CO emission is reduced. Thus, higher IMEP causes higher gross indicated efficiency and lower ringing intensity.

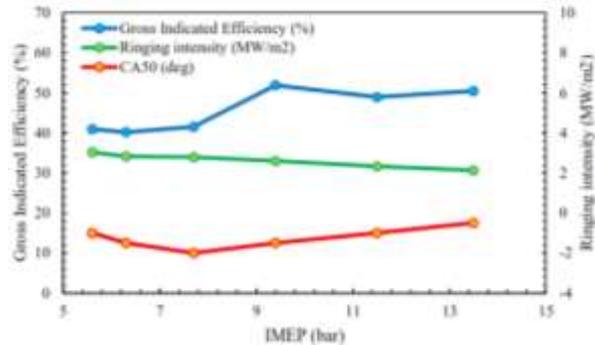
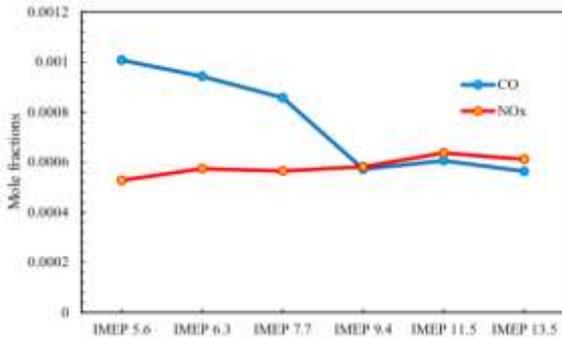


Figure 3. Variations of emissions, GIE, RI, and CA50 versus IMEPs

Different compositions of biogas are listed in Table 4. The gasses are categorized based on methane content from the highest to the lowest one, which is usually found in biogas plants and landfills, respectively.

Table4: Biogas Types

	C1	C2	C3	C4	C5
CO ₂	40	30	20	10	0
Mass CH ₄	60	70	80	90	100

Using each type of biogas leads to different combustion parameters. In other words, the highest in-

cylinder mean pressure and temperature have occurred in C1 since less amount of CO₂ in biogas composition increases combustion enthalpy inside the combustion chamber. Thus, the existence of CO₂ results in the escape of more gaseous fuel and oxygen concentration, and thereby temperature drops. As it is shown in “Figure 4”, increasing the percentage of CO₂ in biogas decreases combustion enthalpy in the combustion chamber, which leads to lower pressure and consequently temperature due to the reduction of the heating value of the fuel.

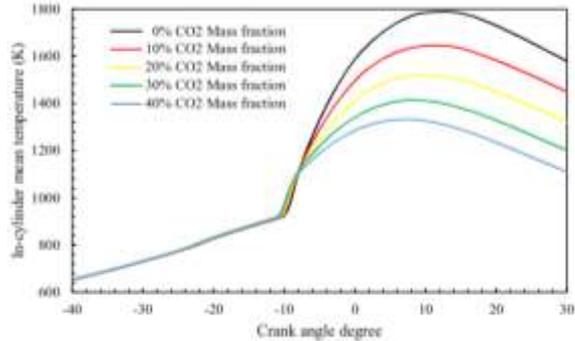
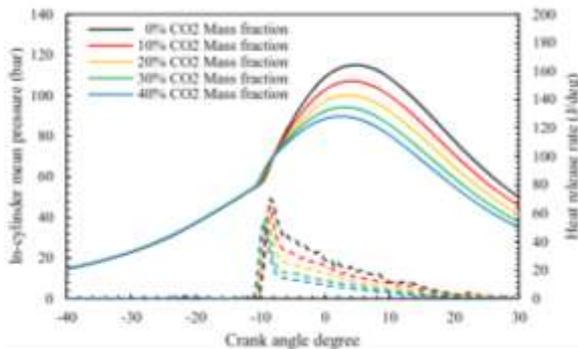


Figure4. Pressure and temperature variations versus crank angle for different mixtures of biogas

As mentioned earlier, NO_x emission mainly depends on temperature. As can be seen in “Figure 5”, increasing the amount of CO₂ in biogas lowers the temperature significantly since CO₂ is an inert gas that does not take part in combustion, resulting in less amount of NO_x emission. However, The amount of CO emission depends on not only incomplete combustion as a result of decreased exhaust temperature but dissociation of CO₂ in biogas as well. Therefore, the higher amount of CO₂ in biogas

composition leads to an increase in CO emission due to the dissociation of CO₂.

By increasing the amount of CO₂ from 0% to 40% in biogas fuel, the NO_x emission drops by 0.0009 ppm, and CO emission rises by 0.0006 ppm, respectively.

Due to the high reactivity gradient as a result of using biogas, the duration of combustion lasts longer; then, the rate of pressure rise decreases the ringing intensity. Thus, gross efficiency is decreased.

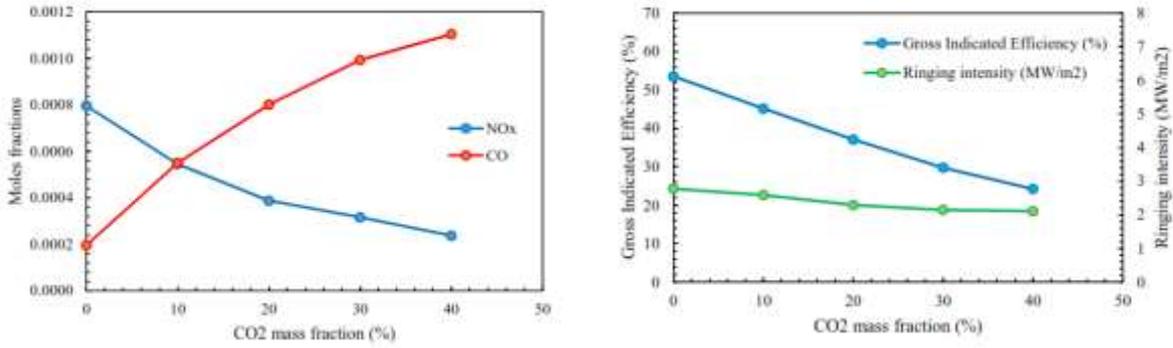


Figure 5. Emission, GIE, and RI variations versus CO₂ mass fractions

“Figure 6” depicts pressure and temperature versus crank angle for different ratios of diesel and biogas in a condition that the total mass keeps

constant at 89 mg. It is noted that mass is injected in two equal times in -40 TDC and -80 TDC, respectively.

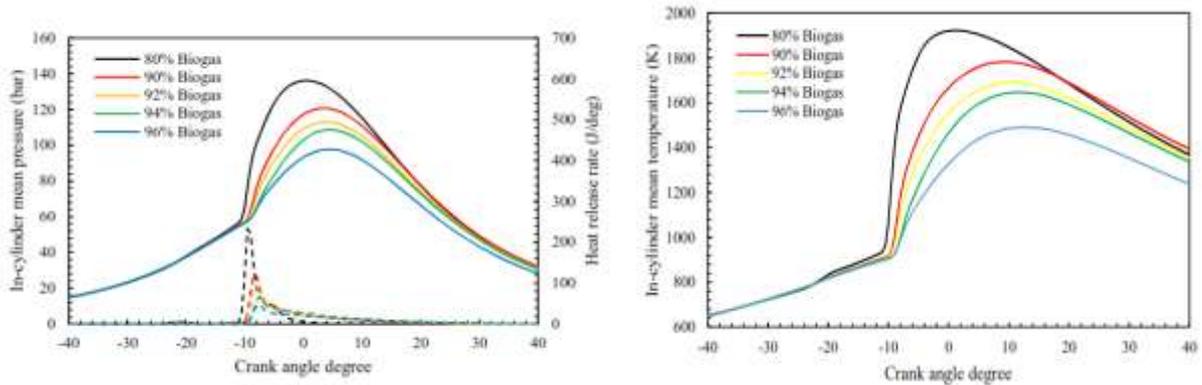


Fig. 6 Variations of pressure and temperature versus crank angle for different ratios of biogas in fuel

Increasing the amount of biogas not only retards the ignition time thanks to having a lower cetane number but also raises the specific heat capacity of the inlet mixture in the compression stroke. Consequently, it takes a longer time for the mixture to reach ignition temperature, leading to a lower temperature rise rate.

lowers the NO_x because of a reduction in combustion temperature. Also, the ignition time is retarded, which leads to a time reduction of NO_x formation. Therefore, NO_x is decreased by increasing the percentage of biogas. Also, CO has a direct relation with biogas percentage. Namely, CO emission rises by increasing the biogas to diesel ratio because of incomplete combustion and dissociation of CO₂ in biogas.

Also, pollution variation is demonstrated in “Figure 7”. Increasing the percentage of biogas in fuel

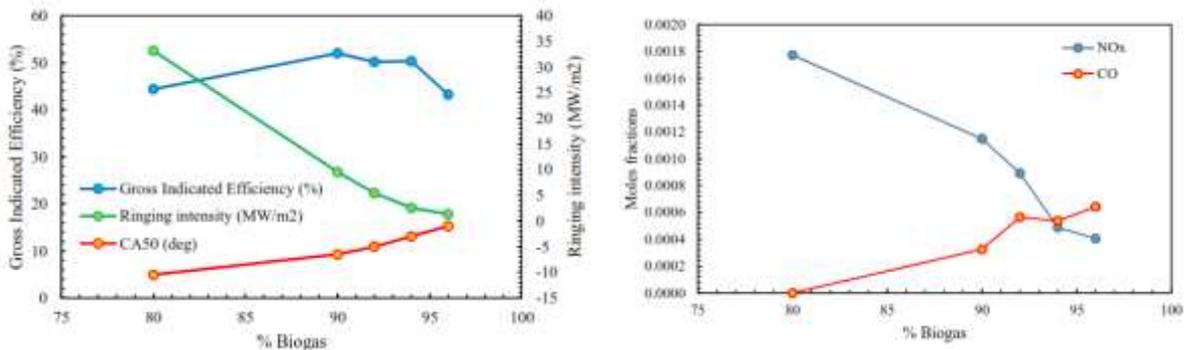


Figure 7. Variations of emissions, GIE, RI, and CA50 versus different ratios of biogas in fuel

Conclusion

In this study, a heavy-duty engine fueled with methane and diesel was considered. Then, the simulation was carried out by comparing

methane/diesel with biogas/diesel combustion in the RCCI engine to study the effects of biogas on combustion characteristics and emission levels. The results showed that CO₂, as an inert gas, played an

important role in maximum pressures and temperatures. The peak flame pressure and temperature in the RCCI engine running on biogas and diesel were lower than the ones in the engine fueled with methane and diesel since CO₂ diluted the cylinder charge and reduced the heating value of the fuel. Although controlling the pressure rise rate in high IMEPs is difficult in the combustion of methane and diesel, using biogas could lower the pressure rise rate. Furthermore, raising the biogas/diesel ratio led to retard in ignition time and, consequently, reduced temperature rise rate. Increasing the biogas to diesel ratio resulted in lower NO_x emission while higher CO emission.

Reference

- Dec, J. E., & Yang, Y. (2010). Boosted HCCI for high power without engine knock and with ultra-low NO_x emissions-using conventional gasoline. *SAE International Journal of Engines*, 3(1), 750-767.
- Dempsey, A., Adhikary, B. D., Viswanathan, S., & Reitz, R. (2011). *Reactivity controlled compression ignition (RCCI) using premixed hydrated ethanol and direct injection diesel*. Paper presented at the ASME 2011 Internal Combustion Engine Division Fall Technical Conference.
- Dukowicz, J. K. (1979). *Quasi-steady droplet phase change in the presence of convection*. Retrieved from
- Gosman, A., & Loannides, E. (1983). Aspects of computer simulation of liquid-fueled combustors. *Journal of energy*, 7(6), 482-490.
- Han, X., Divekar, P., Reader, G., Zheng, M., & Tjong, J. (2015). Active injection control for enabling clean combustion in ethanol-diesel dual-fuel mode. *SAE International Journal of Engines*, 8(2), 890-902.
- Hanson, R., Curran, S., Wagner, R., Kokjohn, S., Splitter, D., & Reitz, R. (2012). Piston bowl optimization for RCCI combustion in a light-duty multi-cylinder engine. *SAE International Journal of Engines*, 5(2), 286-299.
- Hanson, R. M., Kokjohn, S. L., Splitter, D. A., & Reitz, R. D. (2010). An experimental investigation of fuel reactivity controlled PCCI combustion in a heavy-duty engine. *SAE International Journal of Engines*, 3(1), 700-716.
- Heywood, J. B. (1988). *Combustion engine fundamentals*. 1^a Edição. Estados Unidos.
- Hiroyasu, H., & Kadota, T. (1976). Models for combustion and formation of nitric oxide and soot indirect injection diesel engines. *SAE Transactions*, 513-526.
- Kokjohn, S. L., Hanson, R. M., Splitter, D., & Reitz, R. (2011). Fuel reactivity controlled compression ignition (RCCI): a pathway to controlled high-efficiency clean combustion. *International Journal of Engine Research*, 12(3), 209-226.
- Li, J., Yang, W. M., Goh, T. N., An, H., & Maghbouli, A. (2014). Study on RCCI (reactivity controlled compression ignition) engine by means of statistical experimental design. *Energy*, 78, 777-787.
- Li, Y., Jia, M., Liu, Y., & Xie, M. (2013). Numerical study on the combustion and emission characteristics of a methanol/diesel reactivity controlled compression ignition (RCCI) engine. *Applied energy*, 106, 184-197.
- Liu, A. B., Mather, D., & Reitz, R. D. (1993). Modeling the effects of drop drag and breakup on fuel sprays. *SAE Transactions*, 83-95.
- Naber, J., & Reitz, R. D. (1988). Modeling engine spray/wall impingement. *SAE Transactions*, 118-140.
- Nieman, D. E., Dempsey, A. B., & Reitz, R. D. (2012). Heavy-duty RCCI operation using natural gas and diesel. *SAE International Journal of Engines*, 5(2), 270-285.
- Rahimi, A., Fatehifar, E., & Saray, R. K. (2010). Development of an optimized chemical kinetic mechanism for homogeneous charge compression ignition combustion of a fuel blend of n-heptane and natural gas using a genetic algorithm. *Proceedings of the Institution of Mechanical Engineers, Part D: Journal of Automobile Engineering*, 224(9), 1141-1159.
- Ryan Walker, N., Wissink, M. L., DeVescovo, D. A., & Reitz, R. D. (2015). Natural gas for high load dual-fuel reactivity controlled compression ignition in heavy-duty engines. *Journal of Energy Resources Technology*, 137(4).
- Sjöberg, M., Dec, J. E., Babajimopoulos, A., & Assanis, D. N. (2004). *Comparing enhanced natural thermal stratification against retarded combustion phasing for smoothing of HCCI heat-release rates* (0148-7191). Retrieved from
- Splitter, D., Kokjohn, S., Rein, K., Hanson, R., Sanders, S., & Reitz, R. (2010). An optical investigation of ignition processes in fuel reactivity controlled PCCI combustion. *SAE International Journal of Engines*, 3(1), 142-162.
- Splitter, D., Wissink, M., DeVescovo, D., & Reitz, R. (2014). Improving the understanding of intake and charge effects for increasing RCCI engine efficiency. *SAE International Journal of Engines*, 7(2), 913-927.
- von Kuensberg Sarre, C., Kong, S.-C., & Reitz, R. D. (1999). Modeling the effects of injector nozzle geometry on diesel sprays. *SAE Transactions*, 1375-1388.
- Zang, R., & Yao, C. (2015). Numerical study of combustion and emission characteristics of a diesel/methanol dual fuel (DMDF) engine. *Energy & Fuels*, 29(6), 3963-3971.