DOI: http://dx.doi.org/10.22104/aet.2016.328

Advances in Environmental Technology 1 (2016) 1-10

Advances in Environmental Technology

journal homepage: http://aet.irost.ir

Environmental effects of using methanol as a biofuel into the combustion chamber of a heavy-duty diesel engine

Kianoosh Shojae, Majid Mahdavian*

Department of Chemical Engineering, Quchan University of Advanced Technology, Quchan, Iran

ARTICLE INFO

Article history:
Received 6 Jun 2016
Received in revised form
28 July 2016
Accepted 13 August 2016

Keywords:
HD diesel engine
Exhaust emissions
EGR
Injection timing
Methanol biofuel

ABSTRACT

Methanol as a biofuel is an environmentally friendly substitute for pure diesel and can be obtained from biomasses. The use of biofuels such as methanol for the combustion process is associated with positive impacts on the environment. Using pure methanol or a blend of diesel/methanol fuel in motorized vehicles has been proposed by researchers. In this paper, pure methanol was injected into the combustion chamber of a ISM 370 HD diesel engine and the exhaust emissions were evaluated by using AVL FIRE CFD code software at four engine speeds (1200, 1400, 1600 and 1800 rpm). Additionally, the influences of EGR mass fraction and various injection timings were investigated. In order to validate the simulation results, in-cylinder mean pressure and rate of heat release (RHR) were compared with experimental data, and the results gave an acceptable agreement. The obtained results from the conducted simulation showed that the use of methanol fuel in the combustion chamber dramatically reduced the amount of exhaust emissions such as NO, soot, CO, and CO_2 to 90%, 75%, 40%, and 26%, respectively. In addition, a mass fraction of EGR (20%) caused a reduction in the amount of exhaust NO to about 12%. It was determined that when a system is equipped with a fueling system at 3 deg before top dead center (BTDC), the exhaust NO and soot are reduced by 5.8% and 3%.

1. Introduction

When compared with typical diesel fuel, methanol has shown greater environmental performance. This fuel can be produced from a compound of torrefied biomass and coal [1]. In addition, many studies have been performed to investigate various methods for the production of methanol from biomasses. Methanol fuel is generally produced from natural gas, coal, etc. [1-3]. Different technologies have focused on replacing fossil fuels with renewable energies and biomasses [3, 4]. The formation of NO, PM, CO, soot, etc. during piston movement within the engine cylinder can be very problematic (in terms of increased concentrations of pollutant gases) when engines are run with conventional fuels. To improve environmental conditions and achieve a significant reduction in tailpipe emissions, researchers have emphasized on the advantages of biofuels. [4-9]. Methanol has been employed in studies on combustion and its advantages as an alternative or supplemental fuel [10, 11]. Currently, methanol is widely utilized in China [12] as a fuel in its pure or blended form. Furthermore, there are various ways to reduce tailpipe emissions. Studies show that the addition of H_2 fuel through the intake valve and the injection of a diesel-water blend have an effect on ignition, the improvement of various parameters such as mean pressure and in-cylinder temperature, and finally a reduction of polluting gases such as NO emission [13-15]. In addition, a change in the injection timing and EGR can affect CO_2, CO, soot, and NO emissions. A Ford HSDI diesel engine was considered and the effects of injection timings for different statuses of this engine were analyzed and compared to baseline conditions. Furthermore, it became

*Corresponding author. Tel.: +98-9151087002
E-mail address: m.mahdavian@qiet.ac.ir

clear that the piston bowl geometry, especially bowl depth, had a dramatic impact on exhaust emissions. Investigations showed that with retarded injection timing (0.7 deg BTDC), the amount of exhaust soot increased greatly in comparison to the baseline state, whereas, it causes a reduction in NO emissions [16]. Nitrogen monoxide is one of the most dangerous pollutants produced by diesel engines in high temperatures (approximately 2000 K). To minimize the NO formation in the combustion chamber, an exhaust gas recirculation (EGR) system is suggested. The advantage of this system is that the exhaust gases are returned into the combustion chamber and re-enter into chemical interactions. In a heavy-duty engine (high n-butanol-diesel ratio blend), it has been observed that NOx emission for blended fuel decrease dramatically with rising EGR due to the reduced flame temperature caused by diluting oxygen in the incoming air. In detailed analysis of the trade-off between exhaust soot and NO in engines, it was determined that exhaust soot for blended or pure diesel increased due to diluted oxygen caused by EGR rising [17].

In this paper, a Cummins ISM HD diesel engine fueled with methanol biofuel was simulated for the investigation of effective parameters on tailpipe emissions such as CO, NO, CO_2, etc. Methanol was injected into a cylinder through a multi-hole injector and the environmental advantages of using this fuel were compared with diesel. Additionally, various injection timing (1 2, 3, and 4 deg BTDC) and EGR mass fractions (5%, 10%, 15%, and 20%) were considered to arrive at balanced environmental conditions.

2. Simulation

In this simulation, a k-zeta-f turbulence model was applied. This model was chosen to improve numerical stability. The wave breakup model was considered for the spray process. This model can be used for diesel spray simulation. The wall interaction submodel was chosen for calculating the impact of non-volatile fuel particles that collide with the wall of the in-cylinder engine. Walljet1 spray wall interaction was considered. When simulation was used for this model, some droplets of fuel get a slide upon the in-cylinder wall. The extended Zel'dovich mechanism evaluated the exhaust NO emission and this model considered the influences of hydrocarbon radicals as well as N_2 and O_2 on NO emission. This model was coupled with an ECFM-3Z ignition model. The Lund flamelet model was used in this study for soot formation. For simulation of the combustion chamber of a methanol-burning compression ignition engine, a multi-component evaporation model was chosen [13]. In this study, the exhaust emissions of an ISM370 HD diesel engine that was injected with pure methanol were researched. Simulation was performed under 70% load and 1200-rpm engine speed (for validating software with pure diesel). Table 1 shows the characteristics of the simulated diesel engine.

Table 1. Characteristics of Cummins ISM 370 HD diesel engine

Engine model	ISM 37 (heavy-duty)
Capacity	10.8 L
Bore	0.125 m
Stroke	0.147m
Number of cylinders	6
EGR	0%

The applied temperature conditions of the simulation steps are presented in Table 2. In order to do the ignition simulation, meshes of piston bowl geometry were created by using AVL FIRE ESE software. The simulation was carried out between 60000 and 70000 cells and the piston module at TDC is shown in Figure 1. Considering this range, the variation in cylinder mean pressure was found to be ±0.1percentage. The grid independent assay was performed for ten different sets of cells. As illustrated in Figure 2, the mean pressure graphs (For various cells between 60000 and 70000) were completely coincident.

Table 2. Temperature conditions of simulated engine

Cylinder liner temperature	415 K
Piston temperature	545 K
Cylinder head temperature	515 K

The complex grid geometry of the cylinder at the TDC position can be observed in Figure 1. As can be seen, the piston bowl grid was suitable and the software had good accuracy to create the piston bowl geometry. In this paper, numerical simulation was performed only for the baseline piston bowl under various conditions.

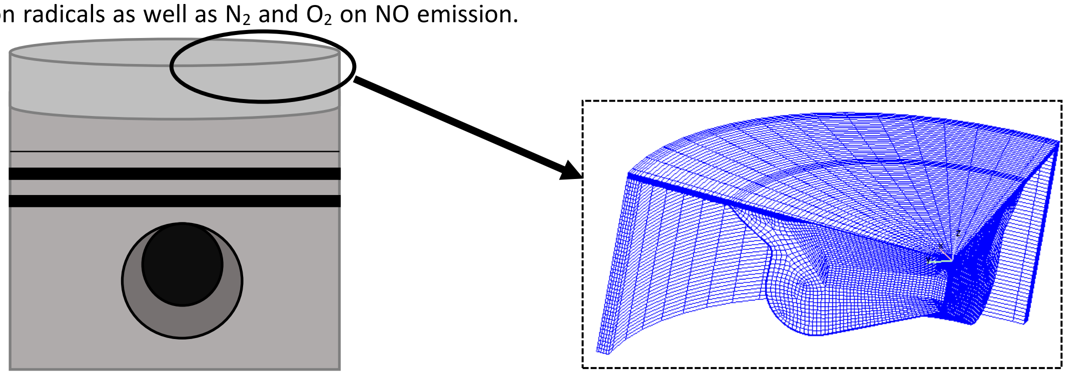


Fig. 1. Piston scheme and in-cylinder computational grid at 720 °CA (TDC).

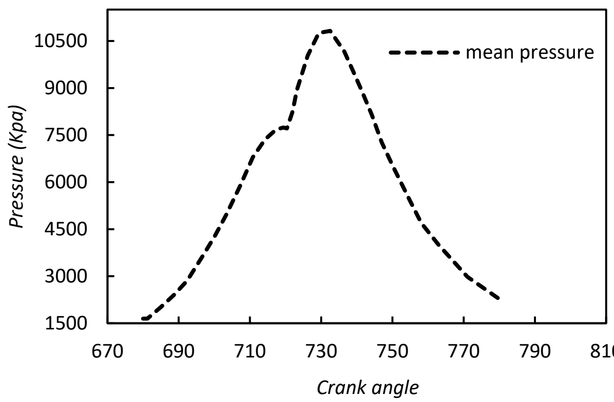


Fig. 2. In-cylinder mean pressure for the range of 60000 to 70000 cells (for pure diesel).

3. Results and discussion

3.1. Validation

For verification and validation of the performed simulation, two parameters were considered. Figures 3 and 4 illustrate the comparison of cylinder mean pressure and rate of heat release for a diesel operation. As observed in Figure 3, the trend of the calculated mean pressure curve and the experimental mean pressure data matched well; the average error was less than 4%. As seen, the ignition timing and the peak pressure were near to the experimental graph. In this simulation, heat transfer through radiation between in-cylinder walls was not considered. The results indicate that, even with considering this simplifying assumption, cylinder mean pressure curves were in good agreement with experimental data [14].

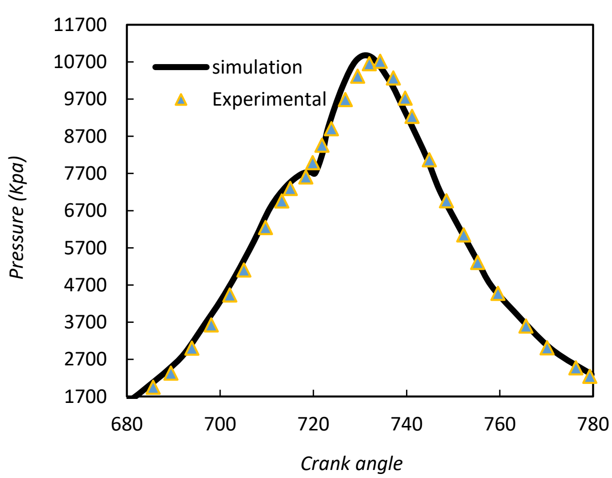


Fig. 3. Comparison between the experimental and predicted in-cylinder mean pressure [14].

As seen in Figure 3, the simulated results were larger than the experimental data between 720 and 730 crank angles (°CAs). This error was created for the indeterminate input data such as baseline injection timing, inlet pressure, temperature, etc.) The predicted data was consistent with the experimental results between 680 and 720 (CAs). The mentioned cases were confirmed for CAs between 730 and 810. As can be seen in Figure 4, the graphs were in basic agreement with each other. The obtained simulation data were higher than the experimental data between 720 and 735 CAs. Detailed investigations showed that errors could be caused by CFD simulation, lack of considers to heat transfer (radiation), etc. [14].

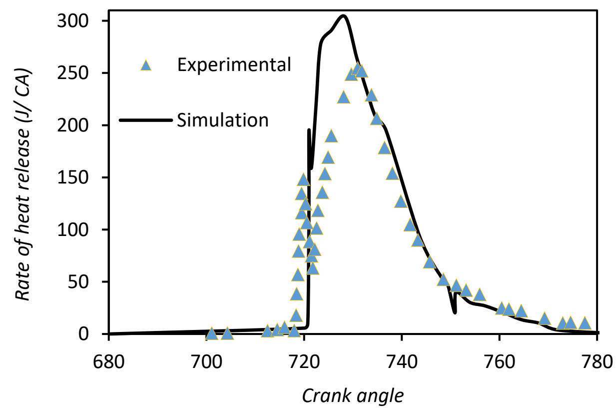


Fig. 4. Comparison between the experimental and predicted in-cylinder rate of heat release (J/ CA) [15].

3.2. Bio-methanol environmental impacts

In-cylinder mean pressure and temperature were calculated to determine the engine performance and the results are presented in Figure. 5. As can be seen, the calculated peak pressure for the methanol-burning engine was lower than the baseline engine. In contrast to diesel fuel, combustion occurred after the TDC point and the delay in ignition was longer than for the pure diesel. It is predicted that by choosing the best piston bowl geometry or increasing injection pressure, the mean pressure and temperature would be enhanced. It is clear that NO was generated under the following conditions: high in-cylinder temperature, rich oxygen, and high temperature duration at wide range of process. These conditions lead to more NO emissions. The type of fuel used to run an engine is the decisive factor on the amount of exhaust emissions produced. Figure 6 indicates that at EVO (exhaust valve are open by 810 CA) and by taking advantage of methanol fuel, the amount of exhaust NO are strongly reduced in comparison with pure diesel by about 90%. This reduction in NO formation is very noteworthy. As observed in Figure 7, at EVO with using the methanol fuel with reduction of in-cylinder pressure as well as temperature, the soot oxidation is not well performed and the exhaust soot emissions increased by approximately 75%. Nevertheless, it should be noted that the amount of produced soot in contrast with NO formation was negligible. As observed in Figures 7 and 9, when the piston is in BDC (bottom dead center), the chamber volume increased extremely in comparison to TDC; and at EVO, the concentration of CO and soot emissions were in lower values. When the piston moves from TDC to BDC, the amount of exhaust CO_2 and NO increased and afterward the amount proved to be steady, as seen in Figures 6 and 8. As shown, the peak CO was reduced along with the methanol until 810 °CA, in each cycle. Moreover, the peak stage lagged occurred with this fuel (in term of CO emissions) when compared to the diesel. The distribution of the mass fraction of CO_2 and NO emissions for a methanol-burning engine is presented in Table 3 at 730, 780, and EVO crank angles.

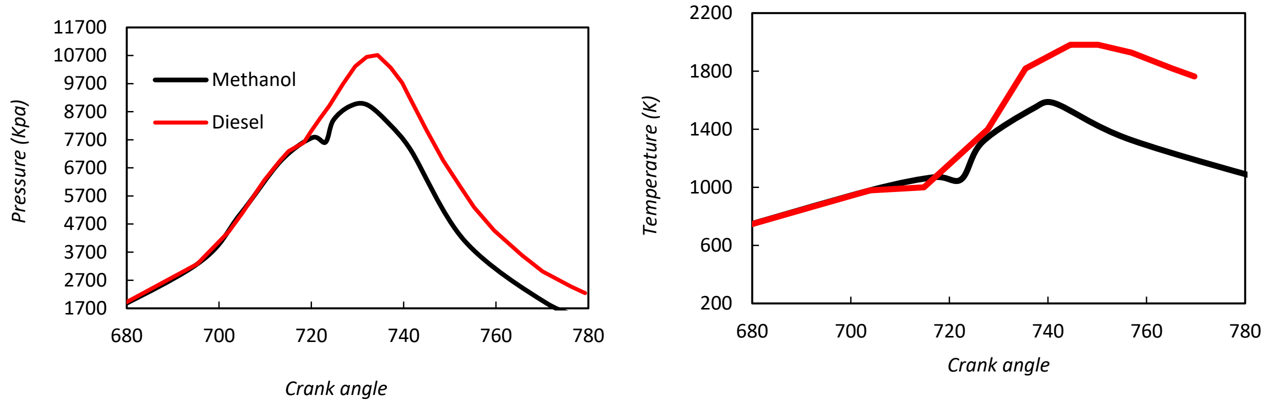


Fig. 5. Mean pressure and temperature distributions for two considered fuel (diesel and methanol).

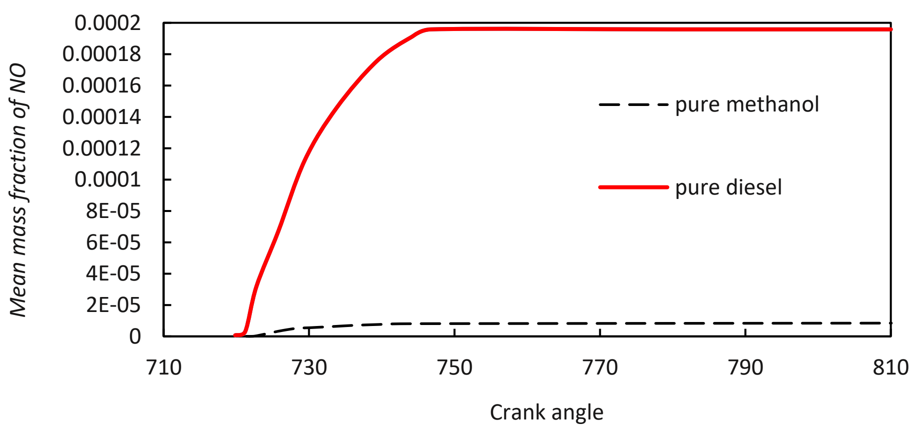


Fig. 6. Comparison of NO formation for two considered fuels (at 1200 rpm).

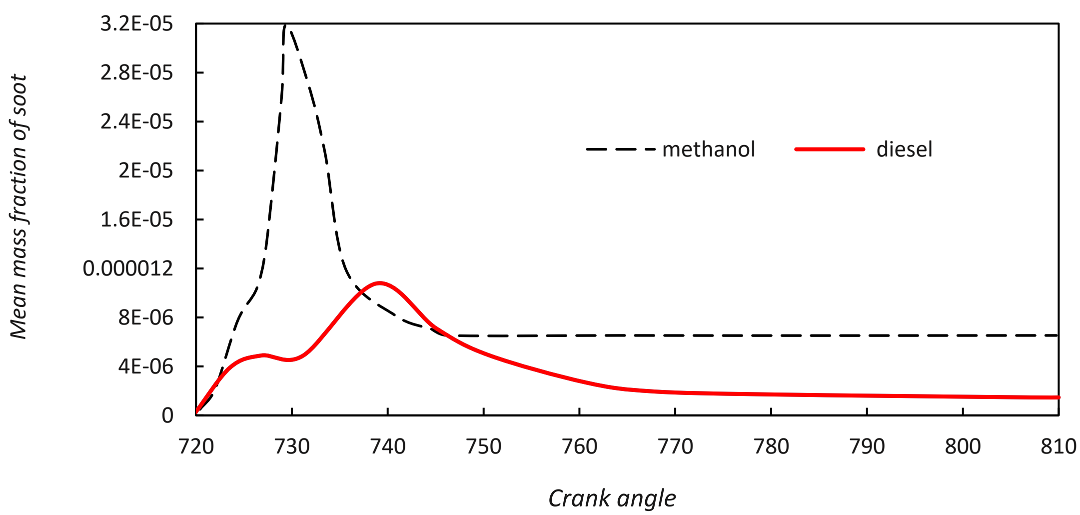


Fig. 7. Comparison of soot formation for two considered fuels (at 1200 rpm)

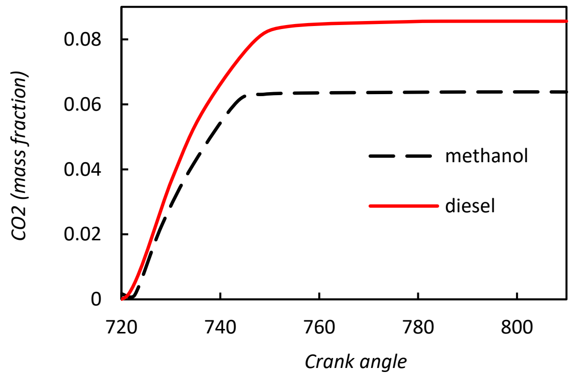


Fig. 8. Comparison of CO_2 formation for two considered fuels (at 1200 rpm).

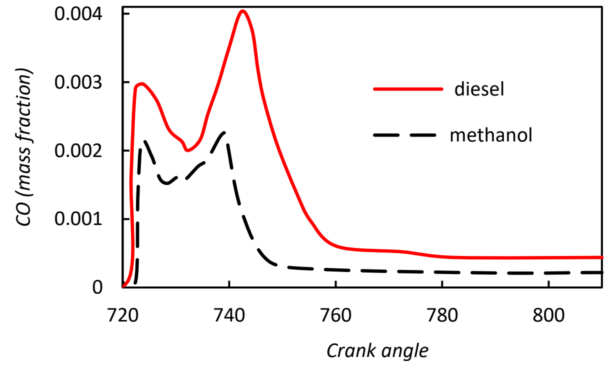
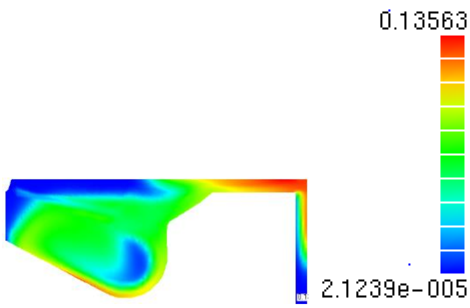
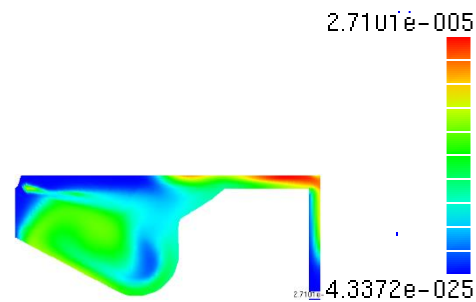
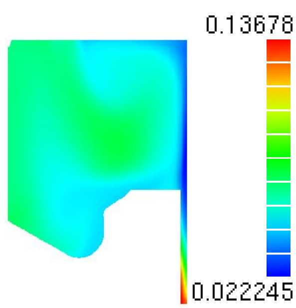
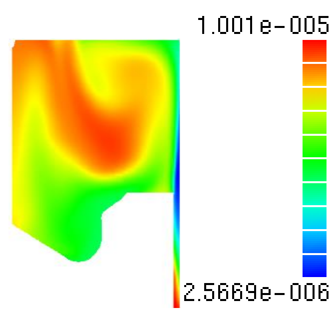
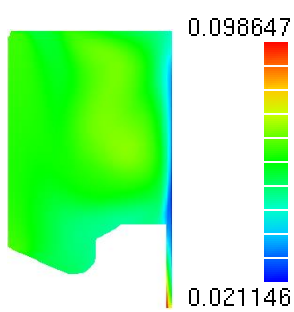
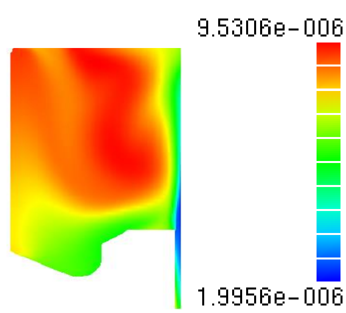


Fig. 9. Comparison of CO formation for two considered fuels (at 1200 rpm).

Table 3. Comparison of in-cylinder CO_2 and NO distribution at various crank angles

Z cut	Mass fraction of CO_2	Mass fraction of NO
730 °CA		
780 °CA		
EVO		

After fuel injection at 718.5 °CA, emissions were dramatically formed. As observed in Table 3, at 730 °CA and around the cylinder center, amount of exhaust NO and CO_2 is in the highest concentration regarding the rest of another in-cylinder areas at 780 and 810 CA. When the outlet valve was opened (at EVO), whole pollutant gases were evacuated through the vehicle tailpipe. Despite lower exhaust emissions, the methanol biofuel had a little drop in engine power performance as opposed to the diesel fuel. A relatively small power loss of engine due to an intense reduction in emissions was negligible.

3.3. Environmental effects of changing engine speed on NO and soot emissions

The parameters of this investigation were to quantify the influences of engine speed at a constant injected mass on NO, soot emissions at EVO, and diesel engine as well as to compare the obtained results in various engine speeds with each other. It was determined that the pressure and temperature of cylinder were reduced by rising engine speed. Higher temperature (and high temperature duration time), enough oxygen, and the presence of N_2 were the main reasons of increasing exhaust NO. It should be noted that lower temperature was associated with higher soot and CO formations (with reducing temperature soot and CO oxidation reduced dramatically). Thus, NO and soot emissions were greatly affected by the variation of speed. As seen in Figures 10 and 11, NO emissions were reduced by rising engine speed. This case was in contrast to soot formation. When the HD engine was fueled with methanol biofuel, the amount of tailpipe NO were reduced by approximately 51% by changing the engine speed from 1200 to 1800 rpm. Thus, NO emission was increasingly produced at lower speeds. Conversely, more soot formation occurred when the engine speed was in a higher value. For example, with a rising engine speed from 1200 to 1800 rpm, the amount of soot formation increased by around 271%.Our investigations showed that the amount of exhaust CO increased, and mutually, CO_2 formation was reduced by increasing engine speed.

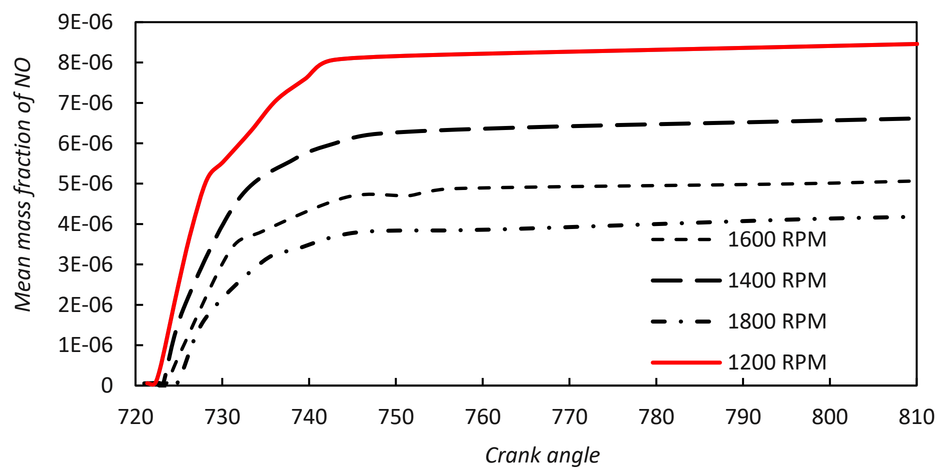


Fig. 10. Comparison of NO formation at various engine speeds.

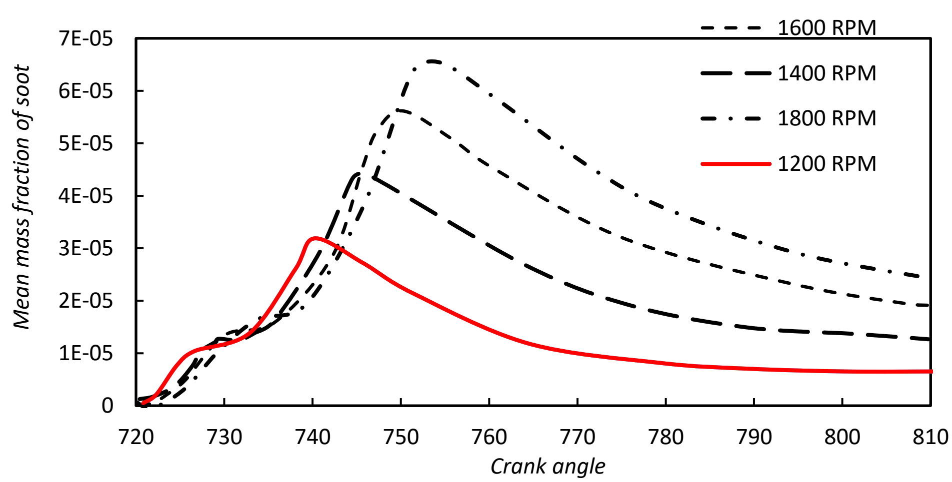


Fig. 11. Comparison of soot formation at various engine speeds

3.4. EGR mass fraction

EGR is an exhaust NO reduction technique which can be utilized in diesel engines. EGR acts by recirculating a combination of tailpipe gases back to the combustion chamber. This attenuates the supply of oxygen in the intake airflow and provides inlet gases to work as absorbents of ignition warmth to decrease combustion chamber temperatures. Most diesel engines such as ISM 370 HD diesel engine require EGR to meet NO emissions standards. As can be observed in Figure 12, by taking advantage of an EGR mass fraction from 5% to 20%, the amount of NO emissions was reduced by around 12%. This reduction for an extremely toxic gas (NO) was very significant. Thermal efficiency is a performance parameter of an engine such as ISM 370 that uses thermal energy. This parameter was calculated for four EGR mass fractions. As seen in Figure 13, thermal efficiency varied with EGR mass fraction. Thermal efficiency for 20% EGR mass fraction was lower than 15% EGR mass fraction by around 11%. However, taking into account a balance between NO emission and thermal efficiency, a 20% EGR mass fraction was preferable. In these conditions, due to choose lowest EGR composition, oxygen content is in highest concentration.

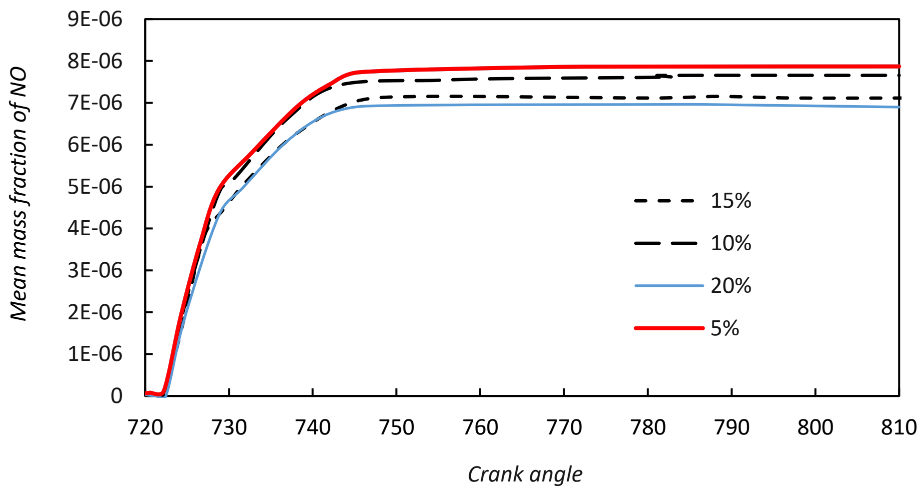


Fig. 12. Comparison of NO formation under various EGR mass fraction (at 1200 rpm).

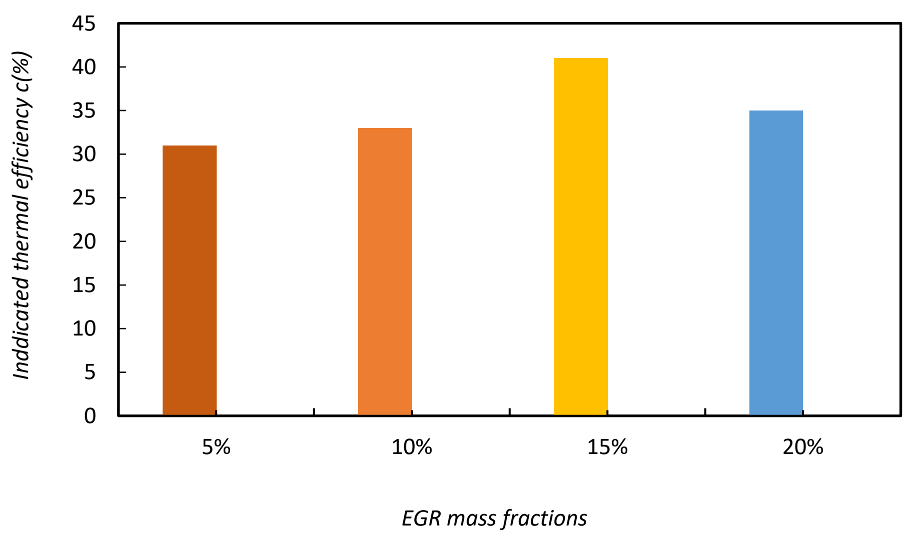


Fig. 13. Thermal efficiency as a function of EGR mass fraction

3.5. Effects of EGR composition on pressure and RHR

In this paper, mean pressure and rate of heat release were calculated in various EGR compositions and mass fractions. This study shows that mean pressure and rate of heat release for two considered fuels as a function of °CA under four EGR mass fractions (5, 10, 15 and 20 percentage) and with the same applied conditions such as 1200-rpm, the engine speeds were identical (0.05 EGR composition). However, when EGR composition was changed from 0.05 to 0.5, the changing EGR mass fraction affected the mean pressure and rate of heat release. As can be seen in Figure 14, the peak pressure was lower than 0.05 EGR composition because of diluted oxygen content.

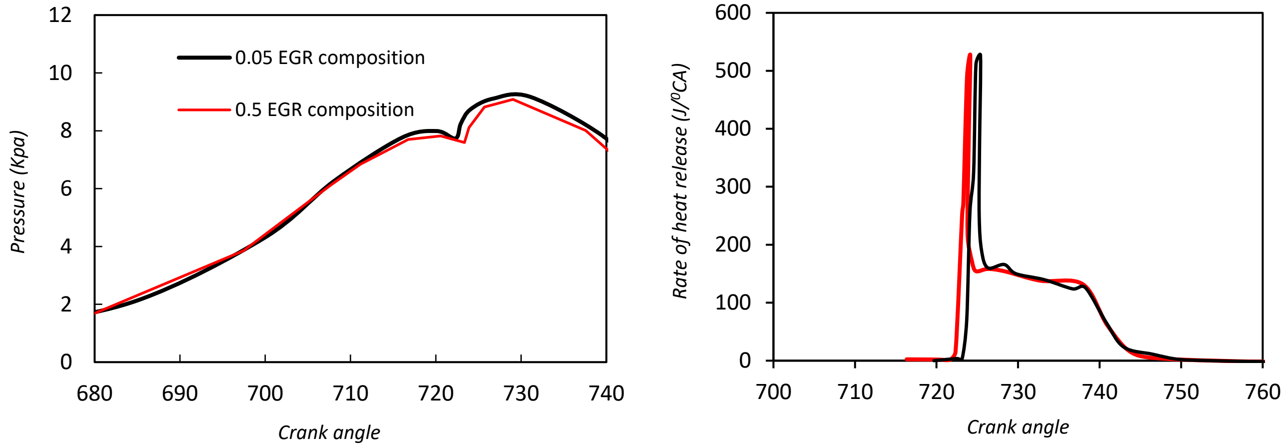


Fig. 14. Comparison of mean pressure and RHR as a function of crank angle for two EGR compositions under 15% EGR mass fraction.

3.6. Injection timing

Fuel injection timing into the combustion chamber has great influence on the amount of exhaust emissions. In order to create a significant comparison of the operation of methanol in pure form, three injection timings were considered. Numerical simulations were carried out with various applied injection timings varying from 2 to 4 before piston is arrived to TDC (BTDC). The calculations in terms of soot and NO emissions were presented against CA. As can be illustrated in Figures 15 and 16, the set injection timing at 2 deg BTDC in comparison to 3 deg BTDC had higher NO and soot emissions and with a set injection timing at 4 deg BTDC, the amount of exhaust NO was in the highest concentration. It was found that when the fueling system through nozzles was set at 3 deg BTDC, the amount of exhaust NO and soot emissions was reduced by 5.8% and 3% in comparison to a 2 deg BTDC injection timing. As seen, the concentration of whole exhaust emissions varied considerably when the piston moves away from the top dead center and turns back to this point. After all the interactions, whole emissions were evacuated through the vehicle tailpipe in EVO crank angle. As observed, with the use of 3 deg BTDC injection timing, the concentration of NO and soot were at the highest level in comparison to another injection timing. Taking advantage of this injection timing is not suitable for the ISM 370 HD engine (under a constant engine speed and injected mass).

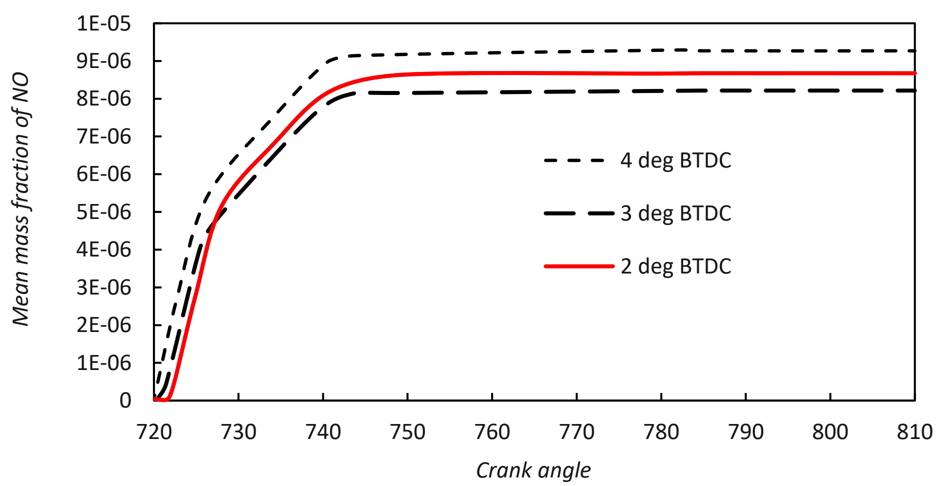


Fig. 15. Comparison of NO formation under 3 injection timing (at 1200 rpm).

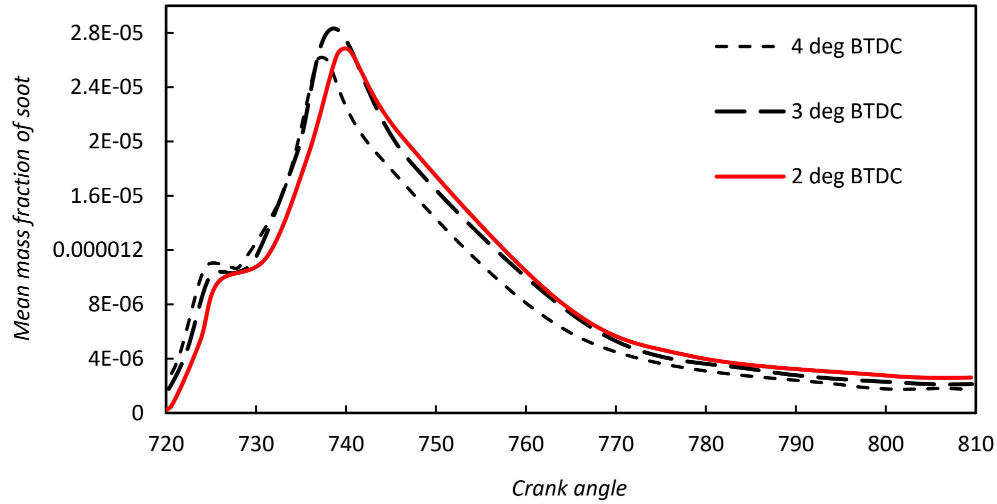


Fig. 16. Comparison of soot formation under 3 injection timing (at 1200 rpm).

3.7. BSFC

Brake specific fuel consumption (BSFC) at different injection timing, EGR, etc. is an important performance parameter. This parameter was calculated for the intended injection timings. The BSFC of a diesel engine such as ISM 370 depends on the relationship between injection timing and properties of fuel such as specific gravity, viscosity, etc. [18]. Figure 17 shows that by retarding the fuel injection timing into the cylinder from 4 to 3 deg BTDC, the BSFC increased approximately 2%. The results of this study showed that advancing the fuel injection timing reduces the brake specific fuel consumption. Thus, advancing fuel injection timing and lower BSFC means that a smaller amount of fuel is required to make the same produced power in comparison to 3 and 2 deg BTDC injection timings.

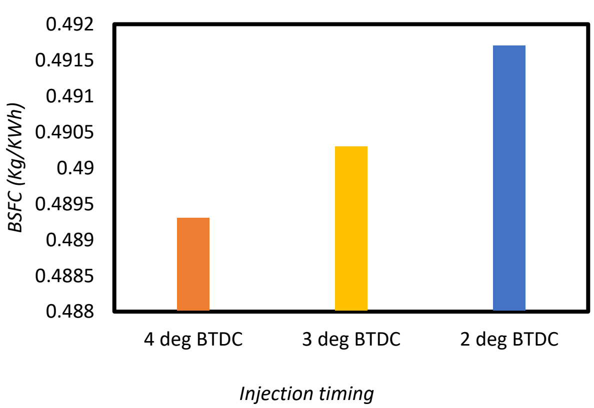


Fig. 17. Influences of injection timings on BSFC

4. Conclusions

In the present work, the exhaust emissions of a HD diesel engine fueled with bio-methanol were evaluated. The results of simulation showed that by taking advantage of methanol fuel in a constant speed (1200 rpm), the amount of exhaust emission such as_NO, soot, CO, and CO_2 was reduced by 90%, 75%, 40%, and 26%, respectively. It was determined that the best injection timing for having a balance between tailpipe emissions (NO and soot) and BSFC was 3 deg BTDC for a methanol-burning HD diesel engine. It was found that a 20% EGR mass fraction can reduce NO caused by high temperatures by approximately 12%. Furthermore, the indicated efficiency was improved by applying this EGR mass fraction. Based on the obtained results, it was clear that methanol as a clean and environmentally friendly fuel is a feasible option to arrive at conditions that reduce the hazardous effects on the environment.

References

[1] Trop, P., Anicic, B., Goricanec, D. (2014). Production of methanol from a mixture of torrefied biomass and coal. *Energy*, *77*, 125-132.

[2] Holmgren, K. M., Andersson, E., Berntsson, T., Rydberg, T. (2014). Gasification-based methanol production from biomass in industrial clusters: Characterisation of energy balances and greenhouse gas emissions. *Energy*,*69*, 622-637.

[3] Manenti, F., Adani, F., Rossi, F., Bozzano, G., Pirola, C. (2016). First-principles models and sensitivity analysis for the lignocellulosic biomass-to-methanol conversion process. *Computers and chemical engineering*, *84*, 558-567.

[4] Thomas, G., Feng, B., Veeraragavan, A., Cleary, M. J., Drinnan, N. (2014). Emissions from DME combustion in diesel engines and their implications on meeting future emission norms: A review. *Fuel processing technology*, *119*, 286-304.

[5] Park, S. H., Lee, C. S. (2013). Combustion performance and emission reduction characteristics of automotive

DME engine system. *Progress in energy and combustion science*, *39*(1), 147-168.

[6] Chen, Z., Wu, Z., Liu, J., Lee, C. (2014). Combustion and emissions characteristics of high n-butanol/diesel ratio blend in a heavy-duty diesel engine and EGR impact. *Energy conversion and management*, *78*, 787-795.

[7] Hou, J., Wen, Z., Jiang, Z., Qiao, X. (2014). Study on combustion and emissions of a turbocharged compression ignition engine fueled with dimethyl ether and biodiesel blends. *Journal of the energy institute*, *87*(2), 102-113.

[8] Paul, A., Bose, P. K., Panua, R., Debroy, D. (2015). Study of performance and emission characteristics of a single cylinder CI engine using diethyl ether and ethanol blends. *Journal of the energy institute*, *88*(1), 1-10

[9] Tudu, K., Murugan, S., Patel, S. K. (2015). Effect of diethyl ether in a di diesel engine run on a tyre derived fuel-diesel blend. *Journal of the energy institute*, *55*, 1-11.

[10] Li, Y., Zhang, C., Yu, W., Wu, H. (2016). Effects of rapid burning characteristics on the vibration of a common-rail diesel engine fueled with diesel–methanol dual-fuel. *Fuel*, *170*, 176-184.

[11] Vancoillie, J., Sileghem, L., Verhelst, S. (2014). Development and validation of a quasi-dimensional model for methanol and ethanol fueled SI engines. *Applied energy*, *132*, 412-425.

[12] Chen, H., Yang, L., Zhang, P. H., Harrison, A. (2014). The controversial fuel methanol strategy in China and its evaluation. *Energy strategy Reviews*, *4*, 28-33.

[13] Soni, D. K., Gupta, R. (2015). Comparison of performance and emission characteristics of diesel and diesel-water blend under varying injection timings. *International journal of engineering, science and technology*, *7*(4), 49-59.

[14] Yang, Z., Chu, C., Wang, L., Huang, Y. (2015). Effects of H_2 addition on combustion and exhaust emissions in a diesel engine. *Fuel*, *139*, 190-197.

[15] Liu, S., Li, H., Liew, C., Gatts, T., Wayne, S., Shade, B., Clark, N. (2011). An experimental investigation of NO_2 emission characteristics of a heavy-duty H 2-diesel dual fuel engine. I*nternational journal of hydrogen energy*, *36*(18), 12015-12024.

[16] Mobasheri, R., Peng, Z. (2013). CFD investigation of the effects of re-entrant combustion chamber geometry in a HSDI diesel engine.*World academy of science, engineering and technology, International journal of mechanical, aerospace, industrial, mechatronic and manufacturing engineering*, *7* (4), 770-780.

[17] Chen, Z., Wu, Z., Liu, J., Lee, C. (2014). Combustion and emissions characteristics of high n-butanol/diesel ratio blend in a heavy-duty diesel engine and EGR impact. *Energy conversion and management*, *78*, 787-795.

[18] Ge, J. C., Kim, M. S., Yoon, S. K., Choi, N. J. (2015). Effects of pilot injection timing and EGR on combustion, performance and exhaust emissions in a common rail diesel engine fueled with a canola oil biodiesel-diesel blend. *Energies*, *8*(7), 7312-7325.