Parametric study of intake manifold temperature on a HCCI combustion engine

Chang Don

Parametric study of intake manifold temperature on a HCCI combustion engine

Chang Don

Department of Chemical Engineering, Suzhou University, China

Abstract

Homogenous Charged Compression Ignition (HCCI) is one of the new combustion strategies developed recently for Internal Combustion (IC) engines to fulfill the stringent emissions regulations while it can keep the thermal efficiency of the engine as high as diesel engines. In this type of engines, the homogenous mixture of fuel and air is inducted to the cylinder and when the piston reached to the top dead center (TDC), the mixture will be ignited due to auto ignition of fuel and air mixture. In this study, a natural gas fueled HCCI engine is considered to study the effect of intake manifold temperature on engine outputs such as power and Indicated Mean Effective Pressure (IMEP), and Fuel Conversion Efficiency (FCE). On the other hand, exhaust characteristics such as pressure and temperature were reported as well as emissions such as carbon monoxide (CO) and oxides of nitrogen (NOx). The exhaust parameters can help to have a maximum efficiency from the engine considering a waste heat recovery system in the exhaust flow. The results showed that FCE is maximum when the intake temperature is minimum. Also, the power output reduced uniformly when the temperature increased. On the other hand, the amount of NOx production increased uniformly, at higher intake temperatures. Furthurmore, with increasing the intake temperature, the exhasut pressure and the exhasut temperature were reduced monotonically.

Keyword: Internal Combustion Engine, Chemical Kinetics, HCCI, Natural Gas, Exhaust Properties, Emissions.

1. Introduction

Increasing concerns about emissions from internal combustion (IC) engines, as well as the permanent demand for higher thermal efficiency, motivated the researchers for applying the new methods in IC engines. One of this method is application of advanced combustion strategies inside the combustion chamber. Advanced combustion strategies such as lean burn spark ignition combustion [1-3] or Reactivity Controlled Compression Ignition (RCCI) [4-6] can produce low emissions of particulate matter and oxides of nitrogen (NOx).

Homogenous Charged Compression Ignition (HCCI) is one of the strategies which received attentions in the recent years. As it is known from its name, in this combustion strategy, the homogenous mixture of fuel and air is inducted to the cylinder at different temperatures and pressures. When the piston reached to the top dead center (TDC), the mixture will be ignited due to auto ignition of fuel and air mixture. Therefore, combustion of fuel and air in HCCI engines are controlled only with the chemical kinetic of the mixture. On the other hand, due to cumbersome essence of chemical kinetic, auto ignition prediction at different air and fuel mixtures is complicated. Beside high efficiency of HCCI engines and low NOx and PM emissions, however HCCI engines suffer from high unburned hydrocarbons and high cyclic variations [7-9].

HCCI engines have been developed in different aspects [10-12]. Fuel property changes on heavy-duty HCCI combustion has been studied by Bessonette et al. [10]. To cover range of volatility, fuel chemistry, and ignition quality, they considered fuels in the gasoline and diesel boiling range. The results showed that heavy-duty HCCI operation over a broad load range can be achieved by the suitable combination of fuel quality and engine conditions. Thus, gasoline low reactivity made the combustion difficult to occur at low load but it could be used to extend the pre-combustion mixing time. In another research effort, Vuilleumier et. al. [12] used the blends of ethanol and n-heptane to study intermediate temperature heat release in HCCI engines over the range of intake pressures and equivalence ratios. They reported that intermediate temperature heat release increased with increasing the portion of highly reactive fuel.

Another method to increase efficiency of IC engines is application of a waste heat recovery system in the exhaust flow such as Organic Rankine Cycle [13-14]. In this method, a device installs downstream of exhaust pipe to produce work directly or indirectly from the high energy exhaust flow. Recently, Mahabadipour et. al. [15] developed a method to predict crank angle resolved exergy of exhaust flow at different operating conditions. They found that the exhaust energy is higher when engine runs at low boost pressures which we used it to confirm our results.

In the present work, a natural gas fueled HCCI engine is considered to study the effect of intake manifold temperature on combustion phenomena as well as exhaust characteristics such as thermodynamic properties and emissions. These results can help to predict what conditions should be considered for the engine to maximize the work output of waste heat recovery system. Therefore, the total thermal efficiency of the engine will be maximized. In this regard, the intake manifold temperature was swept from 437 K to 477 K and the engine speed was constant at 1000 rpm. Also, the engine was considered at naturally aspirated condition.

2. Engine Specifications and Operating Conditions

This simulation was used to determine the effects of intake manifold temperature on characteristics of advanced low temperature combustion engines. In this regard, a natural gas fueled HCCI engine is considered to study the effect of intake manifold temperature on combustion phenomena as well as exhaust characteristics such as thermodynamic properties and emissions. Therefore, the intake manifold temperature was swept from 437 K to 477 K with increment of 10 K in a naturally aspirated single cylinder engine with the compression ratio of 16.5 running at constant speed of 1000 rpm. The variables considered in the parametric study, such as compression ratio, intake temperature, boost pressure, engine speed and other operating conditions were given in Table 1.

Table1. engine specifications and operating conditions

Engine parameters	**Value**
Type	4 stroke, single cylinder
Bore (mm)	110
Stroke (mm)	110
Displacement (L)	1.05
No. of cylinders	1
Engine Speed (rpm)	1000
Boost Pressure (atm)	1
Intake Temperature (K)	437-477
Compression ratio	16.5
Connecting rod length (mm)	250
Intake Valve Open (CAD)	5
Intake Valve Close (CAD)	220
Exhaust Valve Open (CAD)	500
Exhaust Valve Close (CAD)	715

3. Kinetic Model

Chemical kinetics can be utilized for the auto-ignition and combustion phasing in HCCI engines. Therefore, the detailed reaction mechanism including various species and chemical reactions is required describe with a high accuracy the auto-ignition and combustion of natural gas in HCCI engines. The complexity of the detailed mechanisms of natural gas oxidation is one of their characteristics which includes hundreds of species and thousands of reactions [16-17]. Thus, reduced and skeletal oxidation mechanisms of different fuels have been developed for the usage in computational modeling which needs less cumbersome calculations.

To describe the natural gas oxidation chemistry, in the present work, the GRI-mech 3.0 [18] chemical kinetic mechanism was used. It includes 51 species (H2, H, O, O2, OH, H2O, HO2, H2O2, CH, CH2, CH2(S), CH3, CH4, CO, CO2, HCO, CH2O, CH2OH, CH3O, CH3OH, C2H, C2H2, C2H3, C2H4, C2H5, C2H6, HCCO, CH2CO, HCCOH, N, NH, NH2, NH3, NNH, NO,

NO2, N2O, HNO, CN, HCN, H2CN, HCNN, HCNO, HOCN, HNCO, NCO, N2, AR, C3H7, C3H8, CH2CHO, and CH3CHO) and 309 chemical reactions.

In the combustion of fuels that contain no nitrogen such as natural gas, Nitric Oxide is formed by four chemical mechanisms that involve nitrogen from the air, i.e., the Zeldovich mechanism (or thermal mechanism), the Fenimore mechanism (or prompt mechanism), the N2O-intermediate mechanism, and the NNH mechanism. The Zeldovich mechanism dominates in high-temperature combustion over a fairly wide range of equivalence ratios, whereas the prompt mechanism is particularly important in rich combustion [19]. In the present work, the detailed nitrogen chemistry involved in the combustion of natural gas was considered to evaluate the emission of NO and other N-containing species.

4. Governing Equations

To look for the evolution of species within the combustion chamber, conservation of species is employed which is the result of chemical reactions. The rate of change of the mass fraction of species i is given by below equation [20]

$$\frac{dY_i}{dt} + \frac{\left(Y_i - Y_{i_{in}}\right)}{\overline{\rho} V} = \dot{\omega}_i \tag{1}$$

where Yi is the inlet mass fraction and ωi is the mass reaction rate of the species i.

The instantaneous cylinder volume at any crank angle is calculated by below equation [21]:

$$V = V_c\left[1 + \frac{R_c - 1}{2}\left(R + 1 - \cos\theta - \sqrt{R^2 - \sin^2\theta}\right)\right] \tag{2}$$

where V is for instantaneous volume, Vc is the clearance volume, R is the ratio of connecting rod length to crank radius and Rc is the compression ratio.

Rate of change of cylinder volume was calculated as follows:

$$\frac{dV}{d\theta} = V_c\left[\frac{R_c - 1}{2}(\sin\theta)\left(\frac{1 + \cos\theta}{\sqrt{R^2 - \sin^2\theta}}\right)\right] \tag{3}$$

In the present study, Woschni correlation [22] was chosen to model the heat transfer from cylinder walls. Heat release rate was calculated by considering the cylinder pressure and volume as well as heat transfer rate of the engines, which is expressed as follows:

(4)

$$\frac{dQ}{d\theta} = \frac{\gamma}{\gamma - 1} p \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dp}{d\theta} + \frac{dQ_h}{dt}$$

where, dQ is the heat release dependent on the variation of crank angle dθ and ϒ is the ratio of specific heat values.

Indicated mean effective pressure was calculated by the following equation:

(5)

$$imep = \frac{W_{net}}{V_d}$$

Where Vd is the cylinder swept volume and W_{net} is the net work done which can be calculated by considering pressure and change of volume as mentioned above.

5. Results and Discussion

The following equations show the important reaction during the combustion of natural gas and air mixture combustion in a single cylinder HCCI engine. These reactions are extracted in the middle of combustion while some of elementary species were consumed and still there are other intermediate species that can be seen in the chain reactions. As you can see, OH and CH3 are among the important radicals in the chain reactions.

```
2OH(+M)<=>H2O2(+M)
OH+CH4<=>CH3+H2O
HO2+CH3<=>OH+CH3O
OH+CH2O<=>HCO+H2O
OH+C2H6<=>C2H5+H2O
OH+C2H4<=>C2H3+H2O
OH+H2O2<=>HO2+H2O
HO2+CO<=>OH+CO2
OH+CO<=>H+CO2
H+O2<=>O+OH
OH+C3H8<=>C3H7+H2O
H+HO2<=>2OH
O+CH4<=>OH+CH3
O+CH2O<=>OH+HCO
OH+H2<=>H+H2O
OH+CH3<=>CH2(S)+H2O
O2+CH2CHO=>OH+2HCO
OH+CH3(+M)<=>CH3OH(+M)
CH3+O2<=>OH+CH2O
OH+HO2<=>O2+H2O
O2+CH2CHO=>OH+CO+CH2O
HCCO+O2<=>OH+2CO
OH+CH2CO<=>HCCO+H2O
OH+CH3OH<=>CH2OH+H2O
HO2+C3H7=>OH+C2H5+CH2O
O+C2H6<=>OH+C2H5
OH+CH3OH<=>CH3O+H2O
```

Figure 1 shows the variation of combustion phasing at different intake temperatures in the natural gas fueled HCCI combustion engine. As it is shown, with increasing the intake temperature from 437 K to 477 K, Combustion phasing advanced from expansion stroke to the compression stroke. It is worth to mention that CA50 is corresponded to the crank angle which 50 percent of fuel is burned. In other words, CA50 is corresponded to the 50 percent fuel mass fraction. If combustion phasing occurs at compression stroke, a vast amount of produced energy due to combustion will be wasted by the compression of hot gas during the compression stroke. Therefore, as expected, advancing combustion phasing from expansion stroke to the compression stroke should lead to reduction of thermal efficiency. The reduction of thermal efficiency was shown in figure 2.

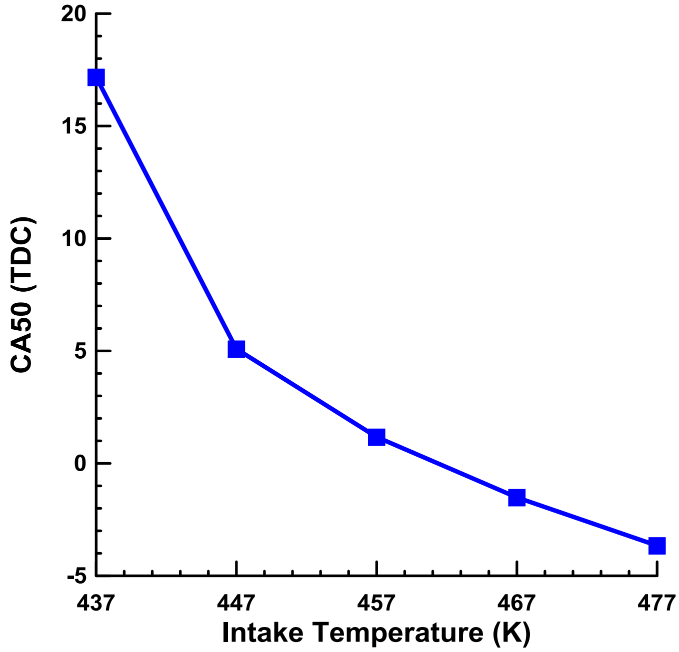

Figure 1. Combustion phasing at different intake temperatures

Figure 2 shows the variation of fuel conversion efficiency at different intake temperatures in the natural gas fueled HCCI combustion engine. It is evident that with increasing the intake temperature from 437 K to 477 K, the fuel conversion efficiency reduced from more than 45 percent to less than 39 percent. As it was mentioned before, change of combustion phasing from expansion stroke to the compression stroke with increasing the intake temperature is the main reason for reduction of fuel conversion efficiency.

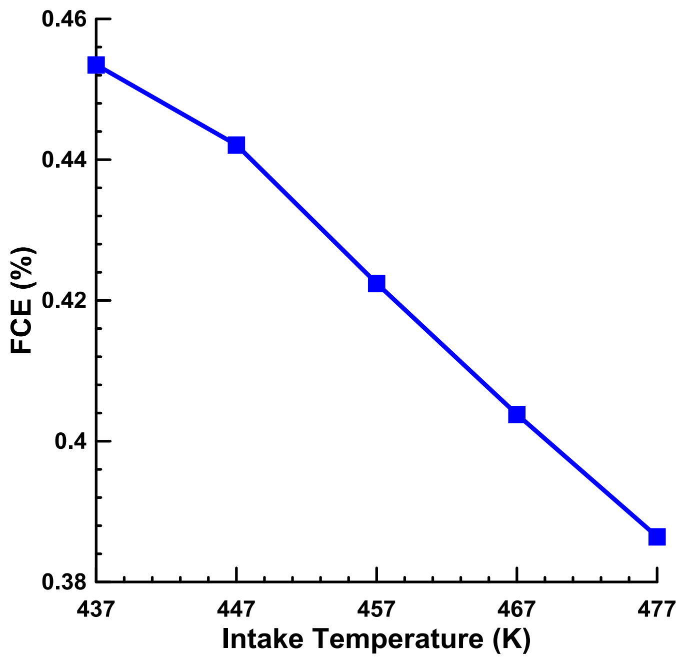

Figure 2. Fuel conversion efficiency at different intake temperatures

Figure 3 shows the variation of indicated mean effective pressure (IMEP) at different intake temperatures in the natural gas fueled HCCI combustion engine. Since the amount of fuel was constant at different intake temperature, it is obvious that with increasing the intake temperature, IMEP should be reduced. Because based on definition of IMEP, it is related to the amount of output work from the engine as well as the displacement volume. Since the displacement volume is constant, IMEP has a direct relation with output work from the engine. Since at higher intake temperatures, combustion phasing occurs at compression stroke, some portion of produced work due to combustion was wasted by compression of gases with piston. Thus, the work output was reduced with increasing the intake temperature from 437 K to 477 K and in the same trend IMEP reduced uniformly.

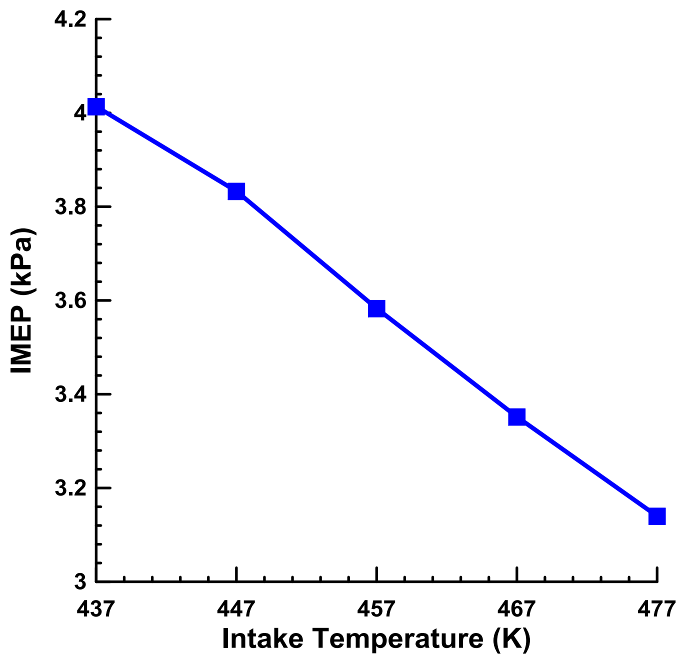

Figure 3. IMEP variation at different intake temperatures

Figure 3 shows the variation of power output at different intake temperatures in the natural gas fueled HCCI combustion engine. As you can see, the trend of power, IMEP are similar which with increasin the intake temperature, power reduced monotonically. Also, the reson is similar to IMEP which is change of combustion phasing from expansion stroke to the compression stroke.

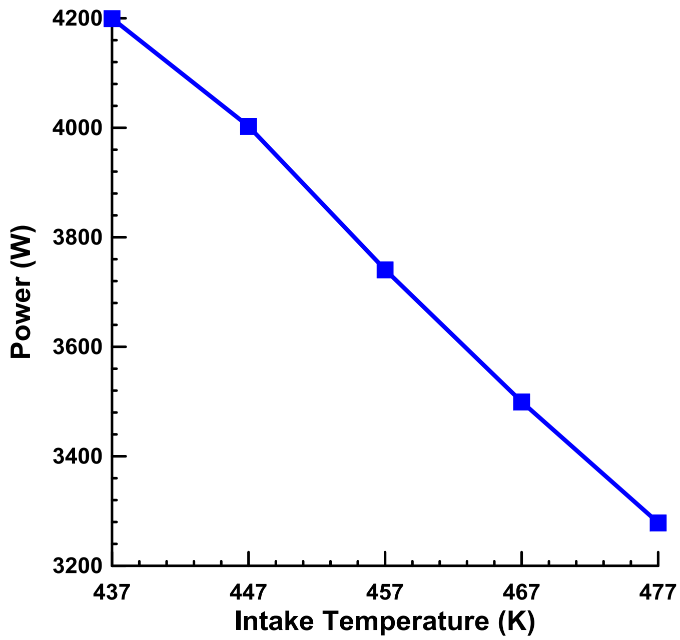

Figure 4. Power output at different intake temperatures

In the following figures, the exhaust characteristics of natural gas fueled HCCI combustion engine simulation are provided. They are the emissions and thermodynamic properties of gases at the exhaust valve opening (EVO). These results are important for design of after treatment and waste heat recovery systems. Figure 5 shows the variation of CO production rate at different intake temperatures in the natural gas fueled HCCI combustion engine. It is evident that with increasing the intake temperature from 437 K to 477 K, CO production rate decreased, especially after 347 K. It shows that the combustion inside the chamber is closer to a complete combustion.

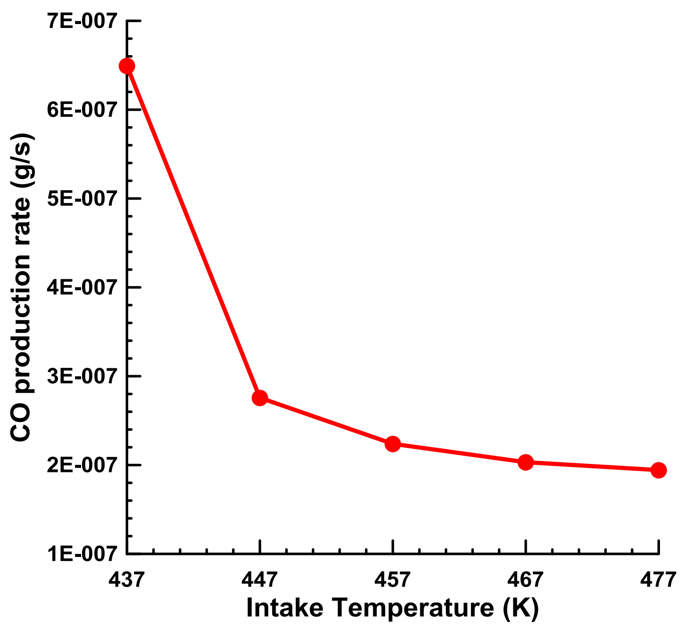

Figure 5. CO production rate at different intake temperatures

Figure 6 shows the variation of NO production at different intake temperatures in the natural gas fueled HCCI combustion engine. It is shown that with increasing the intake temperature from 437 K to 477 K, the amount of NOx production increased uniformly. In the other words, with increasing the intake temperature from 437 K to 477 K, the maximum cylinder temperature increased monotically which led to increase of NOx.

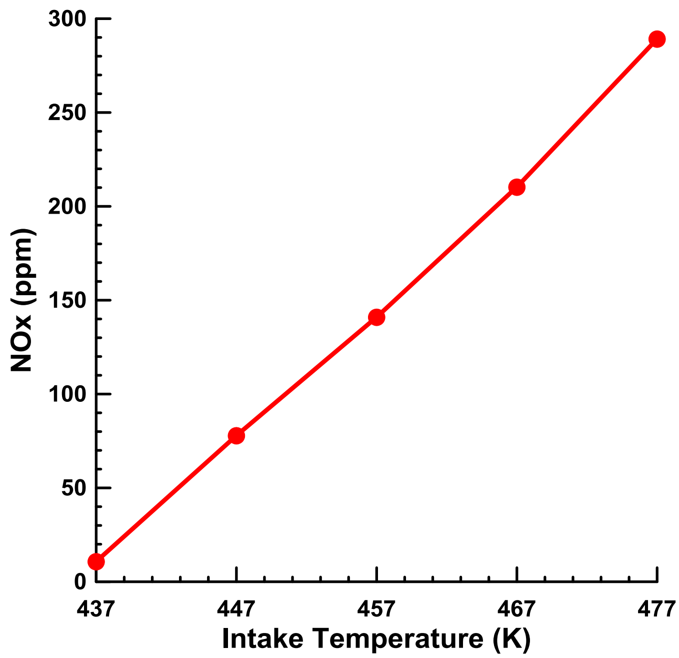

Figure 6. NOx production at different intake temperatures

Figure 7 shows the variation of exhaust pressure at different intake temperatures in the natural gas fueled HCCI combustion engine. This figure shows that with increasing the intake temperature, the exhasut pressure reduced uniformly for higher intake temperature. Therefore, for a direct wast energy recovery system which extracts the exhasut pressure, its is better that the engine runs at lower intake temperature.

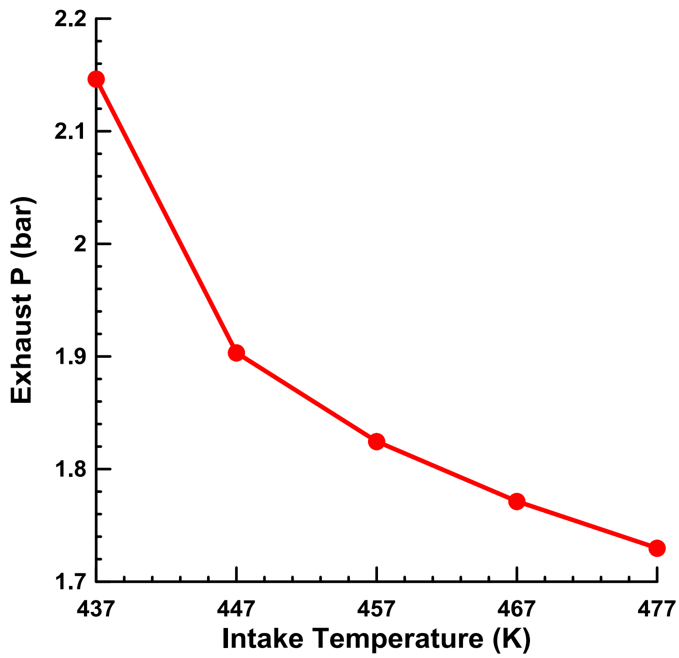

Figure 7. Exhaust pressure at different intake temperatures

Figure 8 shows the variation of exhaust temperature at different intake temperatures in the natural gas fueled HCCI combustion engine. It is evident that with increasing the intake temperature, the exhasut temperature was reduced. It might be due to misadjustment of combustion phasing at higher intake temperature which waste a lot of energy and finally the exhasut temperature will be colder than lower intake temperatures. Therefore, if a oraganic rankine cycle is going to be used as the waste energy recovery system, it is better than the engine run at lower intake temperatures.

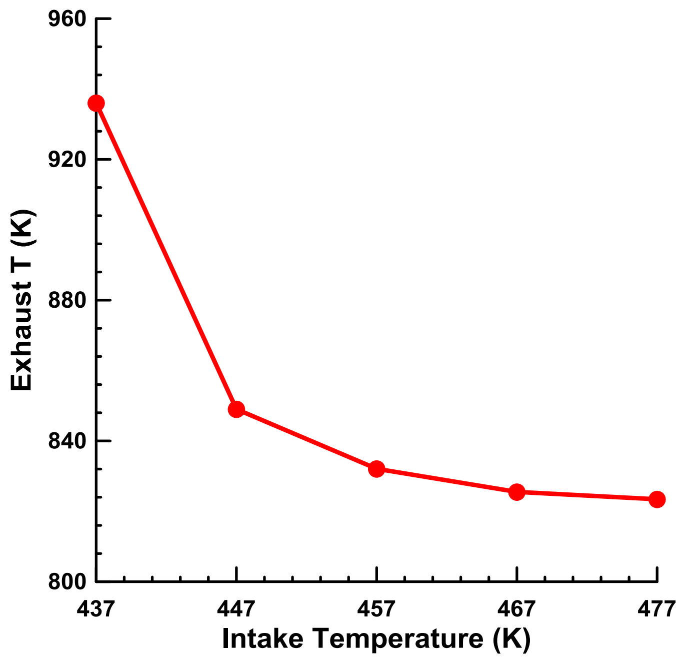

Figure 8. Exhaust temperature at different intake temperatures

Conclusions

In this study, a natural gas fueled HCCI engine is considered to study the effect of intake manifold temperature on combustion phenomena as well as exhaust characteristics such as thermodynamic properties and emissions. In this regard, the intake manifold temperature was swept from 437 K to 477 K and the engine output parameters were studied.

It is found that OH and CH3 are among the important radicals in the chain reactions. Also, with increasing the intake temperature from 437 K to 477 K, Combustion phasing advanced from expansion stroke to the compression stroke. It led to reduction of output power and IMEP from the engine at higher intake temperatures. Therefore, Since the amount of fuel was constant at different intake temperature, FCE reduced at higher intake temperatures.

Regarding to the engine exhaust characteristics, it is found that with increasing the intake temperature from 437 K to 477 K, CO production rate decreased significantly, especially after 347 K. On the other hand, the amount of NOx production increased uniformly, at higher intake temperatures. Furthurmore, with increasing the intake temperature from 437 K to 477 K, the exhasut pressure reduced uniformly for higher intake temperature and the exhasut temperature was reduced monotonically.

References

[1] Ji, Changwei, and Shuofeng Wang. "Experimental study on combustion and emissions performance of a hybrid hydrogen–gasoline engine at lean burn limits." International journal of hydrogen energy 35, no. 3 (2010): 1453-1462.

[2] Chen, Rong-Horng, Li-Bin Chiang, Ming-Hsun Wu, and Ta-Hui Lin. "Gasoline displacement and NOx reduction in an SI engine by aqueous alcohol injection." Fuel 89, no. 3 (2010): 604-610.

[3] Rousseau, S., Bernard Lemoult, and Mohand Tazerout. "Combustion characterization of natural gas in a lean burn spark-ignition engine." Proceedings of the Institution of Mechanical Engineers, Part D: Journal of Automobile Engineering 213, no. 5 (1999): 481-489.

[4] Splitter, Derek, Reed Hanson, Sage Kokjohn, and Rolf D. Reitz. Reactivity controlled compression ignition (RCCI) heavy-duty engine operation at mid-and high-loads with conventional and alternative fuels. No. 2011-01-0363. SAE Technical Paper, 2011.

[5] Li, Yaopeng, Ming Jia, Yaodong Liu, and Maozhao Xie. "Numerical study on the combustion and emission characteristics of a methanol/diesel reactivity controlled compression ignition (RCCI) engine." Applied energy 106 (2013): 184-197.

[6] Li, Yaopeng, Ming Jia, Yachao Chang, Yaodong Liu, Maozhao Xie, Tianyou Wang, and Lei Zhou. "Parametric study and optimization of a RCCI (reactivity controlled compression ignition) engine fueled with methanol and diesel." Energy 65 (2014): 319-332.

[7] Maurya, Rakesh Kumar, and Avinash Kumar Agarwal. "Statistical analysis of the cyclic variations of heat release parameters in HCCI combustion of methanol and gasoline." Applied Energy 89, no. 1 (2012): 228-236.

[8] Flowers, Daniel L., Salvador M. Aceves, Joel Martinez-Frias, and Robert W. Dibble. "Prediction of carbon monoxide and hydrocarbon emissions in iso-octane HCCI engine combustion using multizone simulations." Proceedings of the Combustion Institute 29, no. 1 (2002): 687-694.

[9] Olsson, Jan-Ola, Per Tunestål, Jonas Ulfvik, and Bengt Johansson. The effect of cooled EGR on emissions and performance of a turbocharged HCCI engine. No. 2003-01-0743. SAE Technical paper, 2003.

[10] Bessonette, P. W., Schleyer, C. H., Duffy, K. P., Hardy, W. L., & Liechty, M. P. “Effects of fuel property changes on heavy-duty HCCI combustion.” No. 2007-01-0191. SAE Technical Paper, 2007.

[11] Shi, Lei, Yi Cui, Kangyao Deng, Haiyong Peng, and Yuanyuan Chen. "Study of low emission homogeneous charge compression ignition (HCCI) engine using combined internal and external exhaust gas recirculation (EGR)." Energy 31, no. 14 (2006): 2665-2676.

[12] Vuilleumier, D., Kozarac, D., Mehl, M., Saxena, S., Pitz, W. J., Dibble, R. W., ... & Sarathy, S. M. "Intermediate temperature heat release in an HCCI engine fueled by ethanol/n-heptane mixtures: An experimental and modeling study." Combustion and flame 161, no. 3 (2014): 680-695.

[13] Wang, E. H., H. G. Zhang, B. Y. Fan, M. G. Ouyang, Y. Zhao, and Q. H. Mu. "Study of working fluid selection of organic Rankine cycle (ORC) for engine waste heat recovery." Energy 36, no. 5 (2011): 3406-3418.

[14] Arias, Diego A., Timothy A. Shedd, and Ryan K. Jester. Theoretical analysis of waste heat recovery from an internal combustion engine in a hybrid vehicle. No. 2006-01-1605. SAE Technical Paper, 2006.

[15] Mahabadipour, Hamidreza, Kalyan Kumar Srinivasan, Sundar Rajan Krishnan, and Swami Nathan Subramanian. "Crank angle-resolved exergy analysis of exhaust flows in a diesel engine from the perspective of exhaust waste energy recovery." APPLIED ENERGY- 216, no. 1 (2018): 31-44.

[16] Chaos, Marcos, Andrei Kazakov, Zhenwei Zhao, and Frederick L. Dryer. "A high-temperature chemical kinetic model for primary reference fuels." International Journal of Chemical Kinetics 39, no. 7 (2007): 399-414.

[17] Mehl, Marco, William J. Pitz, Charles K. Westbrook, and Henry J. Curran. "Kinetic modeling of gasoline surrogate components and mixtures under engine conditions." Proceedings of the Combustion Institute 33, no. 1 (2011): 193-200.

[18] Smith, G. P., Golden, D. M., Frenklach, M., Moriarty, N. W., Eiteneer, B., Goldenberg, M., ... & Lissianski, V. V. (2011). GRI-Mech 3.0, 1999. URL http://www. me. berkeley. edu/gri_mech.

[19] Turns, Stephen R. An introduction to combustion. Vol. 499. New York: McGraw-hill, 1996.

[20] K.K. Kuo, Principles of combustion, 1986.

[21] Heywood, John B. "Internal combustion engine fundamentals." (1988).

[22] Woschni G. A universally applicable equation for the instantaneous heat transfer coefficient in the internal combustion engine. No. 670931. SAE Technical paper; 1967.