

## **EFFECTS OF INTERNAL FUEL REFORMING AND INITIAL TEMPERATURE ON HCCI COMBUSTION OF LEAN ETHANOL/AIR MIXTURES - A COMPUTATIONAL STUDY**

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### **Abstract**

*Homogeneous charge compression ignition (HCCI) engine has great potential to operate with high efficiency, ultra-low NO<sub>x</sub> emissions and low particulate matter. The major disadvantages of HCCI engine are the low power output and inherent absence of combustion on-set control. We investigated the expansion of the HCCI operating range and combustion control by use of internal fuel reforming. The study is focused on multi-step simulation of the engine cycle, comprised of fuel reformation cycle and HCCI combustion cycle. In the fuel reformation cycle the valve timing was manipulated to create a negative valve overlap during which a fraction of fuel undergoes a reformation process. The reformate gas, composed mainly of hydrogen, carbon monoxide and other products of incomplete combustion, is then mixed with remainder of fuel/ air mixture and enters the HCCI combustion cycle. The study is carried out using a single-zone well-stirred reactor model and established reaction mechanisms. The HCCI engine cycle is fueled with lean mixtures of air and ethanol. This study demonstrated that the fuel internal reforming does extend the operational range of HCCI engine into partial load region and is effective in the combustion on-set control. The model requires however, several enhancements in order to moderate the cycle pressure rise and pressure magnitude, lower cycle temperatures and NO emissions.*

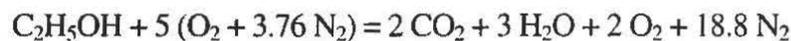
### **1. Introduction**

The homogenous charge compression ignition (HCCI) engine combines a use of premixed air/fuel mixture, which is usually associated with spark ignition (SI) engine, with that mixture self-ignition induced by high compression ratio, which is usually encountered in compression ignition (CI) engine. There are numerous consequences of such an organization of the engine combustion process. To prevent an onset of engine knock the air/fuel mixtures need to be lean or even ultra-lean. With concurrent benefits of increased thermal efficiency, lower cycle temperatures and reduced NO<sub>x</sub> emissions the HCCI combustion is well suited for engine partial load operation. At the same time the requirement to run on very lean mixtures limits the HCCI operational range to partial loads only [11]. The HCCI combustion lacks means of combustion onset and subsequent pressure rise control, since both the spark ignition timing (SI engine) and the injection timing (CI engine) are absent from the engine operation. The HCCI engines and various strategies of HCCI combustion control, which include use of recycled exhaust gas (EGR), preheating of combustion air, and steam injection, are discussed in a recent comprehensive review compiled by Zhao et al [15]. The two approaches of fuel/air enrichment with products of external fuel reforming and EGR were examined with use of numerical simulation by Ng and Thomson [6]. The strategy of HCCI combustion control by means of internal fuel reformation is examined in this study with use of the same ChemkinCollection [4] simulation tools as in [6].

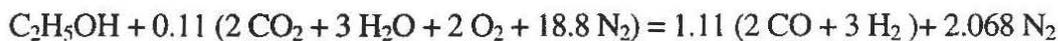
## 2. Methodology

The model used in this study is comprised of a single zone well-stirred reactor that undergoes compression and expansion processes. Studies by Aceves et al [1] and Callhan et al [2] showed that the single zone stirred reactor predictions of NO<sub>x</sub> agreed well with experimental results. In contrast, a study by Sobiesiak et al [8] showed that the well-stirred reactor coupled with Zeldovich NO<sub>x</sub> mechanism failed to accurately predict the measured levels of NO<sub>x</sub> in low temperature reactions zones that were highly diluted with recycled products of combustion. The fuel modeled in our study is ethanol, which is a bio-fuel and has the advantage of lower carbon dioxide emissions per unit of energy released than gasoline. The simulation procedure of a HCCI engine with internal reforming consists of three major steps. Each step is a simulation of the engine cycle that includes compression and expansion strokes only. The simulation is set up as variable volume, single zone well-stirred reactor with convective heat losses.

**Step 1:** The first step is the calculation of the HCCI combustion with lean fuel/air mixture. The ideal balance equations representing the lean combustion, reforming, and fully reformed fuel combustion of ethanol at the equivalence ratio  $\Phi = 0.6$  may be written as:

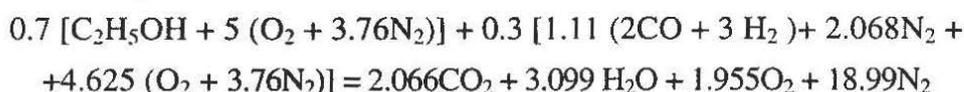


**Step 2:** The combustion products from the first step are used in this step, which involves the calculation of the reforming process. In this cyclic process, the compression ratio is reduced to simulate the early exhaust valve closing and recompression of the retained products of combustion from the preceding cycle and fraction of fuel.

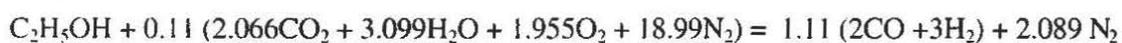


In the above ideal reforming reaction, all hydrogen is converted into H<sub>2</sub>, all carbon into CO, and no molecular oxygen is left. According to the above equation, the H<sub>2</sub> yield is 43%, with a clear indication that in order to achieve the high degree of conversion the volume fraction of retained products of combustion should not be more than 11%. If more of the products of combustion are retained, the H<sub>2</sub> yield will be lower since the paths for hydrogen oxidation will open due to higher oxygen concentrations. Concurrently, it is feasible that under those conditions some of the CO will oxidize into CO<sub>2</sub>.

**Step 3:** In this step, the reformat gas produced in the step 2 is mixed with a fresh lean fuel/air mixture. That new mixture now constitutes a charge for the first HCCI cycle with products of reforming.



It should be noted that the products of combustion from step 3 does not differ much from the products of combustion from step 2. Hence, the need to repeat the reformation step 2 more than once in our procedure with the composition of recycled products of combustion from step 3 is not required (Since there is no major difference between the products of combustion in the two steps). With step 3 combustion products, the reformation of all the fuel will proceed according to this equation:



Furthermore, comparison of the coefficients in the above equation with those in step 2 also indicates that there is little difference between the percentage of the recycled products of combustion and the hydrogen yield as well. The engine parameters and the test conditions for the numerical simulation are discussed in the next section.

### 3. Test conditions

The engine parameters used in the full cycle simulations are as follows: compression ratio,  $r_v = 1:15$ , displacement volume  $V_d = 587.62 \text{ cm}^3$ , cylinder bore diameter  $D = 93 \text{ mm}$ , stroke  $S = 86.5 \text{ mm}$ , and fixed speed of 1000 RPM. It should be noted, the study is focused on the demonstration of the feasibility of internal reforming simulation and the capturing of trends in the onset of combustion and  $\text{NO}_x$  formation without strict adherence to HCCI acceptable operating range.

Lean mixtures of fuel and air at two equivalence ratios of  $\Phi = 0.6$  and  $0.4$  are examined in this study. The portion of the fuel used in the reformation cycle is zero or 30% by mass for each equivalence ratio. All simulations are started at 1 atmosphere but with varying initial temperatures ranging from 410 K to 490 K for both the initial HCCI cycle and the final HCCI cycle with reformat products. The initial temperature of the mixture entering the reforming cycle is calculated under the assumption that the exhaust gas from the preceding HCCI cycle has expanded isentropically to ambient pressure at the end of the expansion process. The duration of the reforming cycle is varied from  $72^\circ$  crank angle (CA) before top dead centre (bTDC) to  $152^\circ$  CA bTDC in  $20^\circ$  intervals, which corresponds to  $327^\circ$  bTDC to  $287^\circ$  bTDC start angle of the reformation compression process. It should be realized that these variations in the start of reformation cycle corresponds to mean variability in the reformation cycle compression ratio and temperatures during reformation process, which in turn affects the composition of the reformation products.

The explicit addition of recycled exhaust gas (EGR) to complement internal fuel reforming was not simulated in this study. It should be noted however, that in our approach the retained in-cylinder products of combustion could be viewed as a form of EGR. The ethanol reaction mechanism and thermodynamic properties data are taken from the well-validated mechanism of Marinov et al [5] and  $\text{NO}_x$  mechanism of University of California, San Diego [3].

### 4. Results and discussion

The discussion of the results is focused on the hydrogen conversion efficiency at varying initial conditions for the reforming cycle, the engine performance with internal reforming in terms of the gross indicated mean effective pressure, the maximum cycle pressure and temperature, the specific fuel consumption, and the  $\text{NO}_x$  and CO emissions.

**Internal Reformation Products:** The  $\text{H}_2$  yield results for equivalence ratio  $\Phi = 0.6$  and  $0.4$  are shown in Figure 1. The  $\text{H}_2$  mole fractions depend on both the initial temperature of the lean charge in the preceding HCCI combustion cycle and the duration of the reforming cycle. The  $\text{H}_2$  yields are higher for the richer mixture over the entire range of the initial temperatures and the durations of the reforming process. In fact, there is almost no  $\text{H}_2$  produced for the two longest,  $152^\circ$  and  $132^\circ$  CA, and the shortest,  $72^\circ$  CA, durations of the reforming cycle when products of combustion of the leaner mixture at  $\Phi = 0.4$  is used. Figure 1 also shows that for  $\Phi = 0.4$  the reforming cycle of  $72^\circ$  CA duration does not produce any  $\text{H}_2$  until the HCCI cycle charge temperature was at 490 K. These trends indicate that optimal conditions for maximum  $\text{H}_2$  yield would involve a medium duration of reforming cycle and high initial temperature of the charge entering the preceding HCCI cycle.

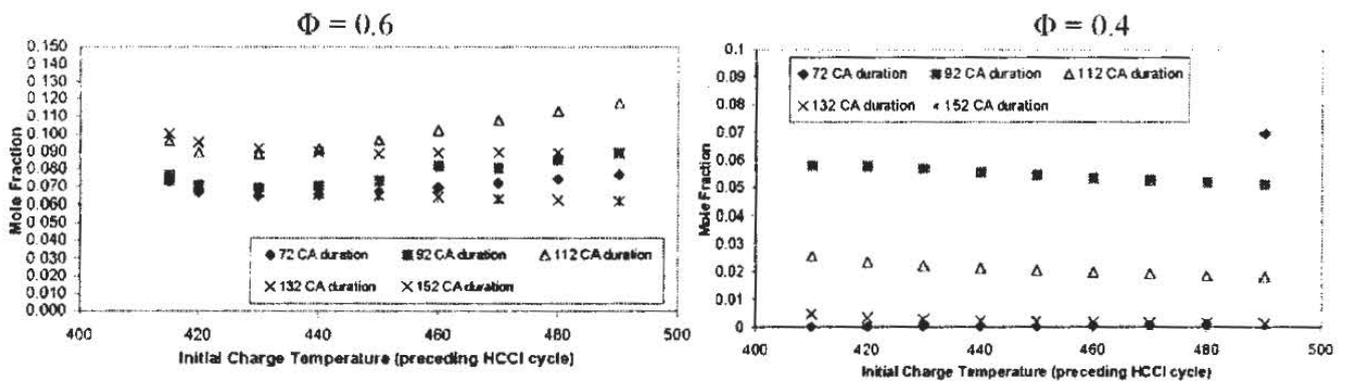


Fig. 1. Hydrogen yield from reforming cycle that used retained products of combustion of HCCI cycle without fuel reformation and lean fuel /air mixture.

For  $\Phi = 0.6$  (Fig. 1), the  $H_2$  yield dependence of the equivalence ratio reflects an impact of higher temperature of the retained products of combustion of the richer mixture and their lower oxygen content. The  $H_2$  yield first decreases and then increases when the initial temperature of the charge entering HCCI cycle is varied and this effect is modified by the reforming cycle duration. The very long and very short reforming cycles yield less hydrogen and are more affected by the HCCI cycle charge temperature. The duration of the reforming cycle should be decreased even more if engine is to be run on very lean mixtures. These conclusions are further supported by the results shown in Fig. 2.

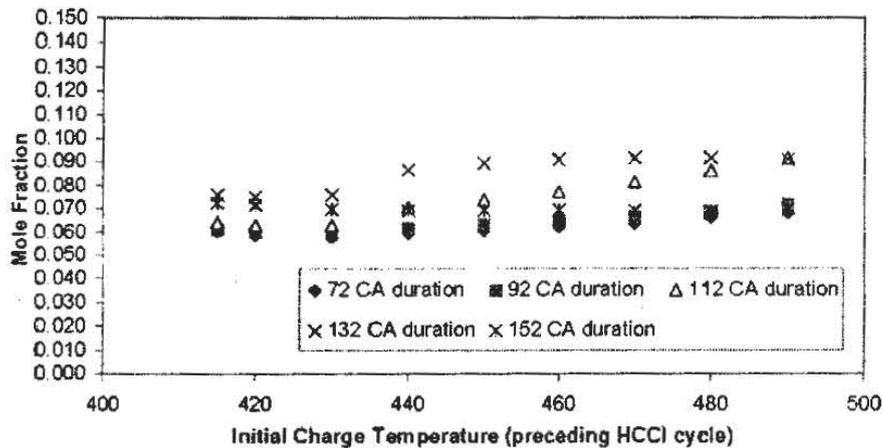


Fig. 2. Hydrogen yield from reforming cycle that used retained products of combustion of HCCI cycle with 30 % fuel reformation and lean fuel/air mixture at  $\Phi = 0.6$ .

Fig. 2 illustrates the  $H_2$  yield from the reforming cycle that used 30 % of fuel of lean fuel/air mixture at equivalence ratio  $\Phi = 0.6$  and retained products of combustion for the preceding HCCI cycle with fuel reformation in the loop. The lower  $H_2$  yields in comparison with Fig. 1 can be explained by the lower temperature of the products of combustion for the HCCI cycle that used only 70% of fresh charge with remaining 30% being reformat gas.

**Engine Cycle Pressure and Temperature:** In-cylinder pressure and temperature versus cycle time for the lowest initial temperature of charge entering the HCCI cycle and mixture equivalence ratio  $\Phi = 0.4$  are shown in Figure 3.

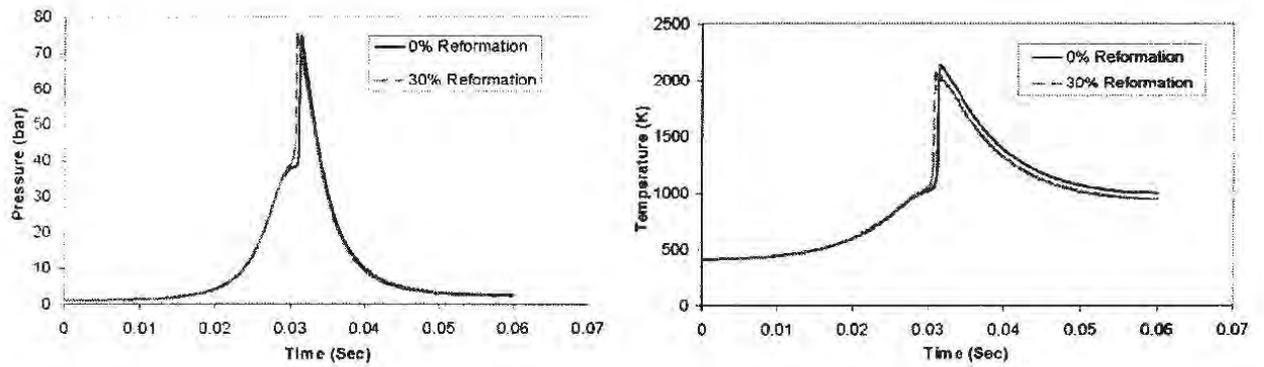


Fig. 3. In-cylinder pressure and temperature changes in HCCI cycle with and without fuel reformation. Mixture equivalence ratio  $\Phi = 0.4$  and initial temperature 410 K.

The curve with somewhat lower pressure peak (solid line) is for the HCCI cycle without fuel reformation and the second with higher-pressure peak (dashed line) is for the HCCI cycle that included 30% fuel reformation. The ignition point occurs short time after top dead center (TDC is at  $t = 0.03$  sec) in both cases and the subsequent combustion process is almost instantaneous with very steep pressure rise. It is important to notice that the ignition event moves towards TDC when fuel reforming is used. The similar shift of the combustion on-set is evident in the temperature trace shown in Fig. 3. The data show that the peak temperature is lower for the HCCI cycle with fuel reformation. It should be said that the predicted pressures and temperatures, and their fast rate of rise after ignition are too excessive and need to be moderated. However, the results for the case with fuel reformation indicate that internal reforming provides means of the combustion on-set control and torque optimization.

**Engine Performance:** In Figure 4 predicted performance in terms IMEP and ISFC is depicted for the entire range of the initial charge temperatures. The results show that fuel reformation decreases IMEP, which is expected due to less charge entering the cyclic process. There is also an optimal charge temperature for which the IMEP is maximized. With fuel reformation that temperature shifts towards lower initial charge temperatures. The interesting outcome is that ISFC decreases for lower initial charge temperatures when fuel reformation is used. This result indicates broadening of the engine operational range into partial loads with the benefit of minimizing specific fuel consumption for lower initial charge temperatures. The similar trend was reported in experimental investigation of internal reforming by Urushihara [12].

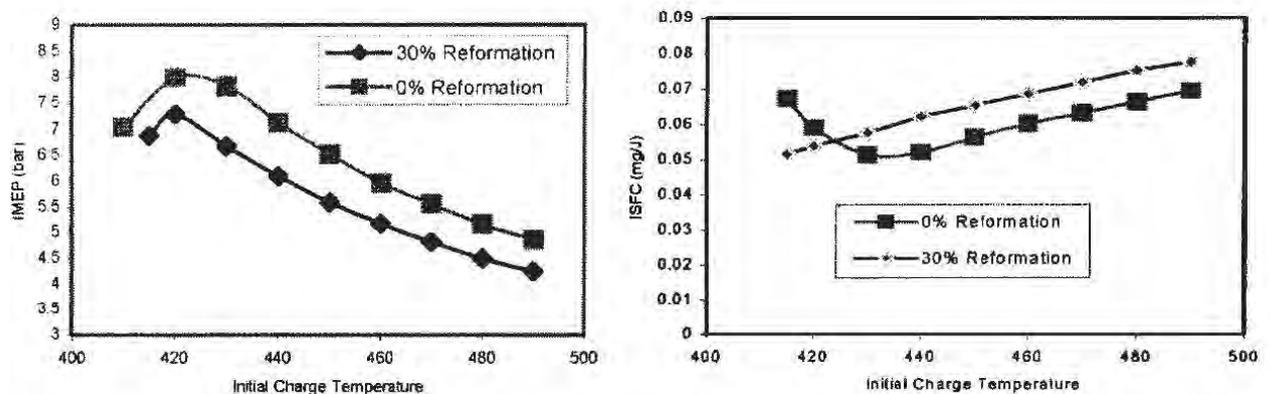


Fig. 4. Indicated mean effective pressure (IMEP) and Indicated specific fuel consumption (ISFC) changes with initial charge temperature for HCCI cycle with and without fuel reformation. Mixture equivalence ratio  $\Phi = 0.4$

**Engine-out NO and CO Emissions:** The calculated engine-out CO and NO emissions for HCCI cycle with and without reformation at equivalence ratio  $\Phi = 0.4$  are shown in Figure 5. The CO emissions are practically negligible over the entire range of the initial charge temperatures. However, for the case without fuel reformation the predicted NO are below 1000 ppm level only if the initial temperatures do not exceed 430 K.

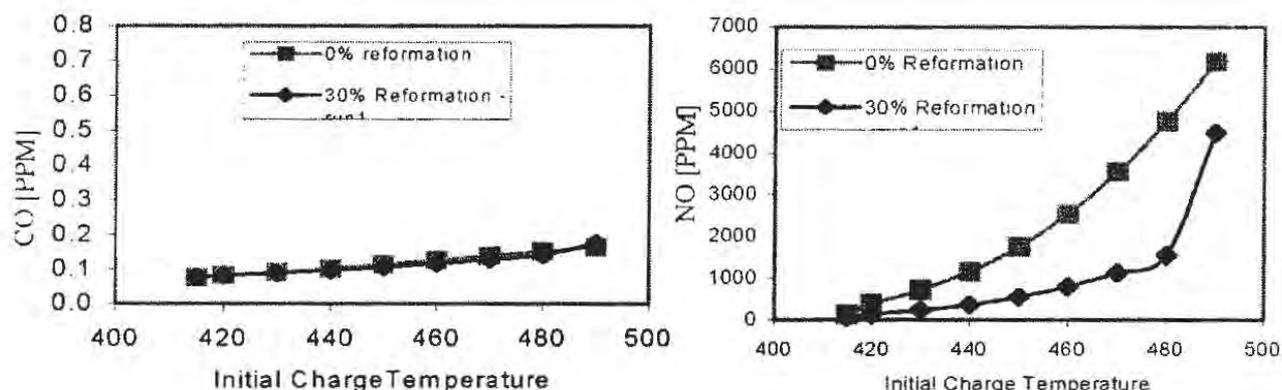


Fig. 5. CO & NO emissions from HCCI cycle with and without fuel reformation. Mixture equivalence ratio  $\Phi = 0.4$ .

The internal fuel reformation extends that range of the initial charge temperatures for which predicted NO is below 1000 ppm level to about 460 K. The discussion of the optimal conditions for high yield of  $H_2$  suggested that higher than 460 K initial charge temperature might be needed. This requirement is in conflict with the high NO emissions at these temperature levels and points towards the need for combustion related means of NO reduction. The elevated NO levels in the simulation are the result of the high cycle temperatures and early occurrence of these temperatures in the cycle.

Furthermore, study was carried out with other NO mechanisms, such as GRI 3.0 NO mechanism, to check whether the NO mechanism used in this study is indeed suitable for this application. Figure 6 shows the NO levels obtained from the NO<sub>x</sub> mechanism of University of California, San Diego and the GRI 3.0 NO<sub>x</sub> Mechanism.

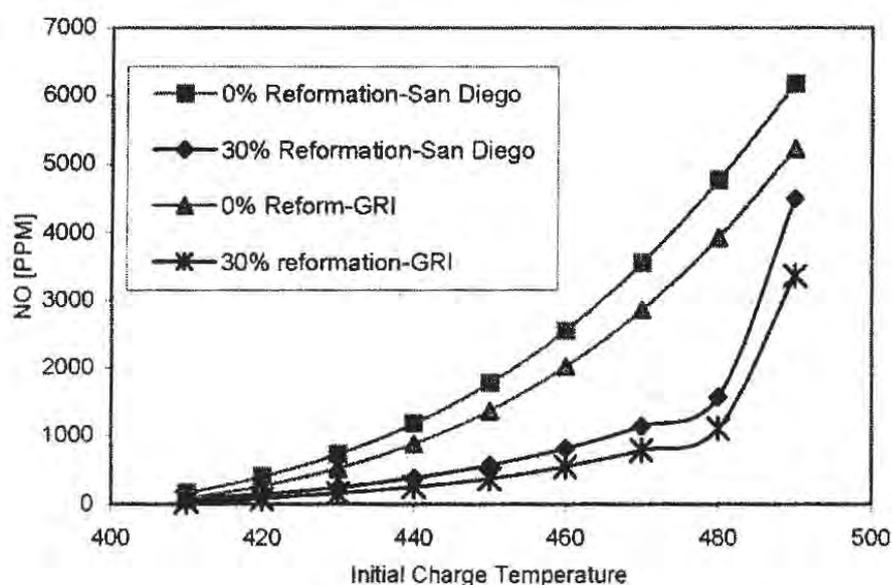


Fig. 6. NO emissions from San Diego and GRI 3.0 mechanism for HCCI cycle with and without fuel reformation. Mixture equivalence ratio  $\Phi = 0.4$ .

From Figure 6 it can be noted that the mechanisms used for simulation does have an impact on the levels of NO predicted, with the GRI 3.0 mechanism predicting NO levels about 1000 ppm less than the San Diego mechanism at elevated temperatures. The reasons for this variation in NO levels associated with the change in mechanism used are not clear and have yet to be studied in detail. Follow-up study will look into the chemical reactions used in both the mechanisms and investigate which mechanism is indeed more suitable for the problem considered in our study.

Furthermore, the cycle peak temperatures are over-predicted and this is due to several reasons. The major cause is the insufficient amount of recycled products of combustion. Use of additional amount of recycled products of combustion in the HCCI combustion will reduce the cycle temperature. The follow up study will also investigate this effect. More difficult to simulate is an impact of fuel/air/reformate gas non-homogeneities. In the present model, the assumption is made that the reactants are perfectly mixed. For that reason, once the temperature is right almost an instantaneous reaction is predicted within the entire cylinder volume. In real HCCI combustion, one can expect regions of different composition and temperature in the cylinder volume. That would result in distributed ignition zones and more moderate rates of the subsequent chemical reactions. Capturing of the initial charge non-homogeneities would require formulation of the mixing model of the reformate gas and fresh charge at the end of the reforming cycle. Further improvements could be gained through incorporation of a more realistic exhaust and retention processes of products of combustion at prior to the reforming cycle.

## 5. Conclusion

The following has been demonstrated in this study:

1. The HCCI engine cycle with internal reforming of fuel has been successfully simulated in multi-step calculations of a well-stirred reactor undergoing compression and expansion processes.
2. The fuel internal reforming extends operational range of HCCI engine into partial load region with concurrent reduction of the specific fuel consumption for lower initial charge temperatures.
3. The fuel reformation is an additional/alternative method of the on-set of combustion control in HCCI combustion.
4. The internal fuel reforming and HCCI combustion models used in this study require several enhancements in order to moderate the cycle pressure rise and pressure magnitude, lower cycle temperatures and NO emissions.

## Acknowledgements

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## References

- [1] Aceves, S. M., Smith, J. R., Westbrook, C. and Pitz, W., "Compression Ratio Effect on Methane HCCI Combustion, ASME Internal Combustion Engine 1998 Fall Conference.
- [2] Callahan, C.V., Held, T. J., Dryer, F. L., Minetti, R., Ribaucour, M., Sochet, R., Faravelli, T., Gaffuri, P. and Ranzi, E., "Experimental data and Kinetic Modelling of Primary Reference Fuel Mixtures", Twenty-Sixth Symposium (International) on Combustion/The Combustion Institute, pp.739-746,1996.

- [3] Hewson, J. C. et al, "University of California NOx Mechanism", San Diego, CA, [Online document]. Available at:  
<http://maemail.ucsd.edu/combustion/cermech/NOx/NOXsandiego20020812.pdf>
- [4] Kee, R. J. et al, "Chemkin Collection, release 3.6", Reaction design, Inc, San Diego, CA, 2000.
- [5] Marinow, N. M., " A Detailed Chemical Kinetics Model for High temperature Ethanol Oxidation', Inter. J. of Chem. Kin, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-131657, 1998. Available at:  
<http://www.cms.lhll.gov/combustion/combustion2.html>.
- [6] Ng, C. K. W. and J. Thomson, M. J., "A Computational Study of the Effects of Fuel Reforming, EGR and Initial Temperature on Lean Ethanol HCCI Combustion", SAE Technical Paper 2004-01-0556.
- [7] Smith, G. P. et al "GRI-Mech 3.0", Available at [http://www.me.berkelev.edu/gri\\_mech/](http://www.me.berkelev.edu/gri_mech/).
- [8] Sobiesiak, A., Rahbar,S. and Becker, H. A., "Performance Characteristics of the Novel Low-NOx CGRI Burner for Use with High Air Preheat", *COMBUSTION AND FLAME*, 115; pp.93-125, 1998.
- [9] Sobiesiak, A., Uykur, C., Ting, D. S-K, and Henshaw, P., "Hydrogen/Oxygen Additives Influence on Premixed Iso-Octane /Air Flame", SAE Technical Paper 2002-01-1710.
- [10] Stone, R. S., "An Introduction to Combustion: Concepts and Applications", McGraw Hill, 1996.
- [11] Tabaczynski, R., "Future Powertrain Technologies", 2000 ASME ICE Meeting, Austin, Texas, USA.
- [12] Urushihara, T., Hiraya, K., Kakuhou, A. and Itoh, T., "Expansion of HCCI Operating Region by the Combination of Direct Fuel Injection, Negative Valve Overlap and Internal Fuel Reformation", SAE Technical Paper, 2003-01-0749.
- [13] Wong, Y. K. and Karim, G. A., "An Analytical Examination of the Effects of Hydrogen Addition on Cyclic Variations in Homogenously Charged Compression-Ignition Engines', *Int. J. Hydrogen Energy*, Vol. 25, No. 12 pp.1217-1224, 2000.
- [14] Yamal, Y and Wyszynski, M. L., "On-Board Generation of Hydrogen-Rich Gaseous Fuels - A Review", *Int. J. Hydrogen Energy*, Vol. 19. No. 7, pp.557-572, 1994.
- [15] Zhao, F., Asmus, T. W., Assanis, D. N., Dec, I.E., Eng, J. A., and Najt, P. M., Editors, " Homogenous Charge Compression Ignition (HCCI) Engines; *Key Research and Development Issues*", SAE PT-94.