



Reforming Controlled Homogenous Charge Compression Ignition -Simulation Results

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Abstract

A computer model was built and a theoretical analysis was performed to predict the behavior of a system containing Homogenous charge compression ignition (HCCI) engine and a methanol reformer. The reformer utilizes the waste heat of the exhaust gases to sustain the two subsequent processes: dehydration of methanol to dimethyl ether (DME) and water, and methanol steam reforming (SRM) where methanol and water react to mainly hydrogen, CO and CO₂. Eventually, a gaseous mixture of DME, H₂, CO, CO₂, water (reused) and some other species is created in these processes. This mixture is used for the engine feeding. By adding water to the methanol and fixing the vaporized fuel's temperature, it is possible to manage the kinetics of chemical processes, and thus to control the products' composition. This allows controlling the HCCI combustion. By a magnification of H₂/DME ratio the ignition delay is increased and so it is possible to synchronize the ignition timing and also to control combustion duration. The simulation results prove feasibility of the suggested approach and a possibility of achieving substantially higher energy efficiency together with zero-impact NO_x emissions in a wide range of engine operating modes.

Introduction

Environmental, health, and political circumstances during the last decades have led humanity to search for alternative energy sources, and to make efforts toward raising the efficiency of energy usage and mitigating the emissions of pollutants. Internal combustion engines (ICE) are both a major consumer of energy, mainly by utilizing fossil fuels, and a significant pollution source. Hence, there is a trend to reduce pollutant emissions and fuel consumption of ICEs, as well as a search for renewable non-fossil fuels. Over the last decades, pollutant emissions from vehicles have been reduced by using exhaust after treatment systems. Climate change challenges and more rigorous regulations on emissions of pollutants from motor vehicles have led to the searching of new technologies to raise engine efficiency, to reduce GHG emissions and to mitigate pollutant emissions towards zero-impact levels [1].

About 30% of the energy supplied to ICE with a fuel is wasted along with the exhaust gases. There are several ways to utilize a part of this energy and improve the performance of an engine. The most common way is turbocharging. Another way is by using this energy to promote endothermic reactions of fuel reforming. This method is called thermo-chemical recuperation (TCR) [2]. The idea of TCR is not new and some studies have addressed the 80s - early 90s. Most of them were summarized by Pettersson et al. [3]. Major shortcomings were reported that resulted in substantial reduction of research activities in this field. The main drawbacks that were found are: cold start, transient behavior, backfire, coke formation on the reformer, lower maximal power due to reduced air charging, and pre-ignition [4, 5, 6].

Tartakovsky et al. [7] analyzed the performance of a spark ignition (SI) engine fueled by ethanol steam reforming (SRE) products. The optimal water to ethanol ratio and reaction temperature were found to achieve highest reformer-ICE system efficiency and the lowest CO emission. They reported on a possibility of efficiency increase by 11-16%, CO emission reduction by a factor of 10, and NO_x emission reduction by a factor of 4 compared with a gasoline-fed engine. Tartakovsky et al. [8] made a comparative theoretical analysis of performance of a SI engine fed by reforming products of two different alcohols: ethanol and methanol. Three compositions of the reforming products: SRE, SRM, and products of the low-temperature ethanol reforming were examined. The authors used in their analysis a model of the heat release process that takes into account the influence of fuel composition and air excess factor on fuel burning velocity.

Poran et al. [9] suggested a modeling approach to simulate the joint operation of an ICE with an SRM reformer. Poran & Tartakovsky [10] later expanded this model to a direct-injection ICE with high-pressure thermo-chemical recuperation process. In order to achieve higher gaseous fuel density required for direct injection into the engine cylinders, this method suggests compressing the liquid fuel and then vaporizing it, eventually reforming the vaporized fuel by an SRM process. Compression of liquid fuel requires much less power than the compression of a gaseous fuel. Combustion of the gaseous hydrogen-rich fuel is resulting in very clean combustion reflected by

low pollutants formation [11]. Moreover, direct injection of a gaseous reformat is a useful method to overcome some of the major TCR drawbacks, such as: backfire, pre-ignition, reduced maximal power and lower volumetric efficiency.

HCCI has been proposed both to improve the thermal efficiency and to reduce simultaneously formation of nitrogen oxides (NO_x) and particles, as compared with conventional combustion processes. The HCCI combines combustion of homogenous air-fuel mixture as in SI engines and compression ignition as in a Diesel engine [12, 13, 14]. An HCCI engine follows the Otto cycle, but unlike SI engines is able to work at high compression ratios. This means that its thermodynamic efficiency potential is higher compared with conventional SI engines. An HCCI engine is not limited to the stoichiometric air-fuel ratio and thus can work with leaner mixtures and at lower temperatures than a conventional engine. Using a fuel rich in H_2 allows for even wider flammability limits. According to the Zeldovich mechanism, formation of thermal NO_x occurs at high temperatures. Thus HCCI combustion produces relatively low NO_x levels compared with other combustion processes. Burning homogeneous lean fuel-air mixture ensures simultaneously low particle formation rates.

However there are several challenges that must be overcome in order to make the HCCI engine commercial-ready. The main one is the controllability of the ignition timing [14]. While in an SI engine the ignition timing is determined by the spark appearance, and in a compression ignition (CI) engine it is determined by the injection timing, HCCI is a kinetically-controlled process. Thus, in the HCCI engine the ignition timing depends on thermal and chemical parameters such as thermal cylinder history, equivalence ratio, fuel reactivity, chemical reactions rate, etc. [15]. There are some other challenges in HCCI engine development such as operating range [14], noise, HC and CO emission [16], cold start [14], preparation of a homogenous mixture etc. [17].

Several solutions of main HCCI challenges have been proposed over the years. A large part of these methods is summarized in [14] and in [18]. Some of these methods are designed to improve the mixing rate of air and fuel applying advanced injection strategies [14, 18, 19, 20]. Some of them are designed to control ignition delay using exhaust gas recirculation (EGR), variable compression ratio and variable valve actuation [20, 21, 22]. A very interesting method is that of fuel modification. In this method two or more kinds of fuels are blended together in different compositions, in order to change the autoignition and combustion characteristics. This method is usually called Reactivity-Controlled Compression Ignition (RCCI) and was suggested by the researchers of the University of Wisconsin - Madison [23]. They suggested using a mixture of gasoline and diesel as a fuel for HCCI engine. Higher gasoline fraction and higher EGR rates are used at higher load for more auto-ignition resistance. They achieved a significant reduction in NO_x and soot emissions, and an increase in gross indicated efficiency compared to a typical diesel engine [26].

Using TCR to control HCCI process was proposed by [27]. Following their approach, methanol enters into two reformers, one for dehydration of methanol to water and DME, and another - for thermal decomposition of methanol to H_2 and CO. Part of the fuel is streamed into the first reformer and the rest is streamed into the second reformer. By changing the mass flow through each reformer,

one can control the reforming products composition and thus - the reactivity of the gaseous reformat mixture entering the cylinder. The researchers also investigated the reformat composition after dehydration, depending on the vaporized fuel's temperature with different types of catalysts [28-29].

Concept Description

The concept suggested and described in this paper (see scheme in Figure 1) also utilizes TCR as a tool for HCCI combustion control.

Following this concept a mixture of methanol (CH_3OH) and water (H_2O) is evaporated using heat of the exhaust gases and then is entered into a single adiabatic reformer. The reformer consists of two sections (Figure 2). The first one is intended for dehydration of methanol to water and DME ($2\text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{OCH}_3 + \text{H}_2\text{O}$) and is supported by $\gamma\text{-Al}_2\text{O}_3$ acid catalyst. The second section is intended for steam reforming of methanol (SRM). In this section, supported by the $\text{CuO}/\text{ZnO}/\text{Al}_2\text{O}_3$ metal catalyst, the reactions of SRM ($\text{CH}_3\text{OH} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + 3\text{H}_2$), methanol decomposition (MD) ($\text{CH}_3\text{OH} \rightarrow \text{CO} + 2\text{H}_2$) and water-gas shift (WGS) ($\text{H}_2\text{O} + \text{CO} \rightarrow \text{CO}_2 + \text{H}_2$) take place simultaneously. Note that DME produced in the first section does not react in the second section and this is because of the fact that dehydration does not occur in presence of metal catalysts [30]. According to Faungnawaki et al. [31], at the temperatures higher than $\sim 650\text{-}670\text{ K}$, methane (CH_4) and CO are created during the methanol dehydration. To avoid formation of these undesired species, we limit the dehydration temperature below these values.

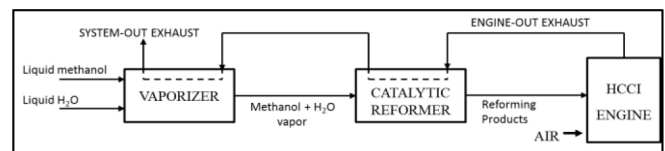


Figure 1. A scheme of TCR utilizing for HCCI control.

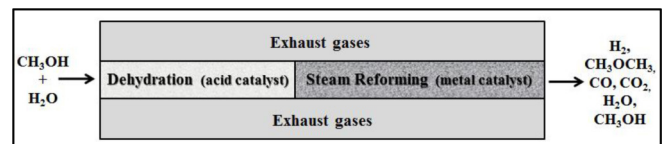


Figure 2. Schematic description of the reformer's structure consisting of two sections.

Composition of the reforming products depends on a number of factors: the vaporized fuel's temperature, the reformer's geometry, the methanol-to-water ratio, and the catalyst type. For the given reformer's geometry and the catalysts type (cannot be changed in a real time), two parameters are available for controlling the reforming products' composition. Adding more water to the methanol decelerates the dehydration reaction rate and thus fewer methanol dehydrates. As a consequence, more unreacted methanol is left for the SRM reactions, and thus more hydrogen is produced. Changing the vaporized fuel temperature impacts the kinetics of reactions too, thus affecting the reformat composition. Eventually a gaseous mixture of DME, hydrogen, carbon dioxide, water, carbon monoxide, and residues of methanol comes out of the reformer. The water condenses during the intermediate cooling process and can be reused. The relevant properties of combustible constituents presenting in the reformat, such as DME, hydrogen, carbon monoxide, and unreacted methanol, are listed in Table 1

homogenous, counter-current packed-bed reactor (PBR). In this model the exhaust gases are first utilized to evaporate the fuel mixture and then enter into the reformer. The reason is that by setting the vaporized fuel's temperature, it is possible to give the fuel almost all the required heat for dehydration and it takes a little more from the reformer.

Unlike the model described in [9], the developed and described here modeling approach is based on two sets of reactions: one for each reformer section, which requires two Global Reactions templates.

The job of these Global Reactions templates is to calculate the reactions' kinetics depending on the physical conditions in the reformer. The reactions' kinetics was modeled by applying two different kinetic models: one for dehydration of methanol and another for the SRM, MD and WGS reactions.

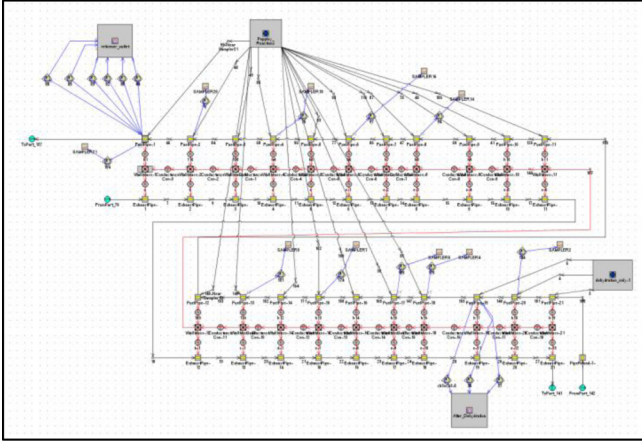


Figure 4. The reformer sub-model.

Reaction Kinetics Modeling

Kinetics of Methanol Dehydration

Kinetic models of methanol dehydration have been proposed by several researchers and are presented in [37]. The model suggested by Bercic et al. [38] is used in this paper. This model was validated for 3 mm γ - Al_2O_3 catalyst, in a temperature range of 523 to 673 K. The reaction rate of dehydration is modeled by the following equation:

$$r_M(T, C_i) = k_s \frac{K_M^2 (C_M^2 - C_W C_E / K_{eq})}{(1 + 2\sqrt{K_M C_M + K_W C_W})^4} \quad (1)$$

$$r_R = \frac{k_R K_{CH_3O}^* (p_{CH_3OH} / p_{H_2}^{0.5}) (1 - p_{H_2}^3 p_{CO_2} / K_R p_{CH_3OH} p_{H_2O}) C_{S_1}^T C_{1a}^T}{(1 + K_{CH_3O}^* (p_{CH_3OH} / p_{H_2}^{0.5}) + K_{HCOO}^* p_{CO_2} p_{H_2}^{0.5} + K_{OH}^* (p_{H_2O} / p_{H_2}^{0.5})) (1 + K_{H^{(1a)}}^{0.5} p_{H_2}^{0.5})}$$

$$r_W = \frac{k_W K_{OH}^* (p_{CO} p_{H_2O} / p_{H_2}^{0.5}) (1 - p_{H_2} p_{CO_2} / K_W p_{CO} p_{H_2O}) C_{S_1}^T}{(1 + K_{CH_3O}^* (p_{CH_3OH} / p_{H_2}^{0.5}) + K_{HCOO}^* p_{CO_2} p_{H_2}^{0.5} + K_{OH}^* (p_{H_2O} / p_{H_2}^{0.5}))^2}$$

(3)

(4)

Where:

$$k_s = 8.94 \times 10^{10} \exp\left(-\frac{E_a}{RT}\right) \left[\frac{\text{mol}}{\text{ml} \cdot \text{sec}}\right]$$

$$K_M = 5.39 \times 10^{-4} \exp\left(\frac{8487}{T}\right) \left[\frac{\text{m}^3}{\text{kmol}}\right]$$

$$K_W = 8.47 \times 10^{-2} \exp\left(\frac{5070}{T}\right) \left[\frac{\text{m}^3}{\text{kmol}}\right]$$

C_i is the molar concentration [kmol/m³] of component i (M -methanol, W -water, and E -DME); $E_a=143.7$ [kJ/mol] is the activation energy. K_{eq} is the thermodynamic equilibrium constant and is given by the following equation for temperature range of 498-623 K [39]:

$$\ln(K_{eq}) = \frac{2835.2}{T} + 1.675 \ln(T) - 2.39 \times 10^{-4} T - 0.21 \times 10^{-6} T^2 - 13.36 \quad (2)$$

Kinetics of Methanol Steam Reforming

Reaction kinetics of SRM, WGS and MD was modeled [10] using the rate expressions suggested by Peppley et al. [40] and based on developing the Langmuir-Hinshelwood mechanistic approach as presented in eq. (3), (4), and (5), respectively.

Where: r_i is the reaction rate expression of reaction process i (R -SRM, W -WGS, and D -MD). k_R , k_W^* , and k_D are reaction rate constants (calculated by Arrhenius expression). K_i is the equilibrium constant of reaction i for SRM, WGS, and MD. These constants were taken from [41], and the others were calculated by using van't Hoff equation. C_i^T is the active site concentration for each type of active site on the catalyst. P_i is the partial pressure of species i .

HCCI Engine Sub-Model

The Engine

A single-cylinder engine based on the Lister-Petter AD1 diesel was modeled. The main parameters of this engine are shown in Table 2. The engine has two valves. A gaseous reformate direct injector was modeled and the injection pressure was selected to be high enough to allow injection of all the required fuel into the cylinder in a suitable time. A PID controller was used to maintain constant Lambda during a simulation.

$$r_D = \frac{k_D K_{CH_3O^{(2)}}^* (p_{CH_3OH} / p_{H_2}^{0.5}) (1 - p_{H_2}^2 p_{CO} / K_D p_{CH_3OH}) C_{S_2}^T C_{2a}^T}{\left(1 + K_{CH_3O^{(2)}}^* (p_{CH_3OH} / p_{H_2}^{0.5}) + K_{OH^{(2)}}^* (p_{H_2O} / p_{H_2}^{0.5})\right) \left(1 + K_{H^{(2,a)}}^{0.5} p_{H_2}^{0.5}\right)} \quad (5)$$

Table 2. Main parameters of the modeled engine.

Displaced volume	367 cc
Stroke	73 mm
Bore	80 mm
Connecting Rod	126 mm
Compression ratio	16
Number of Valves	2
Exhaust Valve Open	38° BBDC @ 0.15 mm lift
Exhaust Valve Close	4° ATDC @ 0.15 mm lift
Intake Valve Open	28° BTDC @ 0.15 mm lift
Intake Valve Close	4° BBDC @ 0.15 mm lift

HCCI Combustion Modeling

A completely homogeneous unburned fuel-air mixture and a single-zone HCCI combustion process were assumed in this model. The combustion rate is predicted based on the chemical kinetics equations suggested by Kaiser et al. [42] that appear in the standard CHEMKIN II formatted mechanism file. The thermodynamic properties of the species presenting in the chemical kinetic model are taken from a thermodynamics CHEMKIN II file. The in-cylinder heat transfer was modeled using Woschni correlation for an engine without swirl. The injected reformat composition is taken from the Composition sub-model and injected under high pressure directly into the cylinder during the compression stroke. NO_x formation was predicted using the extended Zeldovich mechanism.

Thermodynamic Analysis

Two thermodynamic control volumes were defined to analyze the system. The first is the engine itself and the second is the entire system (Figure 5). According to these definitions, two efficiencies are defined. The first is the engine efficiency and the second is the HCCI-TCR system efficiency. The mathematical expressions of these efficiencies are shown below:

$$\eta_{engine} = \frac{P_i}{\dot{m}_{f,b} \cdot LHV_{f,b(g)}} \quad (6)$$

$$\eta_{system} = \frac{P_i}{\dot{m}_{methanol,a} \cdot LHV_{methanol,a(l)}} \quad (7)$$

Here: p_i is the indicated power, $\dot{m}_{f,b}$ is the mass flow rate of the reformat injected into the cylinder, $LHV_{f,b(g)}$ is the lower heating value of that reformat. $\dot{m}_{methanol,a}$ is the mass flow rate of the liquid methanol, and $LHV_{methanol,a(l)}$ is the lower heating value of the liquid methanol. The HCCI-TCR system efficiency has to be higher than the engine efficiency due to TCR. The heat recycled raises energy of the fuel, which is reflected in higher LHV of the reformat compared

with the liquid methanol. Of course, higher burning velocity and wide flammability limits of the hydrogen-rich reformat provide additional opportunities for efficiency improvement

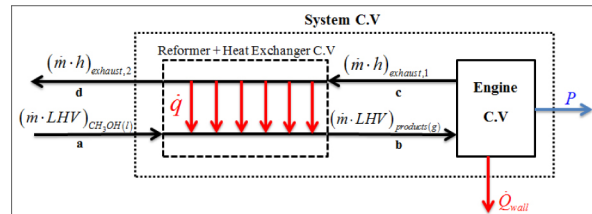


Figure 5. Thermodynamic analysis of the system.

Results and Discussion

The main goals of the analysis reported here were characterization of the system behavior under various operating modes, understanding the influence of various factors on engine performance, exposing weak points of the HCCI-TCR system and finding possible solutions to these weaknesses. The two main control parameters that were studied are water fraction blended with the methanol and the vaporized fuel's temperature. Two additional secondary parameters are EGR ratio and a compression ratio. The objective function of the optimization that has been performed is the HCCI-TCR system efficiency (defined below). There are some constraints that were taken into account: limiting the maximal temperature in the cylinder to reduce temperature-dependent pollutants formation (e.g. NO_x), operating with a lean mixture ($\lambda > 1$), and limiting maximum pressure in the cylinder. The latter was set to about 150 [bar] which is typical for a diesel engine [43]. Maximum allowed NO_x formation was limited to 350 [ppm].

Despite the fact that the results presented hereafter correspond to a specific case of the engine described above and the specific reformer design, we believe that observed trends and factors affecting the HCCI engine-TCR system performance should remain the same. The reformer model that served as a basis of the model described here was validated by Poran et al. [10]. Taking into account that the purpose of this paper was assessing main trends governing the reforming-controlled HCCI process at various operating modes and not predicting performance of a specific engine, and based on the fact that the broadly used worldwide commercial software GT-Power was used for engine modeling, we believe that the reported in this paper results provide useful insights on trends and factors affecting the HCCI engine-TCR system.

Reforming Products Composition under Various Operating Conditions

As was mentioned before, an engine's operating regime has a great impact on the reformer behavior. The engine, as a "customer", has requirements that the reformer should meet. The reformer has to provide the amount of fuel that the engine needs, and the fuel composition should meet the engine's operating mode. At the same time, the engine should provide to the reformer an amount of heat required to sustain the desirable chemical reactions. Adding water to

methanol and limiting the vaporized fuel's temperature allows adapting the reformer products composition to the engine requirements, under different conditions at the engine exhaust. There is a more than one way to achieve the same products composition under the same engine operating regime. For example, under regime of 2500 [RPM], $\lambda=1.1$, and $EGR=0.4$ ($CR=16$) the reforming products composition is very similar under two different sets of variables: in the first set the mass water fraction is 0.05 and the vaporized fuel's temperature is 605 K, and in the second set the mass water fraction is 0.11 and the vaporized fuel's temperature is 650 K.

In both mentioned above cases very similar results are obtained: H_2 to DME ratio is 1.91 and 1.88, respectively; and thus, the engine indicated efficiency is very similar too: 42.5 and 42.4%, respectively. Figure 6 shows an example of the reforming products composition as a function of mass water fraction at constant vaporized fuel's temperature at 2500 [RPM], $\lambda=1.1$, and $EGR=0.3$ ($CR=16$). As can be seen, rising of water fraction indeed increases the H_2/DME ratio.

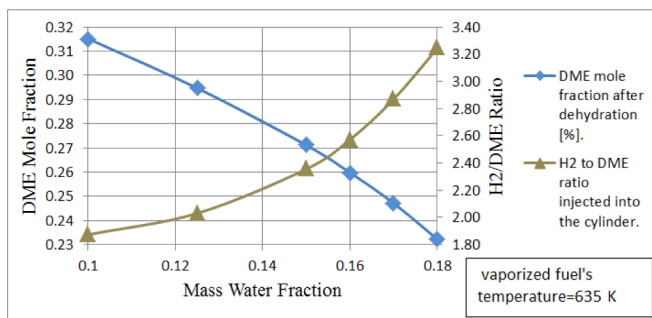


Figure 6. Reforming products composition vs mass water fraction @ 2500 [RPM], $\lambda=1.1$, and $EGR=0.3$ ($CR=16$).

In some cases the vaporized fuel's temperature is limited due to low temperature of the engine exhaust gases. It is mainly typical for low-load regimes. In these cases only a water adding remains as a control tool (Table 3). The vaporized fuel's temperature cannot be used in these cases as a control tool because of the too low exhaust temperature.

Catalyst Deactivation

As was mentioned before, H_2O/CH_3OH ratio has to be maintained greater than 1 during the SRM process to avoid catalyst deactivation [10]. Following [30], catalyst deactivation during dehydration of methanol is less common when using $\gamma-Al_2O_3$ catalyst compared to the HZSM-5 zeolite one. Nevertheless, in the suggested approach when lower H_2/CH_3OH is used, lower temperature is needed and thus the possibility of catalyst deactivation is reduced. Despite the H_2/CH_3OH ratio is low at the reformer inlet (before dehydration), during the dehydration process water is created and as a consequence this ratio increases before the steam reforming process.

HCCI Engine Performance under Different Conditions

As was mentioned above, there are some main parameters that influence the HCCI combustion: fuel properties, EGR, valves timing, compression ratio, injection strategy, cylinder geometry, etc. According to the concept analyzed in this paper, the main control tool is changing fuel properties. Figure 7 shows the influence of reformate composition on the ignition delay and as a consequence - on efficiency. Higher H_2/DME ratios lead to higher auto-ignition

resistance. This allows optimization of the ignition timing to reduce the negative compression work and to leave less time for heat transfer losses. As a consequence, the higher engine efficiency is achieved.

Table 3. Reforming products composition as a function of water mass fraction at @1000[RPM], $\lambda=1.8$ and $EGR=0.2$ ($CR=16$).

Water mass fraction	0.12	0.10	0.08	0.04
Steam/Methanol molar ratio (reformer inlet)	0.24	0.20	0.15	0.07
Actual vaporized fuel's temperature [K].	590	590	590	590
DME mole fraction after dehydration [%].	19.6	25.4	30.3	36.3
H_2O mole fraction after dehydration [%]	37.7	40.6	42.8	42.9
Methanol mole fraction after dehydration [%]	44.0	35.3	27.8	21.0
DME mole fraction after reformer [%].	7.4	15.4	19.9	25.8
H_2O mole fraction after reformer [%]	21.0	8.3	13.4	14.6
Methanol mole fraction after reformer [%]	0.4	0.2	0	0
CO_2 mole fraction after reformer [%]	17.0	17.1	15.4	13.9
CO mole fraction after reformer [%]	0.6	2.5	1.7	1.2
H_2 mole fraction after reformer [%]	53.6	56.4	49.5	44.3
H_2 to DME ratio injected into the cylinder.	7.2	3.7	2.5	1.7

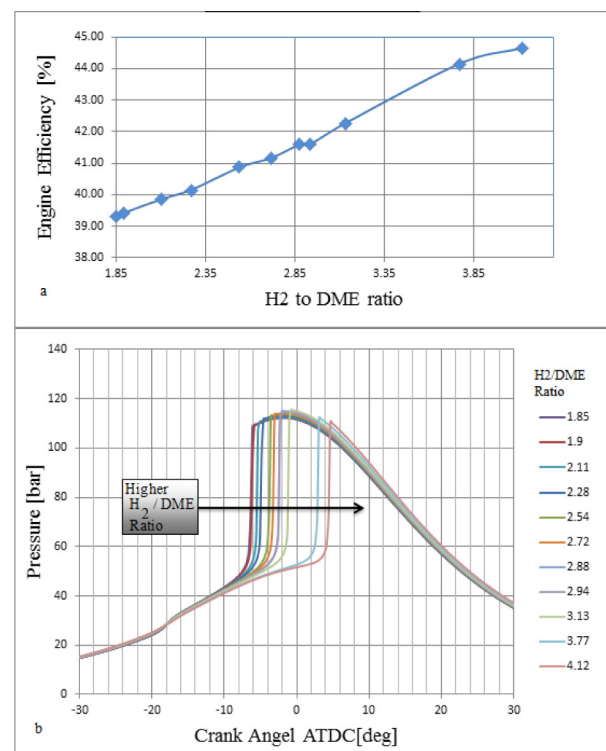


Figure 7. a. Engine efficiency vs H_2/DME ratio. b. In-cylinder pressure-Crank Angle diagram for different H_2/DME ratios. @ 2500 [RPM], $\lambda=1.4$ and $EGR=0.2$ ($CR=16$).

EGR Effects

EGR has several effects on the engine performance [18]. On the one hand it reduces the average temperature in the cylinder during the combustion, and on the other hand it occupies the place of air and thus leads to a power loss (Figure 8 and Figure 9). Subsequently, EGR raises the ignition delay (Figure 9). Under low-load regimes, there is almost no need for EGR and the reforming-controlled compression ignition can be realized. By using the main control tools (water addition and the reformer temperature control), it is possible to gain full control, and avoid a need for using EGR. However, under high-load regimes, where the maximum temperature could be too high, there is a need in EGR to limit that temperature. In these cases EGR using is desirable. Also at low-speed modes use of EGR can be necessary. Because of a low speed, there is a relatively long time available for heat transfer, and thus it is desirable to reduce the in-cylinder temperature, in order to reduce the heat transfer losses.

As shown in figure 8 the efficiency gain can be achieved with increase of the EGR ratio. The reason is that in this case EGR is used as a control tool. Thus, increasing EGR helps to optimize the ignition timing and therefore to achieve higher efficiency values. If the EGR ratio would be higher than the highest value shown in the graph on figure 8, ignition would not occur. Nevertheless, using EGR reduces the power and thus, when it is possible, it would be better to use the reforming-controlled compression ignition, which does not limit the power.

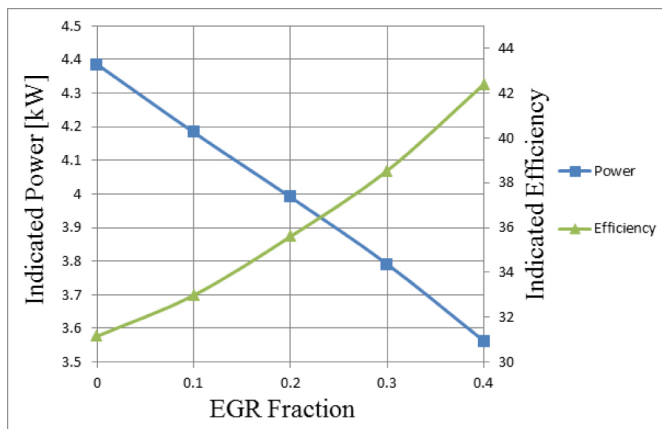


Figure 8. Efficiency and power as a function of EGR under 2000 [RPM], $\lambda=1.4$ (CR=16). Water fraction is 0 and vaporized fuel temperature is 620 K.

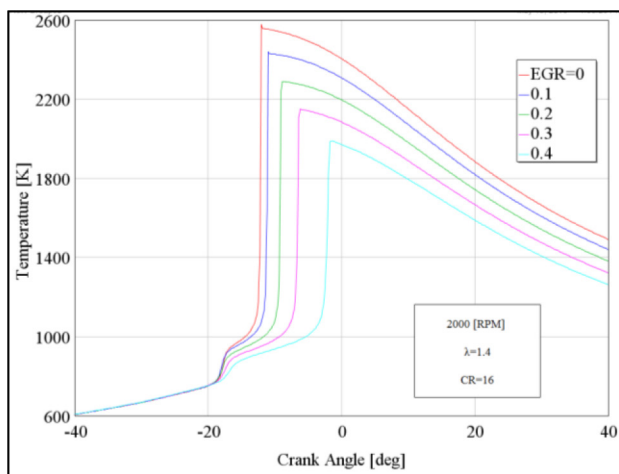


Figure 9. Temperature-Crank angle diagram for different values of EGR.

Pollutants Formation

The developed model version is able to predict the emissions of NO_x , CO , and CO_2 [14]. show that the temperature range over which the formation of NO_x begins is 2300-2400 K. Our predictions provide the similar results. Figure 10 shows the NO_x concentration in the engine exhaust gas under different operating modes, while λ is constant and equal to 1.1. As can be seen, the NO_x concentration approaches very low values when the maximal temperature in the cylinder is less than 2450 K. In our analysis we tried to eliminate operating conditions that lead to NO_x concentrations above 350 ppm.

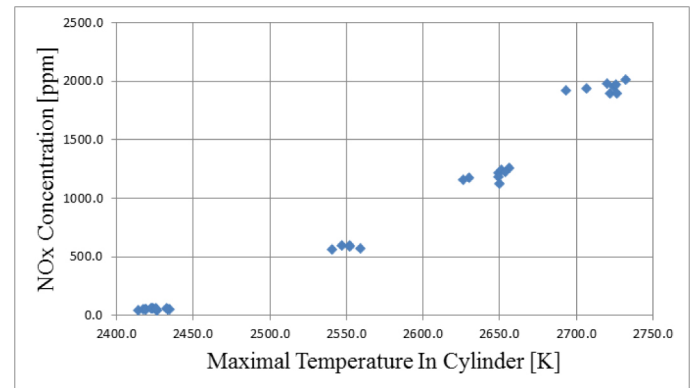


Figure 10. NO_x concentration in the exhaust gas as a function of the maximal temperature in the cylinder.

Maximum Power

The maximum power of the engine was determined under the limiting condition that NO_x concentration should remain lower than ~ 350 [ppm]. In order to comply with this condition, at the rated speed of 3600 [RPM], EGR adding was necessary to reduce the in-cylinder temperature. In the case of high-speed and high-load regimes (number 1 in Table 4), high EGR is required to restrict NO_x formation, but too high EGR ratios can result in misfire (no ignition). However, as more EGR is used, the maximal power is reduced. Thus at this operating mode the water fraction is reduced to zero and the vaporized fuel's temperature is maximal (650 K). A specific value of EGR is selected to achieve a sufficiently low in-cylinder temperature that still allows reformate ignition. In the considered case, the maximum power was achieved with EGR=0.23. In this regime the temperature in the cylinder is about 2500 K and NO_x formation does not exceed 350 ppm. A maximum indicated power of 7.2 [kW] is achieved compared with 6.1 [kW] of the original diesel engine.

Operating Mode Optimization

In order to achieve maximum engine efficiency, it is necessary to operate the engine at optimal reformate composition. Each regime has a specific H_2/DME ratio when the ignition timing is optimal. Table 4 illustrates different regimes representing the entire operating range. As can be seen the reforming-controlled compression ignition has a potential to allow HCCI operating in a wide range of loads and engine speeds.

Table 4. HCCI engine-TCR system performance in the entire operating range

Case	Speed [RPM]	λ	EGR [%]	Water fraction (Reformer inlet)	Vaporized fuel's temperature [K]	Obtained H ₂ /DME Ratio	IMEP [bar]	Engine Efficiency [%]	System efficiency [%]	Power [kW]	Maximal temperature (cylinder) [K]	NOx exhaust concentration [ppm]
1	3600	1.1	23	0	650	1.45	6.6	42	52	7.2	2500	340
2	2500	1.1	40	0.11	620	2.75	7.8	44	55	5.9	2200	negligible
3			30	0.18	635	3.25	8.4	41	53	6.4	2450	43
4	1000	1.1	40	0.12	590	6.20	7.3	40	55	2.2	2150	negligible
5	3600	1.4	7	0	650	1.45	5.9	42	52	6.5	2450	285
6	2500	1.4	20	0.19	635	4.35	7.8	46	52	6.0	2200	negligible
7			35	0	650	1.50	6.1	43	52	4.7	2100	negligible
8	1000	1.4	40	0.13	590	5.80	5.9	44	59	1.8	1800	negligible
9	3600	1.8	0	0.05	635	2.20	5.0	45	57	5.5	2150	negligible
10	2500	1.8	0	0.14	620	3.55	7.14	44	54	5.5	2250	negligible
11			20	0.14	635	2.20	5.76	44	58	4.4	2000	negligible
12	1000	1.8	20	0.12	590	7.24	5.92	44	65	1.8	1800	negligible

Case	Steam/Methanol molar ratio (reformer inlet)	CH ₃ OCH ₃ mole fraction [%]		CH ₃ OH mole fraction [%]		CO ₂ mole fraction [%]		H ₂ mole fraction [%]		CO mole fraction [%]		H ₂ O mole fraction [%]		Exhaust gases before reformer	Exhaust gases after reformer	Fuel engine inlet	Fuel after reforming
		AD ¹	AR ²	AD	AR	AD	AR	AD	AR	AD	AR	AD	AR				
1	0	39.2	27.4	21.6	0	0	9.9	0	40.0	0	5.1	39.2	17.5	890	850	315	640
2	0.22	29.2	17.1	24.5	0	0	16.2	0	52.3	0	1.9	46.3	12.5	750	730	315	610
3	0.39	22.9	15.3	27.5	0	0	15.2	0	49.1	0	1.7	49.6	18.7	780	750	315	610
4	0.24	15.7	4.5	51.7	8.2	0	19.3	0	59.8	0	0.8	33.8	7.4	640	615	315	490
5	0	33.6	23.6	21.0	0	0	10.8	0	40.5	0	4.0	45.4	21.1	840	815	315	650
6	0.42	20.0	13.6	32.9	1.8	0	16.7	0	51.2	0	0.5	47.1	16.2	780	730	315	520
7	0	39.8	28.5	20.4	0	0	12.8	0	41.6	0	1.5	39.8	15.6	670	620	315	620
8	0.26	18.3	8.6	45.1	0.3	0	17.1	0	54.5	0	0.8	36.6	18.7	645	620	315	565
9	0.10	35.6	14.4	20.4	0.8	0	16.2	0	59.8	0	5.7	44.0	3.1	800	750	315	610
10	0.29	23.5	15.1	31.9	0.5	0	17.0	0	53.8	0	1.3	44.6	12.3	710	680	315	560
11	0.29	28.0	20.0	22.0	0	0	13.9	0	43.4	0	0.8	50.0	21.9	650	640	315	600
12	0.24	19.6	7.4	42.4	0.4	0	17.0	0	53.6	0	0.6	38.0	21.0	640	615	590	550

1-After Dehydration, 2- After Reformer

Analysis of cases 9, 10 in Table 4 shows that at the same EGR ratio (0% in the considered case) and the same air excess factor λ (1.8), (3600 and 2500, respectively) higher H₂/DME ratio is required for lower speeds, to achieve optimal combustion. At low speeds more time for the combustion process is available, thus higher ignition delay is required. This is achieved with a higher H₂/DME ratio when the mixture has high auto-ignition resistance.

As can be seen from Table 4, substantial gain in the powertrain efficiency can be achieved by combining advantages of the HCCI process with great benefits of TCR. The system efficiency values that can be achieved are higher than those typical for modern diesel engines, thus confirming great potential of the suggested approach.

Summary and Conclusions

A method of HCCI combustion management by controlled reforming of methanol was presented and analyzed using computational simulation approach. A new technique to produce both DME and H₂ in a single reformer was developed. This technique allows variation of the H₂/DME ratio by changing the water to methanol ratio in the primary fuel entering an on-board reformer, and by changing the vaporized fuel's temperature. Two different catalysts are used to generate two sets of reactions in the reformer: one - for dehydration

of methanol to DME and water, and another - for production of H₂. The waste heat of exhaust gases is utilized to sustain endothermic reactions of DME and H₂ production.

Each engine operating mode has a different desirable H₂/DME ratio that provides the most suitable for this regime resistance to autoignition and combustion phasing.

To analyze a feasibility of the suggested approach, a computational model simulating operation of the complex HCCI engine - TCR system was developed. The model includes an HCCI engine model combined with a reformer model. These models communicate with each other.

The simulation results show that influence of H₂/DME ratio is very significant to the operating of an HCCI engine. The higher this ratio is, the ignition delay is higher. H₂/DME ratio that is too high may result in a misfire where no ignition occurs at all. As we showed on the example of the considered engine and the reformer, the method of reforming-controlled compression ignition allows a wide HCCI operating range with high energy efficiency and low pollutants formation.

The simulation results showed that there is more than one way to create the same composition of the reforming products. Adding of water to methanol or reducing the vaporized fuel's temperature lead to less DME production in the first section and thus higher H₂ production. Thus, higher H₂/DME ratio can be achieved. In cases when the exhaust gas temperature is too low and as a consequence the vaporized fuel's temperature is limited, only the water fraction can be used as a control tool to determine the reforming products composition. This happens mostly at low speeds. At these regimes a H₂-rich fuel is desirable and therefore there is no need in intensive DME production that requires higher temperature.

References

- International Energy Agency, World energy outlook 2011. OECD/IEA, Paris, France, 9 November 2011
- Chakravarthy VK, Daw CS, Pihl JA., Conklin JC. "Study of the Theoretical Potential of Thermochemical Exhaust Heat Recuperation for Internal Combustion Engines." *Energy Fuels*, 2010: 1529-1537.
- Pettersson, Lars, and Sjöström Krister. 1991. "Decomposed Methanol as a Fuel-A Review." *Combustion Science and Technology* 80 (4-6): 265-303. doi:10.1080/00102209108951788.
- Finegold, Joseph G. "Dissociated Methanol Vehicle Test Results." Inst of Gas Technology, 1984.
- Sakai, T., Yamaguchi, I., Asano, M., Ayusawa, T. et al., "Transient Performance Development on Dissociated Methanol Fueled Passenger Car," 1987.
- Brinkman, N. and Stebar, R., "A Comparison of Methanol and Dissociated Methanol Illustrating Effects of Fuel Properties on Engine Efficiency-Experiments and Thermodynamic Analyses," SAE Technical Paper [850217](#), 1985, doi:10.4271/850217.
- Tartakovsky, L., Baibikov, V., Gutman, M., Mosyak, A. et al., "Performance Analysis of SI Engine Fueled by Ethanol Steam Reforming Products," SAE Technical Paper [2011-01-1992](#), 2011, doi:10.4271/2011-01-1992.
- Tartakovsky, L., Baibikov, V., and Veinblat, M., "Comparative Performance Analysis of SI Engine Fed by Ethanol and Methanol Reforming Products," SAE Technical Paper [2013-01-2617](#), 2013, doi:10.4271/2013-01-2617.
- Poran, A., Artoul, M., Sheintuch, M., and Tartakovsky, L., "Modeling Internal Combustion Engine with Thermo-Chemical Recuperation of the Waste Heat by Methanol Steam Reforming," *SAE Int. J. Engines* 7(1):234-242, 2014, doi:10.4271/2014-01-1101.
- Poran, A., and Tartakovsky, L. 2015 "Energy Efficiency of a Direct-Injection Internal Combustion Engine with High-Pressure Methanol Steam Reforming." *Energy*. 88: 506-514. doi:10.1016/j.energy.2015.05.073.
- Tartakovsky L., Amiel R., Baibikov V., Fleischman R., Gutman M., Poran A., Veinblat M.: SI Engine with Direct Injection of Methanol Reforming Products - First Experimental Results. SAE Technical Paper [2015-32-0712](#), 2015
- Ashley, Steven. "A low-pollution engine solution." *Scientific American* 284, no. 6 (2001).
- Najt, P. and Foster, D., "Compression-Ignited Homogeneous Charge Combustion," SAE Technical Paper [830264](#), 1983, doi:10.4271/830264.
- Yao, Mingfa, Zheng Zhaolei, and Liu Haifeng. 2009. "Progress and Recent Trends in Homogeneous Charge Compression Ignition (HCCI) Engines." *Progress in Energy and Combustion Science* 35 (5). Elsevier Ltd: 398-437. doi:10.1016/j.pecc.2009.05.001.
- Stanglmaier, R. and Roberts, C., "Homogeneous Charge Compression Ignition (HCCI): Benefits, Compromises, and Future Engine Applications," SAE Technical Paper [1999-01-3682](#), 1999, doi:10.4271/1999-01-3682.
- Stanglmaier, R., Li, J., and Matthews, R., "The Effect of In-Cylinder Wall Wetting Location on the HC Emissions from SI Engines," SAE Technical Paper [1999-01-0502](#), 1999, doi:10.4271/1999-01-0502.
- Harada, A., Shimazaki, N., Sasaki, S., Miyamoto, T. et al., "The Effects of Mixture Formation on Premixed Lean Diesel Combustion Engine," SAE Technical Paper [980533](#), 1998, doi:10.4271/980533.
- Zhao, Hua. HCCI and CAI Engines for the Automotive Industry. Elsevier, 2007.
- Bression, G., Soleri, D., Savy, S., Dehoux, S. et al., "A Study of Methods to Lower HC and CO Emissions in Diesel HCCI," *SAE Int. J. Fuels Lubr.* 1(1):37-49, 2009, doi:10.4271/2008-01-0034.
- Fang, Qiang, Fang Junhua, Zhuang Jian, and Huang Zhen. "Influences of pilot injection and exhaust gas recirculation (EGR) on combustion and emissions in a HCCI-DI combustion engine." *Applied Thermal Engineering* 48 (2012): 97-104.
- Shi, Lei, Cui Yi, Deng Kangyao, Peng Haiyong, and Chen Yuanyuan. "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.
- Feng, Hongqing, Zheng Zunqing, Yao Mingfa, Cheng Gang, Wang Meiyong, and Wang Xin. "Effects of exhaust gas recirculation on low temperature combustion using wide distillation range diesel." *Energy* 51 (2013): 291-296.
- Kokjohn, S. L., Hanson R. M., Splitter D. A., and Reitz R. D.. "Fuel reactivity controlled compression ignition (RCCI): a pathway to controlled high-efficiency clean combustion." *International Journal of Engine Research* 12, no. 3 (2011): 209-226.
- Splitter, D., Hanson, R., Kokjohn, S., and Reitz, R., "Reactivity Controlled Compression Ignition (RCCI) Heavy-Duty Engine Operation at Mid-and High-Loads with Conventional and Alternative Fuels," SAE Technical Paper [2011-01-0363](#), 2011, doi:10.4271/2011-01-0363.
- Nieman, D., Dempsey, A., and Reitz, R., "Heavy-Duty RCCI Operation Using Natural Gas and Diesel," *SAE Int. J. Engines* 5(2):270-285, 2012, doi:10.4271/2012-01-0379.
- Reitz, Rolf D., and Duraisamy Ganesh. "Review of high efficiency and clean reactivity controlled compression ignition (RCCI) combustion in internal combustion engines." *Progress in Energy and Combustion Science* 46 (2015): 12-71.

27. Shudo, Toshio, Shima Yosuke, and Fujii Tatsuya. "Production of dimethyl ether and hydrogen by methanol reforming for an HCCI engine system with waste heat recovery-Continuous control of fuel ignitability and utilization of exhaust gas heat." *International Journal of Hydrogen Energy* 34, no. 18 (2009): 7638-7647.
28. Shudo, Toshio, and Yamada Hiroyuki. "Hydrogen as an ignition-controlling agent for HCCI combustion engine by suppressing the low-temperature oxidation." *International Journal of Hydrogen Energy* 32, no. 14 (2007): 3066-3072.
29. Shudo, T. and Ono, Y., "HCCI Combustion of Hydrogen, Carbon Monoxide and Dimethyl Ether," SAE Technical Paper 2002-01-0112, 2002, doi:10.4271/2002-01-0112.
30. Vicente, Jorge, Gayubo Ana G., Ereña Javier, Aguayo Andrés T., Olazar Martin, and Bilbao Javier. "Improving the DME steam reforming catalyst by alkaline treatment of the HZSM-5 zeolite." *Applied Catalysis B: Environmental* 130 (2013): 73-83.
31. Faungnawakij, Kajornsak, Kikuchi Ryuji, Matsui Toshiaki, Fukunaga Tetsuya, and Eguchi Koichi. "A comparative study of solid acids in hydrolysis and steam reforming of dimethyl ether." *Applied Catalysis A: General* 333, no. 1 (2007): 114-121.
32. Arcoumanis, Constantine, Bae Choongsik, Crookes Roy, and Kinoshita Eiji. "The potential of di-methyl ether (DME) as an alternative fuel for compression-ignition engines: A review." *Fuel* 87, no. 7 (2008): 1014-1030.
33. Tsang, Wing. "Chemical kinetic data base for combustion chemistry. Part 2. Methanol." *Journal of physical and chemical reference data* 16, no. 3 (1987): 471-508.
34. White, C. M., Steeper R. R., and Lutz A. E.. "The hydrogen-fueled internal combustion engine: a technical review." *International Journal of Hydrogen Energy* 31, no. 10 (2006): 1292-1305.
35. Enggcyclopedia.30/5/2016 <http://www.enggcyclopedia.com/2012/01/syngas-producer-gas/>
36. Tartakovsky L., Gutman M. and Mosyak A.: Energy efficiency of road vehicles - trends and challenges. Chapter 3 in the Edited Collection "Energy Efficiency: Methods, Limitations and Challenges", Santos Cavalcanti Emmanuel F. and Barbosa Marcos Ribeiro (editors), Nova Science Publishers, p. 63-90, 2012
37. Bercic, Gorazd, and Levec Janez. "Intrinsic and global reaction rate of methanol dehydration over. gamma.-alumina pellets." *Industrial & engineering chemistry research* 31, no. 4 (1992): 1035-1040.
38. Bercic, Gorazd, and Levec Janez. "Catalytic dehydration of methanol to dimethyl ether. Kinetic investigation and reactor simulation." *Industrial & engineering chemistry research* 32, no. 11 (1993): 2478-2484.
39. Diep, Bang T., and Wainwright Mark S.. "Thermodynamic equilibrium constants for the methanol-dimethyl ether-water system." *Journal of Chemical and Engineering Data* 32, no. 3 (1987): 330-333.
40. Peppley Brant A., Amphlett John C., Kearns Lyn M., and Mann Ronald F.. "Methanol-steam reforming on Cu/ZnO/Al₂O₃ catalysts. Part 2. A comprehensive kinetic model." *Applied Catalysis A: General* 179, no. 1 (1999): 31-49.
41. Graaf, G. H., Sijtsema P. J. J. M., Stamhuis E. J., and Joosten G. E. H.. "Chemical equilibria in methanol synthesis." *Chemical Engineering Science* 41, no. 11 (1986): 2883-2890.
42. Kaiser, E. W., Wallington T. J., Hurley M. D., Platz J., Curran H. J., Pitz W. J., and Westbrook C. K.. "Experimental and modeling study of premixed atmospheric-pressure dimethyl ether-air flames." *The Journal of Physical Chemistry A* 104, no. 35 (2000): 8194-8206.
43. Eilts, P., Stoeber-Schmidt, C., and Wolf, R., "Investigation of Extreme Mean Effective and Maximum Cylinder Pressures in a Passenger Car Diesel Engine," SAE Technical Paper 2013-01-1622, 2013, doi:10.4271/2013-01-1622.

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Definitions/Abbreviations

- CI - compression ignition
- CN - cetane number
- CR - compression ratio
- DME - dimethyl ether
- EGR - exhaust gas recirculation
- GHG - greenhouse gas
- HCCI - Homogenous charge compression ignition
- ICE - internal combustion engine
- MD - methanol decomposition
- ON - octane number
- PBR - packed-bed reactor

RCCI - reactivity controlled compression ignition

SI - spark ignition

SRE - ethanol steam reforming

SRM - methanol steam reforming

TCR - thermo-chemical recuperation

WGS - water gas shift

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