



Comparative Performance Analysis of SI Engine Fed by Ethanol and Methanol Reforming Products

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ABSTRACT

A comparative theoretical analysis of the spark ignition (SI) engine performance is performed for the cases of feeding it by the reforming products of two different alcohols: ethanol and methanol. Energy efficiency of the steam reforming process, optimal reactor temperature and obtainable compositions of the reforming products are showed and analyzed for the considered two fuel types.

Three compositions of the reforming products: ethanol steam reforming (SRE), methanol steam reforming (SRM) and products of the low-temperature ethanol reforming are considered as gaseous fuels in the engine performance simulations. Change in the fuel burning velocity as a function of fuel composition and air excess factor is taken into account in a modeling of the heat release process.

Effect of the selected reforming product compositions on the achievable internal combustion engine (ICE) and reformer-ICE powerplant efficiencies, NO_x and CO emissions are analyzed and compared with the cases of ICE feeding by reference fuels: gasoline, ethanol and methanol.

INTRODUCTION

Results of recent studies suggest that there is a big potential for improvement of ICE technologies [1, 2, 3, 4]. It is well known that about 30% of fuel energy introduced to ICE is wasted with engine exhaust gases. Its utilization can lead to a significant improvement of ICE energy efficiency. One of the ways to recover an engine's waste heat is by using the energy of exhaust gases to promote endothermic reaction of fuel reforming. This method is frequently called thermo-chemical recuperation

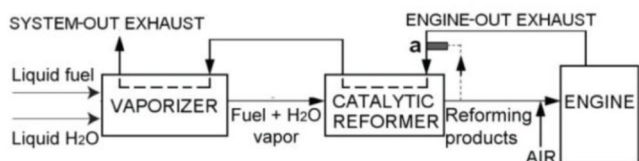
(TCR) [5]. In this case an ICE is fed by the gaseous products of fuel reforming, mainly mixture of hydrogen and carbon monoxide, frequently called syngas. The latter has, as a rule, greater heating value than the primary liquid fuel, and may be burned in the engine using extremely lean air/fuel mixtures with the excess air factor λ values up to 1.5. This should ensure more complete combustion under lower temperatures and, as a result, increase of the engine brake efficiency and decrease of noxious species formation. High hydrogen content of this gaseous fuel provides a possibility of faster combustion compared with the primary liquid fuel, thus resulting in higher engine thermal efficiency. The TCR approach is considered nowadays as one of the possible methods of increasing powertrain efficiency and reducing emissions.

A suitable primary fuel for automotive application has to meet several requirements. The fuel should have as high as possible heating value, be easy to handle and store onboard a vehicle, be cheap, should provide convenient refueling and create as low as possible health, safety and environmental hazards [6]. Use of alternative renewable fuels that can be CO_2 neutral is of growing importance nowadays. The fuel reforming in TCR process should be robust, energy efficient and sustain at as low as possible temperatures. Many studies published on TCR are focused on gas turbine applications [7, 8, 9, 10]. Addition of the simulated reformat gas to gasoline fed engine has been studied at MIT [11, 12] and showed a potential of the engine efficiency improvement by up to 12% under part load conditions. However, if fuel reforming is carried out at too high temperatures, the energy of exhaust gas could be not sufficient to supply a heat required for the reforming. This is overcome by combusting an additional fuel and thus reducing an energy efficiency improvement [13]. Computational analysis of SI engine performance was carried out by Galloni and Minutillo [14] for partial gasoline replacement by a

reformate gas. In their work the reformate gas production by exothermic partial oxidation of gasoline rather than bio-fuel was considered.

Some fuels, such as methanol, can be reformed to the syngas at relatively low temperatures of 270-300 °C [15, 16], thus enabling utilization of the waste heat of exhaust gases without combustion of additional fuel. This feature is an important advantage of methanol as a fuel for the engine with thermochemical recuperation. Many efforts have been made in 80s to feed ICE with methanol reforming products [15, 16, 17, 18, 19]. Obtained results exposed a number of serious problems, mainly caused by the multi-regime nature of the ICE operation in a motor vehicle (cold startability, need to address momentary change of load etc.) and backfiring through the inlet system. In order to enable satisfactory engine operation in the whole range of working regimes, different amounts of liquid methanol were added to the methanol reforming products [15]. This brought up the problems typical for methanol fuel: higher aldehyde emissions, increased wear, poor cold startability etc. These problems remain unsolved, thus precluding further development of the reformer-ICE concept.

In this study we consider a hybrid propulsion system (Fig. 1) having an additional energy source which provides a basis for overcoming these drawbacks. A detailed analysis of this concept and its benefits is provided in [20].



a – optional fuel burner

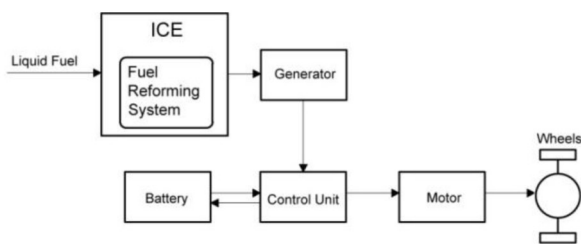


Figure 1. Vehicle hybrid propulsion system (bottom) with onboard fuel reforming (top).

One of the main drawbacks of methanol as a fuel is its relatively high toxicity and corrosivity [21]. Its production is essentially based on reforming non-renewable fossil fuels, mostly natural gas. Its use in this case will release fossil carbon into the atmosphere. However, technologies of methanol production from renewable sources are developed as well [22]. Ethanol appears as an attractive alternative to methanol, since it is

much less toxic and corrosive [23], and is already used as versatile fuel that offers a high octane number and low photochemical reactivity. Moreover, bio-ethanol can be produced in large quantities from biomass fermentation and, therefore, can be considered as a renewable energy source, [24]. A significant advantage of this alcohol over fossil fuels is that it is CO₂ neutral. Carbon dioxide released into the atmosphere during combustion of ethanol or its reforming products is absorbed during the growth of the biomass. Thus, ethanol appears as one of the best candidates that can be used for hydrogen generation. However, previous studies have showed that it is reformed under relatively high temperatures of 600-800 °C [20].

Recently a new reforming technology has been developed [25, 26, 27]. It allows the reforming of ethanol into equal molar fractions of hydrogen, carbon monoxide and methane at temperatures of approximately 300 °C as in methanol reforming.

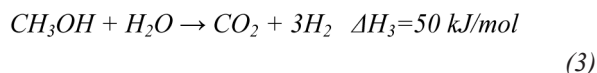
The goal of this study was to perform a comparative theoretical analysis of the SI engine performance under feeding by the reforming products of two different alcohols: ethanol and methanol. Effects of the SRE and the low-temperature ethanol reforming products as well as SRM composition together with exhaust gas temperature limitations (governed by the required reforming temperature) on the achievable ICE and the reformer-ICE powerplant efficiency, as well as pollutant emissions were analyzed and compared with the cases of ICE feeding by reference fuels: gasoline, ethanol and methanol.

ENERGY ANALYSIS OF ALCOHOL REFORMING

Alcohol can be reformed into hydrogen-rich gaseous fuel through steam reforming - ASR [23], partial oxidation [28] and auto-thermal reforming [29]. Partial oxidation and auto-thermal processes have the merit of fast start-up time because of the exothermic nature of the oxidation reaction. However, the steam reforming provides highest hydrogen production. Leung et al. [30] studied different methods of on-board ethanol reforming and found that the steam reforming method makes it possible to generate reformate gas of greater heating value - by 20% higher than primary liquid ethanol.

The thermodynamics of alcohol steam reforming aimed at hydrogen production for fuel cell applications has been widely discussed in the literature. For example, the methanol steam reforming process may be described by three main reactions, namely methanol decomposition (1), water gas shift (WGS) (2) and direct methanol steam reforming (3):





Reactions (1) and (3) are endothermic, whereas WGS is exothermic. In overall, the process is endothermic. Thus, heat should be supplied from an external source. In fuel cell applications, an effort is focused on achievement of maximal possible hydrogen outcome together with prevention of CO formation, which is a poison for the fuel cell catalyst. For these purposes, the reaction (3) is preferable, thus implying that the WGS reaction extent is very high. In contrast with the strict requirement of high-purity hydrogen typical for fuel cells application, ICE is much more flexible and can effectively burn different mixtures of hydrogen, carbon monoxide and other gases. This feature greatly reduces the cost of energy obtained from renewable fuels. In this case alcohol decomposition to CO₂ and H₂ is undesirable, because CO₂ is a diluent gas and does not carry energy. Therefore, for ICE feeding, realization of the reaction (1) would be preferable with negligible WGS reaction extent. In ICE the exhaust heat can be used to promote on-board reforming of alcohol into a mixture of hydrogen and carbon monoxide with some amounts of contaminants (carbon dioxide, methane, soot etc.). Because this reformat has a greater heating value and may be more efficiently burned than the primary fuel, an improvement in engine fuel economy can be expected along with a sensible emissions reduction. CO formed in reaction (1) does not constitute an environmental hazard because it is further oxidized to CO₂ during the combustion in the engine. Therefore, for ICE application alcohol reforming process has to be optimized for the maximal yield of hydrogen and CO together with prevention of contaminants formation and as low as possible reforming temperature.

Method

An important parameter that should be used in reforming optimization is the energy efficiency of the ASR process [20], defined as a ratio of the added enthalpy of combustion ($h_{out} - h_{in}$) to the heat duty, h_d (the sum of the ASR reactions heat, latent heat of vaporization and sensible heat):

$$\eta = (h_{out} - h_{in}) / h_d \quad (4)$$

The lack of detailed kinetic data (reaction rates, residence time, known intermediate species, etc.) has determined a modeling of the steam reforming. Simulation of alcohol steam

reforming was performed for ethanol and methanol by using the equilibrium reactor and Gibbs reactor models of the CHEMCAD [31] software package. We simulated a chemical reactor by solving the heat and mass balances and minimizing the free energy of the components that can be produced during a reforming process. The minimization of total Gibbs free energy is a suitable method to calculate the equilibrium compositions of any reacting system. The method of minimizing the Gibbs free energy is normally preferred in the fuel reforming analysis [32]. For methanol the CHEMCAD calculation results were empirically corrected based on the available experimental data to account for the non-equilibrium reforming behavior. The empiric correction functions were developed using available experimental results for copper based catalysts [33, 34]:

$$\begin{aligned} CO_{cor} &= 1.4 \cdot 10^{-6} \cdot CO_{eq} \cdot T^{1.996} \\ CO_{2cor} &= 10^{-7} \cdot CO_{2eq} \cdot T^{2.827} \\ H_{2cor} &= 0.05 \cdot H_{2eq} \cdot e^{0.01T} \\ CH_3OH_{cor}^{conv} &= 22.44 \cdot 10^{-3} \cdot CH_3OH_{eq}^{conv} \cdot e^{0.013T} \end{aligned} \quad (5)$$

Where: indexes 'cor' and 'eq' relate to corrected and equilibrium molar fractions, respectively; CH_3OH^{conv} - methanol conversion ratio; T - reforming temperature, C.

To validate the suggested empiric correction functions, a comparison of the corrected results with the experimental data [35, 36 and 37], which were not used in the correction function development, was performed. The developed correlations were not validated for catalyst types other than copper-based.

Molar fractions, M_i , of SRE and SRM products were calculated at atmospheric pressure for various water/ethanol (W/E) and water/methanol (W/M) ratios, respectively, and different reaction temperatures. More detailed description of the simulation methodology and results of analysis for ethanol and methanol are provided in [20, 38].

Results and Discussion

Typical examples of the obtained data for both ethanol and methanol are shown in Fig. 2. For ethanol reforming hydrogen yield approaches a value of 60 % at $W/E=1.8$ and $T=1000K$. If methanol is used as a primary fuel, the maximal hydrogen yield of 67% can be achieved at $W/M=1.3$ and $T=570K$. The larger hydrogen yield is explained by the higher H/C ratio of methanol compared with ethanol.

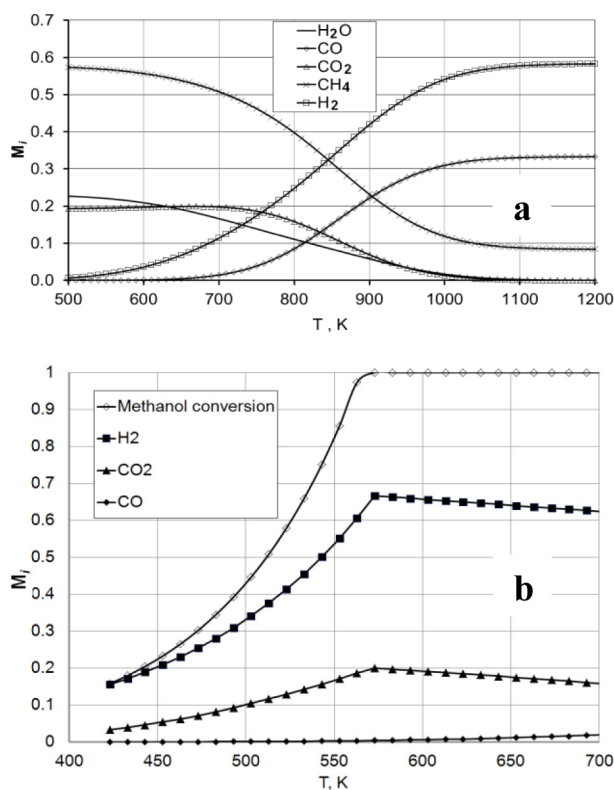


Figure 2. Steam reforming products - example of simulation results: a-ethanol, W/M=1.8; b-methanol, W/M=1.3.

Fig. 3 shows the maximal energy efficiency values of ASR for ethanol and methanol as a function of the water/alcohol ratio. The required values of the reforming process temperature are shown near corresponding points of the plot. Simulation results showed that the energy efficiency of methanol steam reforming approached maximal value of 0.66 at W/M=1.3 and the reaction temperature of approximately 573K. For the all considered W/M ratios maximal energy efficiency of the reforming process was observed in the narrow range of temperatures 570-580K. The maximal energy efficiency of ethanol steam reforming is somewhat lower and more sensitive to the reforming temperature. It was found that for ethanol the efficiency achieved its maximum of approximately 0.59 at W/A=1.2 and T=1100K. However, this temperature is too high to be realized in the reformer heated only by the energy of exhaust gases [31].

The difference between the maximal achievable values of energy efficiency for the compared fuels is not significant. However, for methanol it can be achieved under much lower temperature: 570K compared with 1100K for ethanol. This is a significant benefit of methanol over ethanol in the view of the TCR concept realization.

Utilization of the copper-plated nickel sponge catalyst technology [25] makes possible low-temperature ethanol reforming at approximately 570K, thus neutralizing the important benefit of methanol as a fuel for ICE with TCR. In this case the following reaction path dominates leading to formation of equal molar fractions of methane, carbon monoxide and hydrogen [27]:

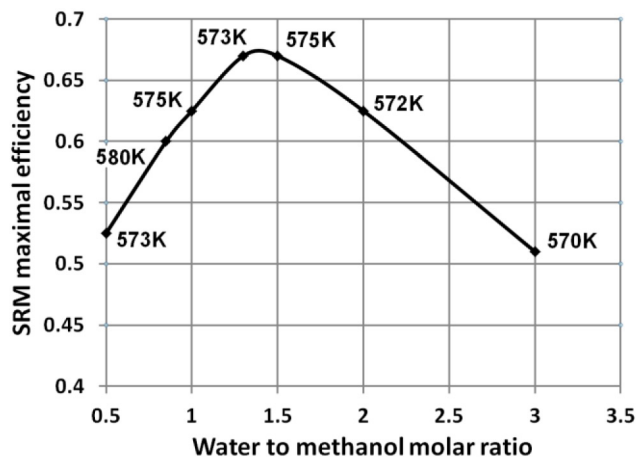
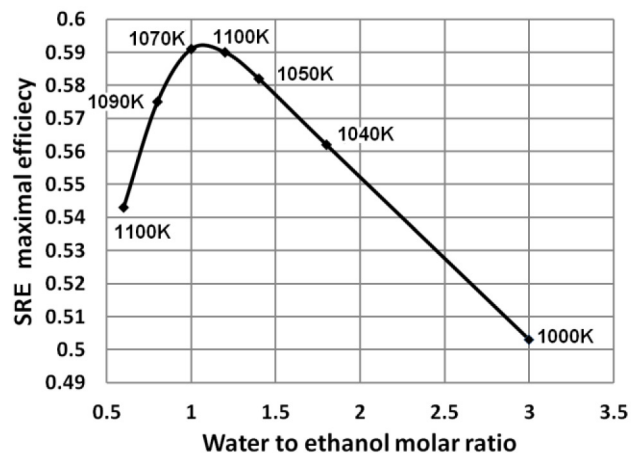
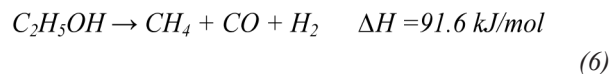


Figure 3. Maximal energy efficiency of alcohol reforming as a function of water to alcohol ratio.



Energy efficiency of the low-temperature ethanol reforming was assessed following the eq. (4). Data from [27] about an increase of the reforming products heating value by 7% compared with the primary ethanol was used. The obtained maximal energy efficiency value of the reforming was 0.42, which is substantially lower compared with the case of the high temperature steam ethanol reforming.

SI ENGINE MODELING

Method

A comparison of the engine performance under feeding it by different fuel types was carried out by modeling with aid of GT-Power software [39] of the GT-SUITE commercial package. GT-Power is the 2- and 4-stroke SI and CI engines simulation tool widely used nowadays by engines researches. GT-Power software has been thoroughly validated by its numerous users in a lot of real-life applications. Prediction of the flow rates in the intake and exhaust systems is performed by using conservation equations. The whole system is discretized into many small sub-volumes, connected by boundaries. At each time step for each the boundary the simultaneous solution of three equations is performed: conservation of mass, energy and momentum. For each sub-volume the pressure, temperature and species concentration are considered uniform. For each boundary area the species velocity and mass flux are considered uniform, as well. For modeling in-cylinder processes the following approaches were applied:

- Since there is no available experimental data that suggest numeric values of the coefficients in the Wiebe model adjusted specifically to gaseous fuel compositions considered in the current work, an approach suggested in [39] was applied. Anchor angle (corresponds to 50% of fuel burned) and combustion duration of 10% - 90% fuel were used as variable inputs for Wiebe model, governing heat release rate as a function of a crank angle;
- Woschni correlation for an engine without swirl was used for calculation of the in-cylinder heat transfer, as described in [40];
- The model of CO formation developed for homogeneous combustion and described by Heywood in [40] was used for CO emission predictions;
- Extended Zeldovich model for NO_x formation predictions;
- The engine cyclic variations and transient operation were not considered.

Main parameters of the engine used in the performance modelling are shown in Table 1. It is the naturally aspirated, fuel direct injection, SI engine.

Table 1. Main parameters of the simulated engine.

Cylinder bore, mm	90
Piston stroke, mm	90
Number of cylinders	4
Compression ratio	10
Rated speed, rpm	4000
Rated brake power, kW	75
BMEP, bar	9.8

The engine performance at the rated power and speed was modeled and analyzed under the engine feeding by gasoline, liquid dehydrated ethanol and methanol, as well as by three gaseous compositions that represent products of ethanol and methanol steam reforming (SRE and SRM) and of the low-temperature ethanol reforming [26, 27]. The main reasons for selection of the rated power regime for the comparative analysis were:

- A need to assess a possibility of reaching the original (as under gasoline feeding) engine rated power value when engine is fueled by the alcohol reforming products;
- A necessity to evaluate a danger of arising the extremely high in-cylinder pressures under the engine feeding by hydrogen-rich gaseous mixtures featured by very high burning velocities;
- A need to assess a possibility of achieving exhaust gas temperatures that are required for the reforming process realization.

Table 2. Alcohol reforming product compositions.

Mixture type (Reformer operation conditions)	Gas composition, molar fraction (%)					Mixture lower heating value, (MJ/kg mix)/ (MJ/kg alcohol)
	H ₂ O	CO ₂	CH ₄	CO	H ₂	
Mixture 1, SRE product (W/E=1.8; T=1000K)	9.4	5.1	2.2	23.5	59.7	18.9/32.2
Mixture 2, SRM product (W/M=1.3; T=570K)	13	20	-	0.4	66.6	12.9/22.3
Mixture 3, Low-temperature ethanol reforming product(T=570K)	-	-	33.3	33.3	33.3	28.7/28.7

Gaseous fuel compositions that have been considered in the engine performance simulations are presented in Table 2. Mixture 1 is the SRE product chosen from the five SRE compositions analysed in [41] as providing maximal energy efficiency of the reformer-engine powerplant. Mixture 2 was selected from the various SRM compositions as providing the maximal energy efficiency of methanol reforming - Fig. 3. Composition of the Mixture 3 was borrowed from [27] and represents the product of low-temperature (570K) ethanol reforming process. Table 2 contains also data on lower heating value for each of these Mixtures, where: in the nominator - the lower heating value of gaseous reforming products calculated per 1 kg of the reforming products mixture and in the denominator - the same calculated per 1 kg of the corresponding primary liquid fuel entering the reforming process.

Main properties of the reference/primary liquid fuels are provided in [Table 3](#).

$$CD_i/CD_{gas} = v_{gas,l}/v_{i,l} \quad (7)$$

Table 3. Main properties of the reference/primary liquid fuels [42].

Parameter	Gasoline	Ethanol	Methanol
Heat of vaporization, kJ/kg	297.3	841.5	1101.1
Lower heating value, MJ/kg	44.38	26.75	19.93
Stoichiometric A/F ratio by mass	14.55	8.99	6.46
Octane number	80 - 95	106	110

Some of the engine simulation assumptions are listed below.

- Due to negligible amounts (less than 0.1%) of non-reformed C_2H_5OH and CH_3OH found in the reforming products at the simulated reforming conditions, ethanol and methanol content in the reformat fuels was assumed to be zero.
- The engine geometry and valves timing was remained the same for all types of the fuels.
- Energy required for cooling, compression and injection of gaseous reforming products into the engine cylinder was not assessed.
- The mass flow-rate of the primary species entering the reformer is equal to the mass fuel consumption of the engine operating on the reforming products.
- Actual burning velocities of the considered fuels inside a cylinder were assumed to be proportional to the appropriate laminar flame velocities (taking into account that the engine geometry and operation regime remained the same with change of the fuel type). Laminar flame velocity for each of the considered gaseous fuel compositions was estimated based on the published experimental data [43, 44, 45]. Only the results obtained under similar values of pressure and temperature were used for these assessments. Laminar flame velocities of gasoline and ethanol have been taken from [46] and of methanol - from [47]. [Fig. 4](#) shows laminar flame velocity of the considered fuels for different excess air factor λ values. High hydrogen percentage in Mixtures 1 and 2 is a reason of their substantially higher flame velocities and ensures combustion of substantially leaner air-fuel mixtures.
- Ratio of actual combustion duration (10% - 90%) of each considered fuel to that of gasoline was assumed to be inversely proportional to the ratio of the laminar flame velocities of these fuels:

where: CD_i and CD_{gas} - actual combustion duration (10% - 90%) of the considered fuel and gasoline, respectively; $v_{gas,l}$ and $v_{i,l}$ - laminar burning velocities of gasoline and the considered fuel, respectively.

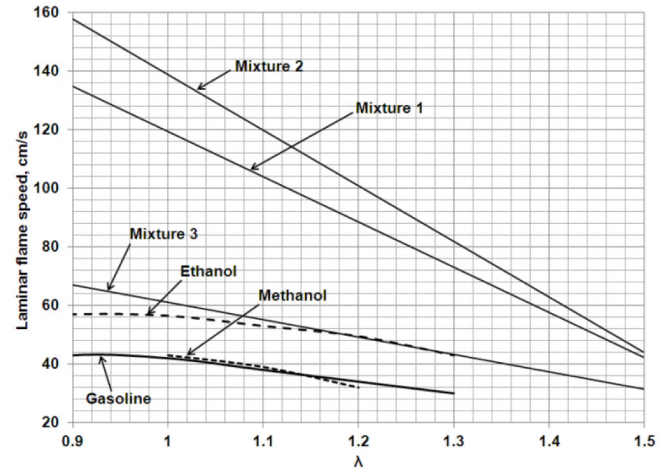


Figure 4. Laminar burning velocity of the considered fuels.

The performance calculations have been carried out with the engine design invariable, i.e. no changes in its geometry, displacement, compression ratio, intake and exhaust valves timing and discharge coefficients etc. were performed. For each of the considered fuel types the engine modelling was carried out at various values of air excess factor and combustion start angle. An optimal engine tuning (air/fuel ratio and combustion start timing) for each fuel was selected based on the following criteria: keeping the same power of 75 kW together with maximal possible brake efficiency and minimal possible NO_x and CO emissions level. Reduction of the engine's power because of the mixture leaning was not acceptable. To limit mechanical stresses and prevent excessive rise of the noise level, combustion start angle and excess air factor values providing reasonable levels of the in-cylinder maximal pressure and maximal pressure rise rate $(dp/dCA)_{max}$ were considered.

When engine was fed by the alcohol steam reforming products, efficiency η_{pp} of the reformer-engine powerplant was calculated using as a basis the primary liquid ethanol/methanol consumption [41]:

$$\eta_{pp} = 3600 / (bsfc_{liq} \cdot LHV_{liq}) \quad (8)$$

Where: $bsfc_{liq}$ is brake specific consumption of a primary liquid fuel, g/(kW·h); LHV_{liq} is a lower heating value of liquid alcohol (ethanol or methanol), MJ/kg.

$$bsfc_{liq} = bsfc_{mix} / m_{mix} \quad (9)$$

Here: $bsfc_{mix}$ is a brake specific consumption of the steam reforming products; m_{mix} is a mass of the reforming products per 1 kg of the primary liquid alcohol. The value of m_{mix} was calculated as follows:

$$m_{mix} = (M_{wat} / M_{alc}) \cdot (W/A) + 1 \quad (10)$$

Here M_{wat} and M_{alc} are molecular weights of water and alcohol, respectively; W/A - water-to-alcohol ratio.

Values of η_{pp} make possible a comparison of the reformer-engine powerplant efficiency with a brake efficiency of the engine fed by gasoline or liquid alcohols.

Modeling Results

A performance of the SI engine was simulated at the WOT operation regime - 75 kW at 4000 rpm (BMEP 9.8 bar). The results for the cases of the engine feeding by liquid methanol, SRM products (Mixture 2), SRE and ethanol low-temperature reformat (Mixtures 1 and 3, respectively) are shown in Figs. 5, 6, 7 and 8, respectively.

For each fuel type an optimal tuning (air excess factor value λ and combustion start angle) was chosen based on the criteria listed above. Start of combustion in this work was defined as the instant where pressure rise due to combustion may be observed. These tunings are marked by a vertical line with dots. As can be seen, the leanest air-fuel mixture ($\lambda=1.45$) and, as a result, the lowest value of NO_x emission may be achieved with the methanol steam reformat (Fig.6).

Evidently, this can be explained by the highest hydrogen content in this fuel, which is resulted in the wide flammability

limits and high burning velocity - Fig. 2 and 4. The latter factor allowed reaching maximal brake efficiency at more retarded combustion start - 10° before TDC. On the other hand, the high burning velocity resulted in greater value of the maximal pressure rise rate, 0.27 MPa/deg. The modeling results show that for the all considered fuels mixture enrichment (decrease of λ) leads to the engine power increase with substantial growth of the pressure rise rate and especially - NO_x emission level. The latter is a result of the maximal combustion temperature increase with the mixture enrichment.

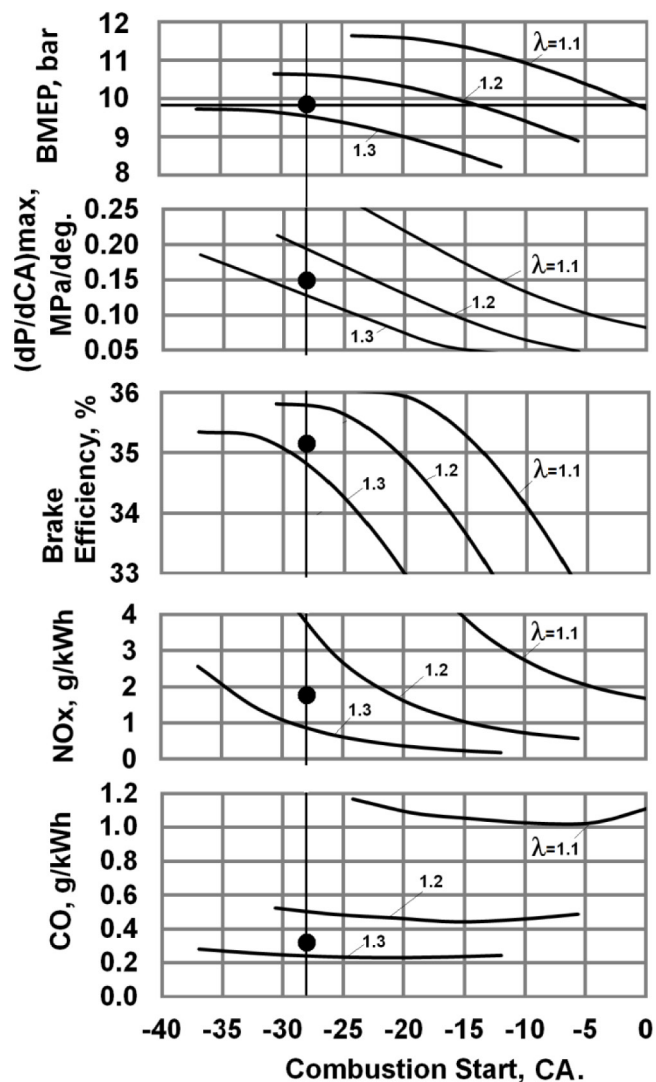


Figure 5. Performance of SI engine fed by liquid methanol.

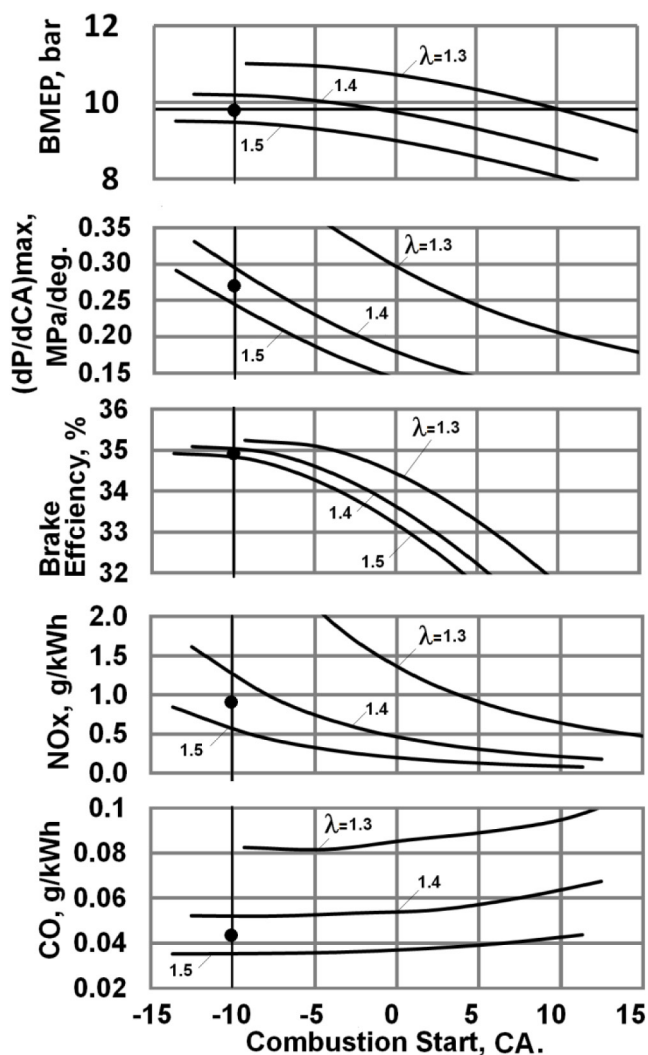


Figure 6. Performance of SI engine fed by SRM product (Mixture 2 in Table 2.).

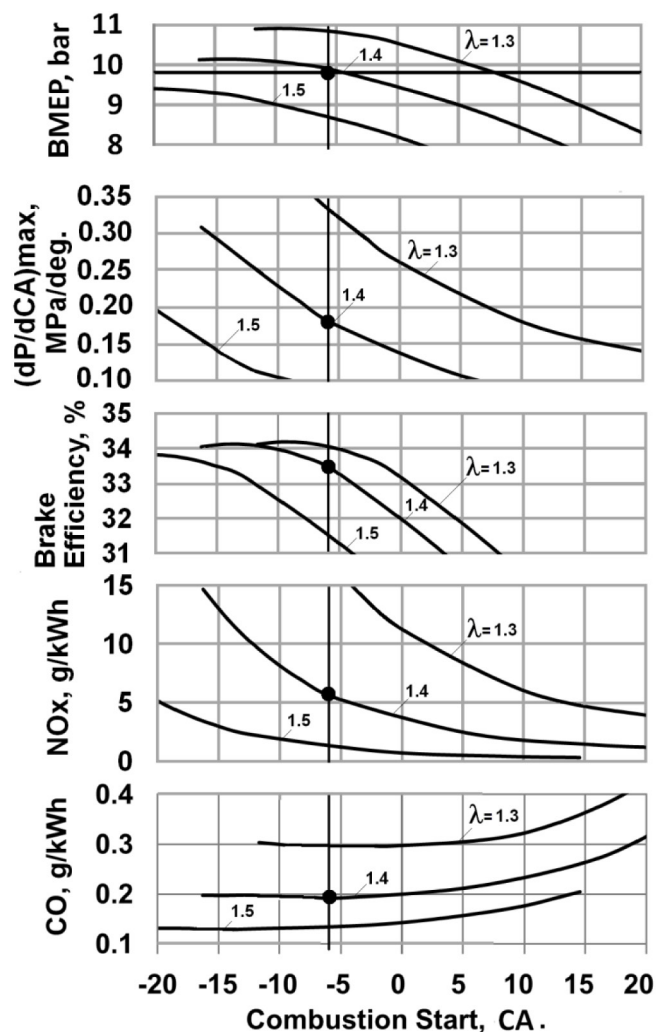


Figure 7. Performance of SI engine fed by SRE product (Mixture 1 in Table 2.).

Figs. 6, 7 and 8 show that practically the same values of maximal brake efficiency of the SI engine fed by gaseous products of the alcohol reforming may be achieved under different combinations of the combustion start angle and air excess factor values. In this work a tuning that ensures achieving the rated power of 75 kW (BMEP 9.8 bar) together with a best possible efficiency and minimal emissions formation was considered as optimal.

As can be seen, engine feeding by the gaseous products of steam reforming (Mixtures 1 and 2) allows its operation with a higher air excess factor λ and thus ensures relatively low levels of NO_x emissions. This is a result of the high hydrogen content of these fuels.

The engine performance parameters, chosen in the way as described above, for the all considered fuel types are summarized in Table 4 and Figs. 9, 10, 11, 12. Performance parameters of the engine fed by liquid gasoline and ethanol were taken from [41]. As can be seen from Table 4, the optimal engine performance with each of the considered fuels was achieved at different air excess factor (λ) values.

A comparison of the brake efficiency predicted for the SI engine fed by the considered fuels is presented in Fig. 9. Feeding engine by ethanol resulted in rise by about 4% of its brake efficiency as compared to gasoline. This is a result of the lower in-cylinder compression work due to more intensive charge cooling and the lower combustion start angle. The former is a result of the substantially higher heat of ethanol vaporization. The latter was possible due to higher burning velocity of ethanol compared with gasoline that allowed combustion phasing optimization.

Table 4. Performance of the SI engine fed by different fuels: 75 kW/4000rpm, optimal tuning.

Performance parameter	Liquid gasoline	Liquid ethanol	Liquid methanol	Mixture 1 (W/E=1.8; T=1000K)	Mixture 2 (W/M=1.3; T=570K)	Mixture 3 (low-temp. ethanol reforming)
Comb. start, CA BTDC	-26.2	-11.8	-28	-5.3	-10	-15
Air excess factor λ	1.2	1.25	1.27	1.4	1.45	1.26
$(dP/dCA)_{max}$, MPa/deg.	0.185	0.185	0.15	0.176	0.27	0.18
Engine brake efficiency, %	34.2	35.6	35.2	33.3	34.9	33.6
T_{exh} , K	1100	1040	1020	1080	950	1000
$bsfc$, (g/kW·h)	242	378	504	572	807	373
$bsfc_{alc}$, (g/kW·h)	-	378	504	336	466	373

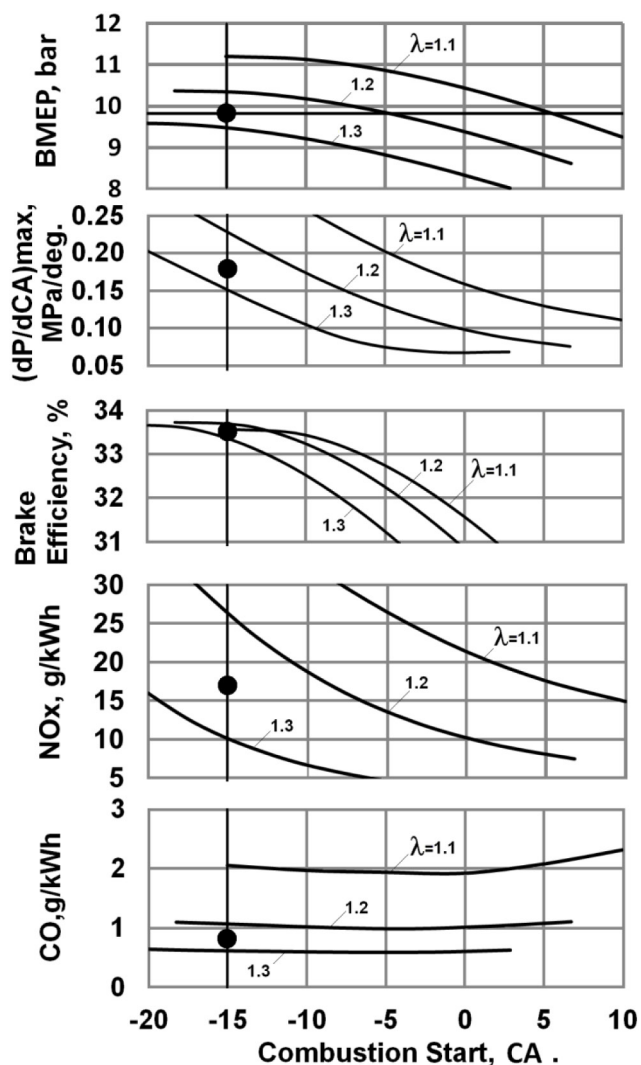


Figure 8. Performance of SI engine fed by low-temperature ethanol reforming products (Mixture 3).

Intensity of the in-cylinder charge cooling by alcohol vaporization in comparison with gasoline at given operation regime may be assessed by a relative cooling intensity (RCI) factor calculated as follows:

$$RCI = (HoV_i / HoV_{gas}) \cdot (bsfc_i / bsfc_{gas}) \quad (11)$$

where: HoV_i and HoV_{gas} - heat of vaporization of the alcohol i and gasoline, respectively; $bsfc_i$ and $bsfc_{gas}$ - break specific consumption of the alcohol i and gasoline, respectively.

Using values of HoV (Table 3) and predicted $bsfc$ (Table 4) for the considered liquid fuels, the conclusion may be done that under considered regime of operation intensity of in-cylinder charge cooling by ethanol and methanol is higher by a factor of 4.4 and 7.7, respectively, than in the case of gasoline.

Engine feeding by methanol also leads to growth of its brake efficiency, but this increase is slightly lower than in the case of ethanol, only by some 3%. This takes place despite the fact that methanol's RCI and, therefore, in-cylinder charge cooling is much higher and, consequently, compression work is lower than in the case of ethanol. However, burning velocity of methanol is substantially lower as compared with ethanol (Fig.4): 31 compared with 47 cm/sec at λ values relevant for each fuel and mentioned in Table 4. Lower working cycle temperatures contribute to further reduction of burning velocity. Lower burning velocity requires combustion start advancing that leads to a subsequent increase of the compression work and appropriate thermal efficiency reduction. The summary effect of alcohols' heat of vaporization and their burning velocity is reflected in the engine's energy efficiency gain as shown in Fig.9.

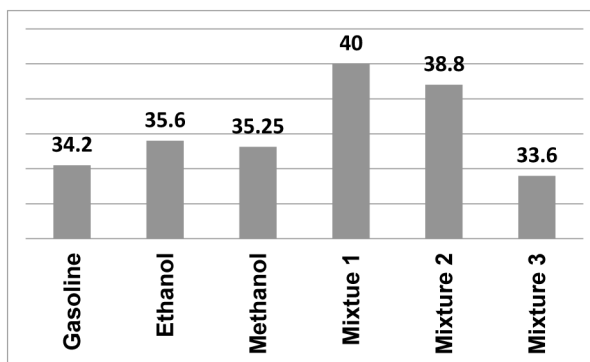


Figure 9. Brake efficiency of reformer-engine powerplant and SI engine fed by liquid fuels, %.

Use of the steam reformer-SI engine powerplant fed by ethanol or methanol allows the efficiency improvement by 12% and 10%, respectively, in comparison with the cases of ICE feeding by the primary liquid alcohols. An appropriate efficiency gain in comparison with the engine feeding by gasoline is 17% and 13%, respectively. This is a result of the combined effect of raising the reformat heating value and working cycle temperatures, shortening combustion duration and better combustion completeness in comparison with liquid fuels [20]. The efficiency improvement at engine operation with Mixture 2 (methanol steam reformat) is somewhat lower compared with that one obtained under operation with SRE products (Mixture 1) because of the slightly longer combustion duration (see burning velocities of Mixtures 1 and 2 on Fig.4 at lambda values of 1.4 and 1.45, respectively) and lower increase of the reforming products heating value (20% and 10% for SRE and SRM, respectively).

It should be noted that, in contrast to the Mixtures 1 and 2, efficiency of the engine fed by the low-temperature ethanol reformat has become worse not only in comparison with the reference liquid fuel - ethanol but even in comparison with gasoline. This result confirms the conclusion of [48] made for the port fuel injection engine that at high load the low-temperature ethanol reforming is not advantageous. This is explained by the lower burning velocity of this reformat (Mixture 3) compared with SRE (Mixture 1) and SRM (Mixture 2) products, absence of the charge cooling, as in the cases of engine feeding by liquid alcohols, and increase of the residual gas fraction due to rise of the reformat volume compared with liquid primary fuels. This finding complements results obtained in [27, 48] that demonstrated substantial rise of the engine efficiency at low partial loads and speeds by using the simulated low-temperature ethanol reforming products. The engine operation at partial loads allowed the authors to work with lean air-fuel mixtures and increase the compression ratio from 9.5 up to 17 [27] and from 10 up to 14 [48] using high knock-resistance of this gaseous composition and not exceeding upper limits of in-cylinder maximal pressure and maximal pressure rise rate. It is clear that this approach is unacceptable for the case of the engine operation at a rated power and high loads because of inadmissible rise of mechanical loads on the engine elements and power loss due to lean-burn operation.

A comparison of maximal in-cylinder pressure values for the considered fuels at optimal tuning is demonstrated in Fig.10. One must pay attention to the very low maximal pressure under methanol feeding as compared to other liquid fuels. This is a result of the very high value of methanol's heat of vaporization and its relatively low burning velocity. The SI engine operation on gaseous reforming products leads to noticeable increase of the maximal in-cylinder pressure as compared to the primary liquid fuel: by 12% for Mixture 1, 46% for Mixture 2 and 31% for Mixture 3. The evident reasons of this result are absence of the vaporization cooling effect

under compression stroke, higher burning velocity of these gaseous mixtures due to the high content of hydrogen and rise of the reformat volume compared with liquid primary fuels. In the case of Mixture 3 (low-temperature ethanol reformat) there is an additional factor - increase of the compression work because of a need in advanced combustion start in comparison with Mixtures 1 and 2.

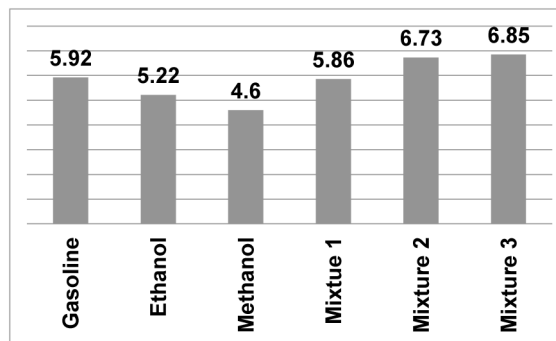


Figure 10. In-cylinder maximal pressure, MPa.

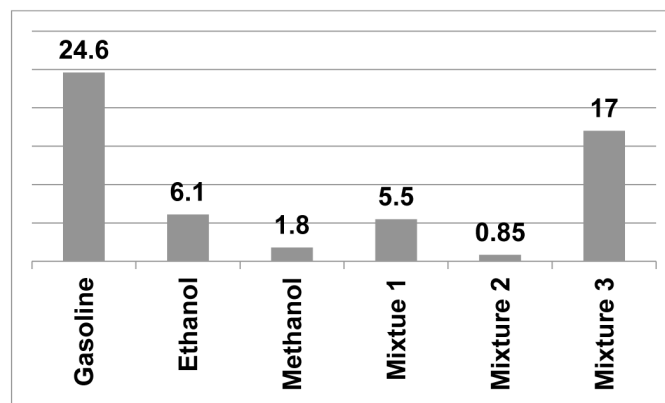


Figure 11. NO_x emissions, g/kWh.

A comparison of engine NO_x emissions for the considered fuels is shown in Fig.11. Reduction of NO_x emissions by almost 4 and 14 times for the cases of engine feeding by liquid ethanol and methanol, respectively, as compared to gasoline was observed. This is a result of the higher intensity of in-cylinder cooling due to vaporization of these fuels and lower flame temperatures, and therefore, reduction of the cycle maximal temperature. Engine feeding by Mixture 1 (SRE) leads to only slight decrease of NO_x emissions in comparison with the reference fuel - ethanol, in spite of the lean-burn operation. Evidently, the latter does not compensate increase of burning velocity and absence of in-cylinder cooling under engine feeding by the gaseous fuel. In the case of engine feeding by SRM products (Mixture 2) the working mixture leaning up to λ=1.45 ensured more than double reduction of NO_x emissions as compared to the reference liquid fuel - methanol. The predicted NO_x emissions under engine feeding by both steam reforming products (Mixtures 1 and 2) were

lower by a factors of 4.5 and 29, respectively, in comparison with the case of gasoline. The low-temperature ethanol reformat (Mixture 3) did not allow such a substantial decrease of NO_x emissions. They dropped down only by a factor of 1.45 compared with gasoline.

CO concentration in engine exhaust gases denotes completeness of the combustion process. Fig.12 shows a possibility of sharp decrease in CO emissions compared with gasoline in the case of engine feeding by liquid ethanol and methanol, as well by their reforming products. Especially low CO emissions were predicted for the case of the engine feeding by Mixture 2 (SRM products) - lower by a factor of 29 than in the case of gasoline. It is a result of the lean-burn operation.

Possibility of NO_x and CO emissions drastic decrease in the case of SI engine feeding by SRE products was experimentally confirmed by Li et al. [49].

Our results showed that level of CO emissions in the case of gaseous fuel is proportional to CO content in it (Table 2), and in the case of a liquid fuel it is proportional to a number of carbon atoms in the fuel molecule.

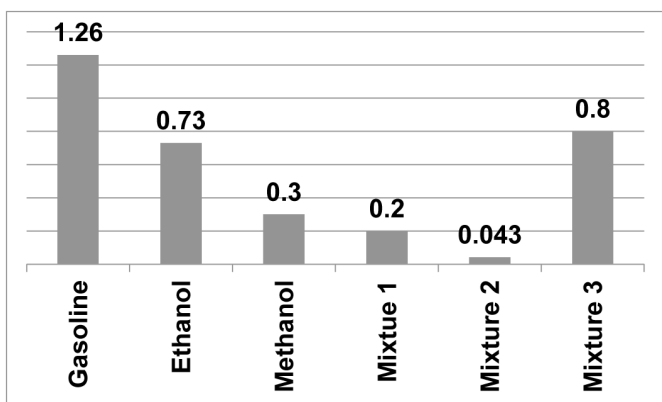


Figure 12. CO emissions, g/kWh.

Since the discussed reformer-engine powerplant is considered for a potential use in vehicle propulsion, it is of great interest to assess change that would be required in a volume of a fuel tank compared with the case of gasoline feeding - Fig.13. The data were calculated based on the fuel consumption of the reformer-engine powerplant and density values of the considered primary fuels. As can be seen, the largest increase of the fuel tank volume by a factor of 2.8 would be required in the case of engine feeding by Mixture 2 (SRM products). ICE feeding by the rest of considered fuels would require significant increase of the fuel tank volume, as well. If the water required for sustaining the steam-reforming process would be utilized from the engine exhaust gases, the required increase of the fuel tank volume would be much lower - by a factor of 1.3 and 1.7 only for SRE and SRM products, respectively.

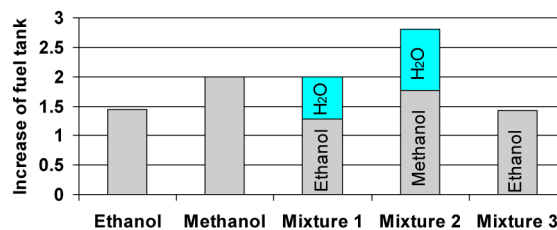


Figure 13. Required increase of a fuel tank in comparison with the case of gasoline feeding.

CONCLUSIONS

Simulation of alcohol steam reforming processes confirmed that use of methanol as a primary fuel allowed effective reforming at low temperatures of approximately 570 K compared with 1000-1100 K for ethanol. Low-temperature ethanol reforming process suggested in [25] may be realized at the temperature of 570K as well. Maximal energy efficiencies of SRE, SRM and low-temperature reforming processes were assessed as 0.59, 0.66 and 0.42, respectively. For the case of methanol reforming the equilibrium calculation results were empirically corrected to account for the non-equilibrium reforming behavior. The empiric correction functions were developed using available experimental results for copper based catalysts.

Modeling results showed that engine feeding by SRE and SRM products allows lean-burn operation with λ value up to 1.45. Efficiency of the reformer-engine powerplant increased by 12% and 10%, respectively, in comparison with the appropriate primary liquid fuels, and by 17% and 13%, respectively in comparison with the case of the engine feeding by gasoline.

In contrast to the cases of the engine feeding by SRE and SRM products, efficiency of the engine fed by the low-temperature ethanol reformat has become worse not only in comparison with the reference liquid fuel - ethanol, but even in comparison with gasoline. This result confirms the conclusion of previous studies that at high loads the low-temperature ethanol reforming is not advantageous.

The engine operation on gaseous hydrogen-rich reforming products led to noticeable increase of the maximal in-cylinder pressure up to 69 bar, as compared to 59 bar for gasoline. The maximal pressure rise rate did not exceed 0.3 MPa/deg for all the considered fuels under the engine optimal tuning. A danger of knock arising was not revealed.

NO_x formation depends strongly on the oxygen content and temperature. The latter is influenced not only by air excess factor, but also by the heat of fuel vaporization, combustion phasing, etc. NO_x behaviour obtained in our work is a result of the mutual influence of all mentioned factors. The lowest NO_x

emissions were obtained with the engine feeding by SRM products. These emissions are lower by a factor of 29 and 2 compared with gasoline and methanol, respectively.

Sharp decrease of CO emissions in comparison with gasoline was predicted for the case of the engine feeding by the alcohol reforming products, as well as by liquid ethanol and methanol. The lowest CO emissions were achieved in the case of engine feeding by the SRM products - lower by a factor of 29 compared with gasoline. Our results showed that level of CO emissions in the case of gaseous reformat fuel is proportional to CO content in it, and in the case of a liquid fuel it is proportional to a number of carbon atoms in the fuel molecule.

ICE operation with SRM products would require the largest increase of the vehicle's fuel tank volume - by a factor of 2.8 compared with gasoline. If the water required for sustaining the steam-reforming process would be utilized from the engine exhaust gases, the required increase of the fuel tank volume would be much lower - by a factor of 1.7 only.

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SRM - steam reforming of methanol

TCR - thermo-chemical recuperation

TDC - top dead center

W/E - water-to-ethanol molar ratio

WGS - water gas shift

W/M - water-to-methanol molar ratio

WOT - wide open throttle

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ABBREVIATIONS

ASR - alcohol steam reforming

BMEP - brake mean effective pressure

BSFC - brake specific fuel consumption

CA - crank angle

CD - combustion duration

CI - compression ignition

HoV - heat of vaporization

ICE - internal combustion engine

RCI - relative cooling intensity

SI - spark ignition

SRE - steam reforming of ethanol

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