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Internal combustion engine with thermochemical recuperation fed by ethanol steam reforming products – feasibility study

O Cesana¹, M Gutman¹, M Shapiro¹, and L Tartakovsky¹

¹Faculty of Mechanical Engineering, Technion Israel Institute of Technology, Israel

E-mail: orcesana@gmail.com

Abstract. This research analyses the performance of a spark ignition engine fueled by ethanol steam reforming products. The basic concept involves the use of the internal combustion engine's (ICE) waste heat to promote onboard reforming of ethanol. The reformer and the engine performance were simulated and analyzed using GT-Suite, Chem CAD and Matlab software. The engine performance with different compositions of ethanol reforming products was analyzed, in order to find the optimal working conditions of the ICE - reformer system. The analysis performed demonstrated the capability to sustain the endothermic reactions in the reformer and to reform the liquid ethanol to hydrogen-rich gaseous fuel using the heat of the exhaust gases. However, the required reformer's size is quite large: 39 x 89 x 73 cm, which makes a feasibility of its mounting on board a vehicle questionable. A comparison with ICE fed by gasoline or liquid ethanol doesn't show a potential of efficiency improvement, but can be considered as a tool of additional emissions reduction.

1. Introduction

It is known that about one-third of fuel energy introduced to an ICE is wasted with engine exhaust gases [1, 2]. Even its partial utilization can lead to a significant improvement of the ICE energy efficiency. One of the ways to recover an engine's waste heat is by using exhaust gases energy to promote fuel endothermic reactions that produce hydrogen-rich reformate. The basic concept involves the use of the engine's exhaust heat to promote on board reforming of ethanol into a mixture of hydrogen and carbon monoxide with some amounts of carbon dioxide, methane, etc. (frequently called syngas) [3, 4]. The resulted fuel has greater heating value than primary liquid fuel and may be more efficiently burned in the engine in comparison to the original fuel. Also the ICE working cycle approaches the theoretical Otto cycle as a result of the higher burning velocity of a hydrogen-rich reformate [5, 6]. The efficiency also can be improved by utilizing lean burning (due to wide flammability limits of a hydrogen-rich reformate) that leads to reduction of heat transfer energy loses and a possibility of increasing the engine compression ratio (CR) [5].

Because the reforming reactions are endothermic they provide an opportunity for recovery of exhaust gas energy in a thermochemical form that otherwise would have been wasted. This approach, called thermo-chemical recuperation (TCR) [2,7], has been receiving renewed interest as one of the possible methods of increasing efficiency and reducing emissions of ICE.

Bio-ethanol is widely recognized as a promising renewable energy source [2]. A significant advantage of this alcohol over fossil fuels is that it is CO2 neutral. Thus, ethanol appears as one of the candidates that can be used for hydrogen generation onboard a vehicle.

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It is known that an onboard reformer cannot work efficiently in a wide range of engine operation regimes typical for a conventional road vehicle especially at transient modes and cold-start conditions [8]. In case of a hybrid propulsion system, which always has an additional energy source, these shortcomings can be successfully overcome [9].

This research is a feasibility study of an internal combustion engine with thermochemical recuperation fed by ethanol steam reforming products. The engine is part of a series hybrid propulsion system and works at a steady-state single operating regime. In this work and attempt was made to optimize performance of the reformer – ICE system, to compare it with the performance of the same ICE fed by gasoline and ethanol and finally – to design a reformer-heatexchanger.

2. Methodology

Figure 1 shows the schematically layout of the considered reformer - ICE system.



Figure 1.Scheme of the integrated reformer – SI engine system.

Engine performance optimization for different types of primary and reformate fuels was carried out using the GT-Power software. GT-Power is the 2-and 4 stroke SI and CI engines simulation tool widely used nowadays by engine developers and researchers. GT-Power software has been thoroughly validated by its numerous users in many real-life applications [10-12].

A 1-D simulation approach is used in engine modeling. Prediction of the flow rates in the intake and the exhaust system is performed by using conservation equations (energy, mass, momentum). The entire system is divided into many small sub-volumes, separated by boundaries. At each time step for each sub-volume, the conservation equations: of mass, energy and momentum are solved. In each sub-volume the pressure, temperature and species concentration are considered uniform. For each boundary area the species velocity and mass flux are considered constant as well.

For modelling in-cylinder processes the following approaches were applied:

The fuel mass fractionx_bburned in the ICE cylinderswas modelled using the Wiebe function [13]:

$$x_{b} = \left\{ 1 - \exp\left[-a \left(\frac{\theta - \theta_{0}}{\Delta \theta} \right)^{m+1} \right] \right\}$$
(1)

Where: θ is the current crank angle; θ is the start of combustion angle; $\Delta \theta$ is combustion duration from 10% to 90% of the fuel, measured in degrees of crank shaft rotation; *m* is a form factor; *a* is a coefficient dependent on the combustion duration.

The in cylinder heat transfer coefficient h_c was calculated using the Woschni correlation for an engine without swirl [14]:

$$h_c = 3.26B^{-0.2} p^{0.8} T^{-0.55} w^{0.8}$$
⁽²⁾

where: h_c is the heat transfer coefficient [W/m*K]; B is the cylinder bore [m]; p is the motored cylinder pressure [kPa]; T is the volume average cylinder gas temperature [K]; w is the average gas velocity in the cylinder [m/s].

NOx and CO emissions were predicted by using the extended Zeldovich mechanism and a Kinetic model respectively, [7].

Main parameters of the engine used in the engine modeling are shown in table 1. The ICE simulated was a naturally aspirated direct injection (DI) SI engine.

	Tabl	e 1	l:	Main	parameters	of	the	SI	engine	ethat	was	used	in	the	simu	lation	s.
--	------	-----	----	------	------------	----	-----	----	--------	-------	-----	------	----	-----	------	--------	----

Cylinder bore (mm)	90
Piston stroke (mm)	90
Number of cylinders	4
Compression ratio	10
Rated speed (rpm)	4000
Rated brake power (kW)	75

The engine performance at the rated power and speed was modeled and analyzed for conditions of the engine feeding by products of steam reforming of ethanol (SRE) with properties taken from [9]. The reactions occurring in the reformer were modeled by using CHEM-CAD software applying chemical equilibrium approach.

We selected the rated power regime for the comparative analysis taking into account the following considerations:

• A necessity to evaluate maximal in-cylinder pressure and rate of the pressure rise under the engine feeding by hydrogen-rich reformate fuel featured by high burning velocities.

• A need to assess availability of exhaust gas energy and temperatures required for the reforming process.

Some of the assumptions applied in engine simulation are listed below:

• Due to negligible amounts of non-reformed ethanol found in the SRE products (less than 0.1% [9] at the simulated reforming conditions, ethanol content in the reformate fuels considered in the ICE modeling was assumed to be zero.

- Valves timing remained the same for all considered types of fuels.
- The engine geometry remained the same with a change in the fuel type.

• The energy required to cool gaseous SRE products and inject them into the engine's combustion chamber during the compression stroke was not assessed.

• High-pressure reforming was assumed to be applied thus enabling negligible energy investment to achieve high pressure of the SRE products.

• There are no leaks in the reformer – ICE system and no fuel accumulation between the reformer and the engine. Therefore, the mass flow-rate of the primary water / ethanol mixture entering the reformer is equal to the mass fuel consumption of ICE operating on SRE products.

• Actual burning velocities of the considered fuels inside a cylinder were assumed to be proportional to the appropriate laminar burning velocities (taking into account that the engine geometry remained the same with change of the fuel type).

• Ratio of actual combustion duration (10%-90%) of each SRE mixture to that of gasoline was assumed to be inversely proportional to the ratio of the laminar burning velocities of thesefuels [11]:

$$\frac{CD_i}{CD_{gas}} = \frac{v_{gas,l}}{v_{i,l}} \tag{3}$$

Where: CD_i and CD_{gas} are the actual duration (10%-90%) of the considered SRE mixture and gasoline, respectively; $v_{gas\ell}$ and $v_{i\ell}$ are the laminar burning velocities of gasoline and the considered SRE mixture, respectively.

Water-to-ethanol ratio W/E in the performed analysis was changed from 1 to 2.4 by intervals of 0.2. As mentioned above, the required energy for the reformer activation is intended to be supplied by the engine exhaust gases. Therefore, it is desired to minimize the reformer temperature. The minimum acceptable reformer temperature (900 K) is defined as the temperature where coke is still not formed in the process of ethanol reforming.

Air excess factor(λ) was considered in the range 1 to 1.7.

When the engine was fed by the reformate fuels, the efficiency (η_{sys}) of the reformer-engine system was calculated using as a basis the primary liquid ethanol consumption [10].

$$\eta_{system} = \frac{1}{Q_{LV_{Ethanol}} \cdot bsfc_{Ethanol}}$$
(4)

Where $bsfc_{Ethanol}$ is the brake specific fuel consumption of primary ethanol, [g/KWh]; $Q_{LV_{Et}}$ is the lower heating value of ethanol (26.75 MJ/kg).

$$bsfc_{Ethanol} = \frac{bsfc_{mix}}{m_{mix}}$$
(5)

Here $bsfc_{mix}$ is brake specific consumption of SRE products; m_{mix} is a mass of SRE products per 1 Kg of primary ethanol; m_{mix} is the mass of the reforming products per 1 Kg of liquid ethanol and was calculated as follows:

$$m_{mix} = \frac{M_{water} \cdot W + M_{Ethanol} \cdot E}{M_{Ethanol} \cdot E}$$
(6)

Here M_{water} and $M_{Ethanol}$ are the molecular weights of water and ethanol, respectively; W and E are the number of moles of water and ethanol, respectively.

Values of η_{sys} enabled a comparison of the reformer – ICE system efficiency with this one of the engine fueled by gasoline or liquid ethanol.

The power wasted with exhaust gases was calculated using the following equation:

$$P_{ex} = \dot{m}_{ex} \cdot Cp_{ex} \cdot \Delta T \tag{7}$$

Where \dot{m}_{ex} is the flow-rate of exhaust gases, [Kg/sec]; Cp_{ex} is the specific heat of the exhaust gases [J/kgK] and ΔT is the difference between the exhaust gases temperature $-T_{ex}$ and the reformer temperature T_{ref} , [K],

$$\Delta T = T_{ex} - T_{ref} \tag{8}$$

In order to compare the engine performance at various combinations of engine parameters and select the optimal one, several mathematical methods can be used. Sensitivity analysis can provide information about optimal combination of engine parameters. In this work sensitivity analysis was not performed. Instead, the following optimization function was suggested:

$$f = \frac{\eta_{sys}}{\eta_{sys}} \cdot w_{\eta_{sys}} + \frac{NOx_{\min}}{NOx} \cdot w_{NOx} + \frac{(\Delta T - 200)}{(\Delta T_{\max} - 200)} \cdot w_{\Delta T}$$
(9)

Where η_{sys} , NOx and ΔT are the system efficiency,NOx emission value and the temperature gap at specific values of λ and $\theta o.\Delta T = T_{ex}-T_{ref}$. $\eta_{sys_{max}}$, NOx_{min} and ΔT_{max} are the maximum system efficiency, minimum NOx emission and the maximum temperature gap that are obtained for each type of

considered fuel (defined by W/E ratioandT_{ref}). $w_{sys_{max}}$, $w_{NOx_{min}}$ and $w_{\Delta T}$ are the weighting factors in the optimization function (f). $\Sigma w_i = w_{sys_{max}} + w_{NOx_{min}} + w_{\Delta T} = 1$.

Three scenarios with different relative weight of engine efficiency, NOxemission and the temperature gap were studied to assess sensitivity of the final result to relative importance of each of the mentioned above parameters. The values of $w_{sys_{max}}$, $w_{NOx_{min}}$ and $w_{\Delta T}$ that were considered in this work are shown in table 2.

Scenario #	1	2	3
$\mathcal{W}_{\eta_{sys}}$	1/3	1/4	1/5
$w_{_{NOx}}$	1/3	1/4	2/5
$W_{\Delta T}$	1/3	1/2	2/5

 Table 2: Weighting factors of the optimization function f

These values were selected taking into account the obtained engine simulation results. The changes in the system efficiency were minor compared to the change in the temperature difference. ΔT has the biggest impact on the results due to the requirement to supply energy from the exhaust gases to the reformer. The engine working conditions that yielded the highest value of the optimization function (f) were considered as optimal. These working conditions were determined for each type of fuel considered in this research. Performance of the reformer-ICE systemwas optimized and compared for various fuel types.

The heat exchanger type that was considered in this analysis is Shell & Tube with cross-counter flow in line configuration. The surface (A) required for the heat exchanger was calculated using the following formula:

$$\dot{q} = U \cdot A \cdot \Delta T_{lm}$$

$$A = \frac{\dot{q}}{U \cdot \Delta T_{lm}}$$
(10)

where U is the overall heat transfer coefficient; \dot{q} is the total power required for the reformer in order to get the required reactions; $\Delta t_{\ell m}$ is the log mean temperature drop defined in [16].

$$\Delta T_{lm} = \frac{\Delta T_2 - \Delta T_1}{\ln\left(\frac{\Delta T_2}{\Delta T_1}\right)} = \frac{\Delta T_1 - \Delta T_2}{\ln\left(\frac{\Delta T_1}{\Delta T_2}\right)}$$
(11)

and

$$\Delta T_1 = T_{h,1} - T_{c,1} = T_{h,i} - T_{c,o} \tag{12}$$

$$\Delta T_2 = T_{h,2} - T_{c,2} = T_{h,o} - T_{c,i}$$
(13)

where: $T_{h,i}$, $T_{h,o}$ are the inlet and outlet hot temperatures respectively; $T_{c,i}$, $T_{c,o}$ are the inlet and outlet cold temperature, respectively.

The overall heat transfer coefficient was determined assuming negligible thickness of the heat exchanger tubes [16]:

$$U = (h_h^{-1} + h_c^{-1})^{-1}$$
(14)

The required heat exchanger surface is found using the equation (9) and (10). When the required heat exchanger surface is known, the length of the heat exchanger can be calculated:

$$L = \frac{A}{N \cdot \pi \cdot D} \tag{15}$$

Knowing the number N of the tubes, the heat exchanger dimensions were determined.

3. Results and discussion

3.1. SI engine performance optimization

The engine performance was predicted for the various reformate fuel types. Figure 2 shows an example of the engine performance simulation results.



Figure 2.System performanceVs. θ_0 , W/E=2.4 and T_{ref}=900K.

As can be seen from the results shown figure 2, there is a tradeoff between the requirements for minimum NOx emission and maximum system efficiency together with maximum exhaust gases temperature. In this work we analyzed and map this tradeoff to find the best possible ICE-reformer system performance. It is clear that achieving simultaneously the maximal efficiency together with minimal NOx formation and maximal temperature difference is impossible. Therefore, an analysis was performed using design of experiment to find the conditions that ensure the best possible performance. Also values of optimization function f (equation 8) were analyzed for different scenarios as described in table 2. This analysis was carried out for all types of reformate fuel. The optimal engine operating conditions for every SRE fuel (that meet the threshold value of $\Delta T = 200$ K) are summarized in table 3.

This table is organized from highest to lowest values of the W/E ratio. In order to distinguish between the different types of SRE fuels, they were marked from A to F as shown in table 3. As can be seen from table 3, better results are obtained at lower reformer temperature. Clearly, this is due to the requirement of the highest possible temperature gap between the exhaust gases and reforming temperature (defined as ΔT). Note that higher ΔT values would allow designing a more compact reformer-heat exchanger, which is a very important parameter in assessment of the system's feasibility.

				Inputs				Outputs
Fuel Identification	W /E	T _{ref} (K)	λ	Start of Combustion (deg)	Δ Τ	Exha ust temp. (K)	NOx(p pm)	Syste m efficiency (%)
А	2 .4	90 0	1 .1	19.5	2 52	1152	987	33
В	2	90 0	1 .06	15.7	2 51	1151	1485	34
С	2	10 00	1	18.5	2 43	1243	3050	34
D	1 .8	10 00	1	18.5	2 45	1245	3382	34
E	1 .6	10 00	1	20.5	2 63	1263	3496	33
F	1 .4	10 00	1	20	2 55	1255	3970	33

 Table 3. Optimized engine working conditions for various relevant ERP fuels

3.2. Reformer – ICE performance optimization.

The results of simulations show that maximal difference between the lower and higher system efficiency is about 3%. This variation is not very significant and there is a need to evaluate trends of variation of other factors and performance parameters to select the optimal reformer operating conditions.

As can be shown from table 3, the maximum system efficiency is reached where the reformer temperature is 1000K, and the second best value is reached for reformer temperature about 900K. On the other hand, minimum reformer temperature is required in order to maximize the temperature gap (ΔT) between the exhaust gases and the reformer temperature. There is no clear trend in dependence of the system efficiency on the W/E ratio and on the reformer temperature.

As can be seen, the maximal variation of the temperature gap (ΔT) values is about 20K out of about 263K. Such a variation is not negligible and should be definitely considered in selecting the appropriate reformer operating conditions. The highest temperature gap is obtained at W/E ratio of 1.6 and the reformer temperature is 1000K for SRE fuel type E.

As in the case of the system efficiency, no clear correlation was observed between the W/E ratio, the reformer temperature and the temperature gap. The main reason for this observation is dependency of the considered ICE-reformer system's parameters on a great majority of factors, in addition to the W/E ratio and the reformer temperature.

As can be seen, the obtained range of the NOx emission values varies from maximum of approximately 4000 ppm till minimum of about 990 ppm. It is clear that this variation is significant relative to observed variation in the system efficiency and the temperature gap. The lowest NOx emissions value is obtained at the W/E ratio of 2.4 and the reformer temperature of 900K for fuel type A. Some correlation is observed between the W/E ratio and NOx emissions. In general, NOx emissions decrease when W/E ratio increases. This dependence can be explained by increasing steam and CO_2 amounts that participate in the combustion process with increasing W/E ratio. Steam and CO_2 are diluents that inevitably lead to reduction of the maximal cycle temperature and as a result decrease the NOx formation. SRE fuel type C provides the maximal system efficiency (34%) but at the same time it produces very high NOx emissions (3050 ppm) at the acceptable temperature gap of 243K. SRE fuel type E allows to obtain the maximal temperature gap (263K), but leads to even higher NOx emissions (3496 ppm) at somewhat lower system efficiency of 33%.

It is clear that it is impossible to select the best possible reformer operating regime based only on these results.

Thus, the optimization function as defined in equation (9) was applied. The same three scenarios as defined in table 2 were tested for the purpose of selecting a best possible operating regime. The obtained results are shown in table 4.

Table 4: Selection of a best possible reformer operating regimeoptimization results

#	θ₀	λ	Scenario #1	Scenario #2	Scenario #3
Α	19.5	1.1	0.9278	0.9022	0.9217
В	15.7	1.06	0.8224	0.8192	0.7883
С	18.5	1	0.6687	0.6722	0.6025
D	18.5	1	0.6646	0.6770	0.6000
Ε	20.5	1	0.7471	0.8103	0.7047
F	20	1	0.6996	0.7429	0.6441

As can be seen from table 4, for all three scenarios the SRE fuel of type A provides maximal values of the optimization function of 0.90 to 0.93 as compared to 0.60-0.82 for the rest of compared With the selected reformer operating mode the following ICE-reformer system reformates. performance can be achieved – see table 5.

Fuel T	ype	Engine work conditions	king	yster	n performa	ance	
W/E	T _{ref} (K)	Combustio n start angle (deg)	λ	System Efficiency (%)	N Ox (ppm)	Exh aust Temp. (K)	$^{\Delta}_{T}$
2.4	900	19.5	1 .1	33	98 7	115 2	2 52

Table 5. The selected reformer operating mode and the achieved system performance

Based on the selected performance and operating mode of the ICE reformer system, a preliminary design of the reformer was accomplished.

3.3. Reformer-heat exchanger design

The hot and the cold stream conditions at the entrance to the reformer are known from the simulation. The total heat flowrate that is required to be transferred by the heat exchanger is $\dot{q} = 45 \text{kW}$. The cross flow shell-and-tube configuration of the reformer-heat exchanger was selected for this preliminary design because of the relative simplicity and effectiveness [16].

Dimensions of the designed reformer-heat exchanger geometric are listed in table 6. The reformerheat exchanger size is quite large: 39 x 89 x 73cm, which makes a feasibility of its mounting onboard a vehicle questionable.

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Vertical distance between the tubes, m	Horizontal distance between the tubes, m	Tubes Diameter, m	Reforme r height, m	Refor mer width, m	Reforme r length, m
0.02	0.03	0.015	0.35	0.89	0.73

Table 6 The designed heat exchanger - Geometric dimensions

4. Comparison with other fuels

To evaluate the achieved change in the engine performance by using ICE fed by SRE, a comparison with cases of engine feeding by gasoline and liquid ethanol was performed. For this purpose the available results from [11] were used. Table 7 shows ICE performance comparison for three types of fuel: gasoline (1), ethanol (2) and SRE fuel (3) as were selected in this study.

Performance parameter	Gasoli ne	Etha nol	SRE fuel W/E=2.4, T _{ref} =900K
λ	1.0	1.25	1.1
NO _x (ppm)	4400	510	987
CO (ppm)	10000	193	422
η_{sys} (%)	33	35	33

 Table 7. Comparison between different fuel types

As can be seen from table 7, ICE fed by SRE mixture provides the same efficiency as engine fed by gasoline, however allows much lower pollutant emissions. NOx emissions are reduced by a factor of 4.5, while CO emissions are reduced by a factor of 23.5. At the same time, the best system efficiency and lowest pollutant emissions were obtained when ICE is fed by liquid ethanol without applying the reforming process. It is clear that worsening efficiency of ICE with ethanol steam reformer is a result of the requirement to supply all the heat needed to sustain endothermic reactions of SRE from the engine exhaust gases. This forced a significant ignition retarding and, as anticipated, leads to the efficiency worsening. However, the heat required for SRE sustaining may be supplied not only from the exhaust gases, but also from combustion of additional unreformed ethanol.

Taking into account that combustion of unreformed ethanol in ICE leads to formation of very toxic and carcinogenic aldehydes all possible measures should be undertaken to minimize ethanol burning in engine cylinders. For this reason and considering the arguments reported above, an additional approach was evaluated in this work. The concept of this approach is to supply the required energy to the reformer both from the exhaust gases and the heat released as a result of after burning ethanol in the air-excess conditions. In this approach, the requirement for hightemperature of exhaust gases is not required. A simplified analysis to examine this approach was performed.

The ICE-reformer system's working conditions that were selected are those that allowed best possible engine performance. These ICE-reformer system working conditions are as follows:

W/E = 2.4;
$$T_{ref} = 900K; \theta_o = -11.3; \lambda = 1.41.$$
 (16)

These conditions yield the following performance:

$$\eta_{sys} = 38\%$$
; NOx = 490ppm; CO = 40ppm; T_{ex} = 945K. (17)

For the considered case, according to our simulation, the exhaust gas specific heat value and the exhaust gases flow rate are: 1313.5 J/kgK and 33.5 Kg/h, respectively. The total power required for sustaining endothermic reactions of SRE in the reformer is 45 kW and the ethanol higher heating value is 26.75 MJ/Kg. The outlet exhaust gases temperature will remain 808K. The total available exhaust power is 16.75 Kw, additional 28.25 kW (at least) should be supplied by the ethanol after-burning.

This power supply is achieved when 3.8Kg/h of ethanol are after-burned. Clearly the total system efficiency decreases due to the ethanol after burning. As showed this simplified analysis, the updated total ICE-reformer system efficiency is not higher than 33%. Taking into account that not all the available exhaust gases energy can be utilized, it is clear that the ICE-reformer system's efficiency will be lower. Thus, the updated performance of the ICE-reformer system is: $\eta_{sys} < 33\%$; NOx = 490ppm; CO = 40ppm; T_{ex} = 945 K.

So, the examined approach does not show a potential of efficiency improvement, but can be considered as a tool of emission reduction – table 7. To make a more precise assessment of the potential of emissions reduction, emission formation during ethanol after burning should be evaluated.

5. Conclusions

Analysis results demonstrate the capability of sustaining the endothermic reactions of the SRE in the reformer by using the heat of engine exhaust gases. The cross flow shell-and-tube configuration of the reformer / heat exchanger was selected because of its relative simplicity and effectiveness and designed. The reformer / heat exchanger'ssize is quite large $(0.39 \times 0.89 \times 0.73 \text{ m})$, which makes questionable its possible implementation in a vehicle. ICE with steam reforming of ethanol provides the same efficiency as the engine fed by gasoline. However, it allows obtaining much lower pollutant emissions. NOx are reduced by a factor of 4.5, while CO are reduced by more than order of magnitude (factor of 23.5). The energy efficiency of ICE fed with products of ethanol steam reforming is lower than that of the engine fed by liquid ethanol. An approach with ethanol after-burning where the required energy is supplied to the reformer from both the exhaust gases and the heat released as a result of ethanol burning was also investigated. The examined approach doesn't show a potential of efficiency improvement, but can be considered as a tool of additional emissions reduction.

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