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High-pressure thermo-chemical recuperation – a way toward sustainable propulsion systems

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Abstract

To meet GHG emission targets and to decrease oil dependency, overall energy consumption of road vehicles must be substantially reduced. Various types of propulsion technologies are under consideration, like internal combustion engine (ICE), hybrid electric (HE), plug-in hybrid electric (PHE), range extended electric (REE), electric battery, fuel cell, etc. The article provides a comparison of various propulsion technologies and arrives to the conclusion that internal combustion engines (ICEs) will be a major propulsion option in the foreseen future with massive penetration of hybrid vehicles to global markets. Utilization of more energy-efficient ICEs together with low-carbon-intensity fuels is, therefore, of great importance on a way toward development of sustainable propulsion systems. About one-third of fuel energy introduced to ICE is wasted with engine exhaust gases. A promising way of engine's waste heat recovery is by using the energy of the exhaust gases to sustain endothermic reactions of fuel reforming. This approach is called Thermo-Chemical Recuperation (TCR).
We go beyond the previous studies in this field by applying direct injection of the reformate gas together with the high-pressure steam-reforming process. We aim at developing a high-pressure TCR-ICE set as a part of a series hybrid propulsion system, thus alleviating the acute problems of the reformer's startup and transient behavior. The obtained experimental results showed that engine energy efficiency is improved by 18%-39% (higher values at lower loads) and pollutant emissions are reduced by 73-94%, 90-96%, 85-97%, 10-25% for NO_x, CO, HC and CO_2 emissions, respectively, compared with gasoline in a wide power range, without any need in exhaust gas aftertreatment.

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Keywords: Vehicle propulsion; Internal combustion engine; Waste heat recovery; Thermo-chemical recuperation; Methanol

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1. Introduction

The challenges of climate change require a continuous effort toward reduction of global environmental pollution and fossil oil consumption. Transportation is responsible for a significant share of the energy consumption worldwide. According to the International Energy Agency - IEA, about 23% of global CO2 emissions from fossil fuel combustion in 2013 were caused by transportation (IEA, 2015). It is likely to account for a higher share in the future, unless special measures are taken. Note that in the non-G20 countries the transportation share was 39% compared to 20% in the G20 area. Following the recommendation of the United Nations Intergovernmental Panel on Climate Change (IPCC), annual global greenhouse gas (GHG) emissions must be reduced by 50 - 85% by 2050 in comparison with the emissions level in 2000. Road vehicles are responsible for about three quarters of total energy consumption in the transportation segment and almost entirely dependent on crude oil (IEA, 2009). Thus, to meet GHG emission targets and to decrease oil dependency, overall energy consumption of road vehicles must be substantially reduced. Note that the necessary reduction in GHG emissions by vehicles should be achieved without any disruptions in transportation patterns and population mobility.

Vehicle's GHG intensity is determined by the following factors (Tartakovsky et al, 2012):

1) Energy quantity required by an average vehicle to carry out a given amount of transport activity in each transportation mode. This factor depends on the vehicle energy consumption.
2) Carbon intensity of the used fuel.
3) Total volume of transportation activity that depends on the number of vehicles in operation, their usage patterns, and is a function of the consumer demand.
4) Modal composition of transportation activity, which depends on the consumer choice, the mode pricing and the fiscal measures affecting mode selection.

The first two factors have the biggest impact on vehicle's GHG intensity. According to IEA assessment, above 80% of the reduction in GHG emissions can be attained through vehicles energy efficiency improvement and fuels decarbonization.

2. Comparison of various propulsion technologies

Various types of propulsion technologies are under consideration, like internal combustion engine (ICE), hybrid electric (HE), plug-in hybrid electric (PHE), range extended electric (REE), electric battery, fuel cell, etc. Note that the all mentioned above types of hybrid propulsion, like HE, PHE, REE, include ICE as an inherent part of the powertrain system. A number of studies have been performed to project main trends in vehicles propulsion development out to 2050 (Bastani et al, 2012; McCarthy, 2017). Most of experts agree that internal combustion engines will be a major propulsion option in the foreseen future with massive penetration of hybrid vehicles to global markets (Bastani et al, 2012; Thomas, 2017). Pure battery electric and fuel cell vehicles (designated in Fig.1 as BEV and FCHEV) are expected to remain niche products, with a total market share of about 10-12% by 2050 – Fig.1. Hybrid vehicles benefit from the latest advancements in both ICE and electric propulsion technology. This allows the hybrid vehicles to become a widespread measure of reducing energy consumption and GHG emissions. No substantial differences between the pure battery electric vehicles and the plug-in hybrid electric vehicles could be identified in terms of energy efficiency (Kobayashi et al, 2009; Berggren & Magnusson, 2012; Granovskii et al, 2006).

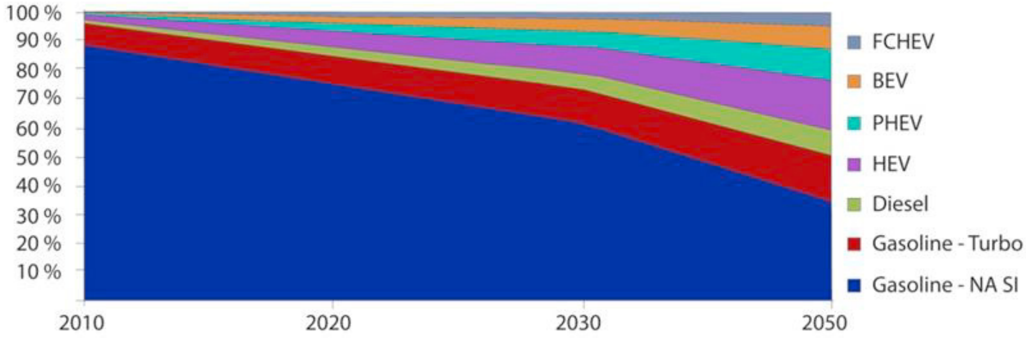

Fig. 1. Projected US sales volume of light-duty vehicles out to 2050, percent of market share (Bastani et al, 2012).

Two main reasons lead researchers to the mentioned above conclusions. First, a very significant gap between the energy density of liquid fuels and the most advanced electricity storage technologies, like Li-Ion batteries – Fig.2. Second, a vast potential of improvement in ICE efficiency and emissions reduction. According to Taylor (2008), efficiency of the gasoline-fueled SI engines can be improved by a factor of two (i.e. from about 30% to 60%). It should be noted also that life cycle emissions induced by battery electric vehicles can differ considerably in various geographic areas depending on the carbon intensity of the power generation mix. In countries with heavy use of coal as a feedstock for electric power generation (USA, China, India, etc.), the overall emissions of diesel cars nowadays can be equal or lower than those of corresponding electric vehicles (Doucette & McCulloch, 2011).

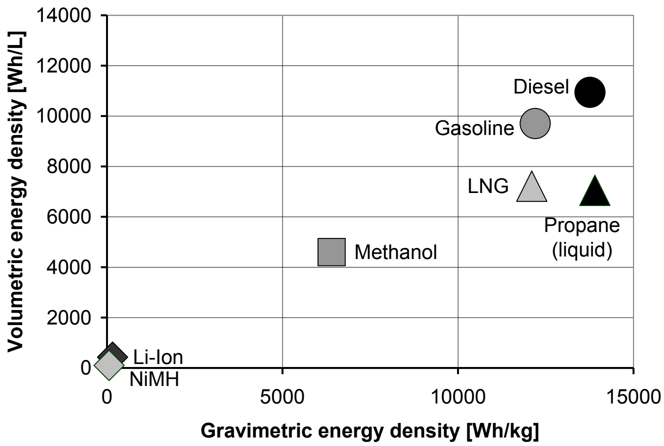

Fig. 2. Energy storage density of various sources (Tartakovsky et al, 2012).

A potential of various technologies to improve ICE energy efficiency is summarized in Table 1. All these technologies are sorted also by the level of market penetration readiness: production-intent – manufacturing is started or anticipated in next five years; emerging – manufacturing is anticipated in 10 years; long-term – manufacturing may be anticipated after 2025-2030.

Table 1 clearly demonstrates that an internal combustion engine is far from realizing its efficiency improvement potential and that the technologies that are expected to penetrate the market in a long-term perspective allow the largest efficiency gain. These technologies will require a considerable increase in the onboard computing power (for data interpretation, pattern recognition, simulation and prediction) together with flexible and adaptive powertrain control systems (Curran, 2017). As mentioned by Kobayashi et al. (2009) and Taylor (2008), some of these technological benefits are additive when multiple advancements are built into a powertrain, though synergistic effects may diminish the total efficiency gain.

Table 1. Increase of energy efficiency due to various engine technologies (Tartakovsky et al, 2012).

ICE technology	Efficiency increase, %	Market penetration readiness
Downsizing	8-10 (potential up to 20)	Production-intent
Friction reduction	1-5	Production-intent
Boosting	2-7	Production-intent
Accessories electrification	1-2	Production-intent
Variable valve train	4-10 (potential up to 20)	Production-intent
Direct injection in SI engine	3-15	Production-intent
Advanced fuel injection strategy	3-5	Production-intent
Engine idle stop	0.5-15	Production-intent
Cylinders deactivation	7.5	Emerging
Waste heat recovery	2-15	Emerging to long-term
Variable compression ratio	2-25	Emerging to long-term
Low temperature combustion concepts	Up to 50%	Long-term

It is important to underline that the mentioned above advancements in ICE energy efficiency are always considered in a conjunction with a need of maximal possible emissions reduction, whereas achieving the "zero-impact emissions" level together with a considerable efficiency improvement is an ultimate goal (McCarthy, 2017). Nowadays, engine exhaust gas aftertreatment is widely accepted as the most efficient way of emissions mitigation. Diesel Particle Filters (DPF) could be a good example. DPF enable reduction in emission of the most harmful ultrafine particles by more than 99 percent (Tartakovsky et al, 2015). Dramatic reduction of pollutants formation inside ICE cylinders can open new opportunities of emissions mitigation towards achieving the "zero-impact" target.

3. Thermo-chemical recuperation

Approximately 1/3 of the energy introduced to ICE with a fuel is wasted along with the hot exhaust gases (He et al, 2011). Thus, partial utilization of this energy, also known as waste heat recovery (WHR), can lead to a significant improvement in the overall ICE efficiency (Shu et al, 2016). One possible method of WHR is utilizing the energy of hot exhaust gases to sustain endothermic reactions of fuel reforming. This method is known as thermo-chemical recuperation - TCR. TCR has two main advantages. First, it increases a heating value of the fuel to be combusted because of the waste heat recovery through endothermic fuel reforming reactions — see Eq. (1-3). Second, a mixture of the gaseous reforming products (reformate) usually has a high hydrogen content, resulting in the increased burning velocity, higher antiknock quality and wider flammability limits (Verhelst & Wallner, 2009). Thus, TCR allows improvement in the ICE efficiency, not only due to the WHR, but also because of the lean-burn operation benefits (reduction in throttling and heat transfer losses), getting closer to the theoretical Otto cycle and the possibility of increasing the engine compression ratio.

Methanol decomposition (MD): $$CH_3OH_{(g)} \rightarrow CO + 2H_2 \ \Delta H = 90\ kJ/mol \quad (1)$$
Methanol steam reforming (MSR): $$CH_3OH_{(g)} + H_2O_{(g)} \rightarrow CO_2 + 3H_2 \ \Delta H = 50\ kJ/mol \quad (2)$$
Ethanol decomposition (ED): $$C_2H_5OH_{(g)} \rightarrow CH_4 + CO + H_2 \ \Delta H = 50\ kJ/mol \quad (3)$$

Ethanol and especially methanol are low carbon intensity alternative fuels which are widely considered as promising oil substitutes because of a possibility of their production from diverse fossil and renewable sources, such as biomass, coal, natural gas and renewable energy-derived hydrogen (Wang et al, 2015; Nguyen & Verhelst, 2017). Methanol and ethanol are also excellent primary fuels for the reforming purposes because they can be reformed at relatively low temperatures of approximately 250-300°C, thus making possible efficient exhaust heat recovery (Wheeler et al, 2011; Liao & Horng, 2016).

Alcohol reforming for ICE applications was investigated in the past and a possibility of up to 40% brake thermal efficiency (BTE) improvement compared to the gasoline counterparts was demonstrated. However, a number of major drawbacks were identified. The main problems that were reported include catalyst deactivation, system's startup and transient behavior, uncontrolled combustion and maximal power loss due to reduced volumetric efficiency (Pettersson & Sjostrom, 1991). The latter is a result of supplying gaseous reformate into the intake system that reduces the partial pressure of the air in the intake manifold, and the absence of an evaporative cooling effect compared to the case of a liquid fuel port injection.

In the previous works (Tartakovsky et al, 2015; Poran & Tartakovsky, 2015), we suggested a novel concept of direct-injection ICE with High-Pressure TCR (Fig.3). Direct injection of the reforming products allows prevention of the uncontrolled combustion and the power loss problems. We showed that performing the reforming reactions at high pressure is essential to enable direct injection of the reformate. Otherwise, a significant fraction of the engine power would be required to compress the reformate prior to its injection. The cold start and transient behavior problems can be resolved by integrating the High-Pressure TCR system in a hybrid-electric propulsion scheme and/or keeping a small on-board pressurized vessel with reformate for startup or injection of some of the primary fuel with a port fuel injector (Tartakovsky et al, 2011).

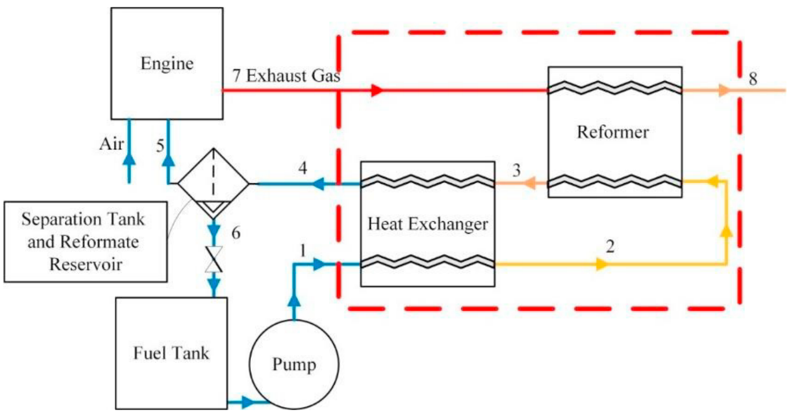

Fig. 3. Schematic layout of the High-Pressure TCR system. 1 – methanol and water mix (1:1 molar ratio) at high pressure; 2 – preheated methanol and water mix; 3 – hot reforming products with residues of unreformed methanol and water; 4 – cooled reforming products with condensed unreformed methanol and water; 5 – cooled gaseous reformate; 6 – condensed unreformed methanol and water; 7 – hot exhaust gas; 8 – cooled exhaust gas (Poran & Tartakovsky, 2017b).

Results of experiments performed with a single-cylinder, direct-injection SI engine designed to operate with direct injection of various gaseous fuels, like MSR or ED reformates, methane (a major constituent of natural gas), as well as a carburetor gasoline-fed engine (baseline configuration), demonstrated great improvement in the combustion process and the resulting engine performance and emissions. A possibility of unthrottled and much more stable engine operation in the entire loads range was demonstrated – Fig.4.

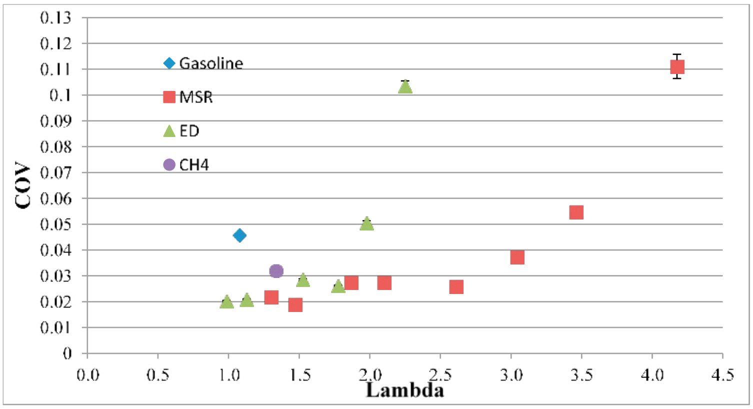

Fig. 4. Cycle-to-cycle variation (COV) as a function of excess air factor (Lambda) for various fuels. Engine speed 2800 rpm. The MSR and ED operation at wide-open throttle and the injection pressure of 40 bar. The error bars show the uncertainty of the calculated COV values (Poran & Tartakovsky, 2017a).

The mentioned in Fig.4 cycle-to-cycle variation is a measure of ICE combustion stability and usually is expressed by the coefficient of variation (COV):

$$COV = \frac{\sigma_{IMEP}}{IMEP} \tag{4}$$

where σ_{IMEP} is the IMEP standard deviation and IMEP is the average indicated mean effective pressure of all considered cycles (at least 100). IMEP is known from thermodynamics as:

$$IMEP = \frac{\int pdV}{V_d} = \frac{W_{i,g}}{V\ \ d} \tag{5}$$

where V_d is the displaced volume; V is the instantaneous cylinder volume; p is the instantaneous in-cylinder pressure; and $W_{i,g}$ is the gross indicated work.

The main reason of better ICE operation stability is higher laminar burning velocity of the hydrogen-rich reformate. Fuel burning velocity has significant influence on the cycle-to-cycle variability since it influences the early flame development and thus affects the overall heat release rate. The higher burning velocity of a fuel-air mixture reduces the cyclic variations and hence has a beneficial effect on engine efficiency and emissions. The results of experimentally achieved improvement in efficiency and pollutant emissions of ICE fed with methanol reforming products are shown in Fig.5.

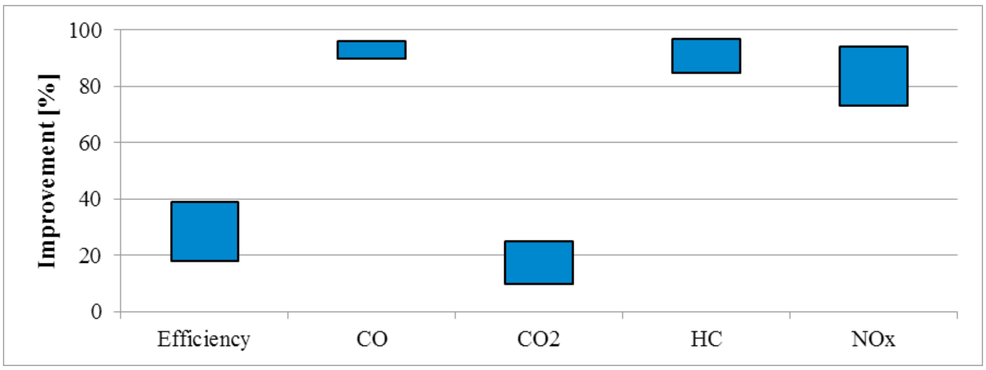

Fig. 5. Improvement in efficiency and pollutants emission of ICE fed with MSR reformate compared to conventional gasoline. Single-cylinder DI SI engine, speed 2800 rpm, injection pressure 40 bar, start of injection 127 CAD BTDC (Poran & Tartakovsky, 2017b).

The obtained experimental results showed that engine efficiency is improved by 18%-39% (higher values at lower loads) and pollutant emissions are reduced by 73-94%, 90-96%, 85-97% for NOx, CO and HC emissions, respectively, compared with gasoline in a wide power range, without any need in exhaust gas aftertreatment.

4. Conclusions

Internal combustion engines have a vast potential of improvement in efficiency and emissions reduction. They will continue to be a major propulsion option in the foreseen future. Hybrid vehicles have a greatest potential to become a widespread measure for reducing energy consumption and GHG emissions.

Any advancements in ICE energy efficiency are always considered in a conjunction with a need of maximal possible emissions mitigation. Achieving the "zero-impact emissions" level together with a considerable efficiency improvement is an ultimate goal of future ICE development.

Thermo-chemical recuperation is a promising method of waste heat recovery that allows simultaneous improvement in ICE efficiency and pollutant emissions. We go beyond the previous studies in this field by applying direct injection of the reformate gas together with the high-pressure steam-reforming process. The obtained experimental results showed that ICE efficiency is improved by 18%-39% (higher values at lower loads) and pollutant emissions are reduced by 73-94%, 90-96% and 85-97% for NOx, CO and HC emissions, respectively, compared with gasoline in a wide power range and without any need in exhaust gas aftertreatment.

A prototype of the direct-injection ICE with High-Pressure TCR was successfully developed and is undergoing extensive study in the Technion ICE Laboratory.

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