Improvement of Engine's Energy Efficiency and Emissions Reduction by Thermo-Chemical Recuperation of Exhaust Gas Energy

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Introduction

Energy efficiency improvement is one of society's most important instruments for mitigating climate change. Transportation is responsible for a large part of the energy consumption worldwide. According to International Energy Agency (IEA) data, about 26% of all energy-related CO_2 emissions in 2007 were caused by transportation (IEA, 2010). It is likely to account for a higher share in the future, unless special measures are taken. To limit the long-term global heating down to acceptable levels, United Nations Intergovernmental Panel on Climate Change (IPCC) recommended that annual global greenhouse gas (GHG) emissions must be reduced by 50 - 85% by 2050 in comparison with the emissions level in 2000 (IPCC, 2007). According to the IEA's BLUE map scenario (IEA, 2010), above 80% of the projected GHG emission mitigation may be achieved by improvement of vehicle efficiency, introduction of alternative fuels and electricity decarbonization – Fig. 1.

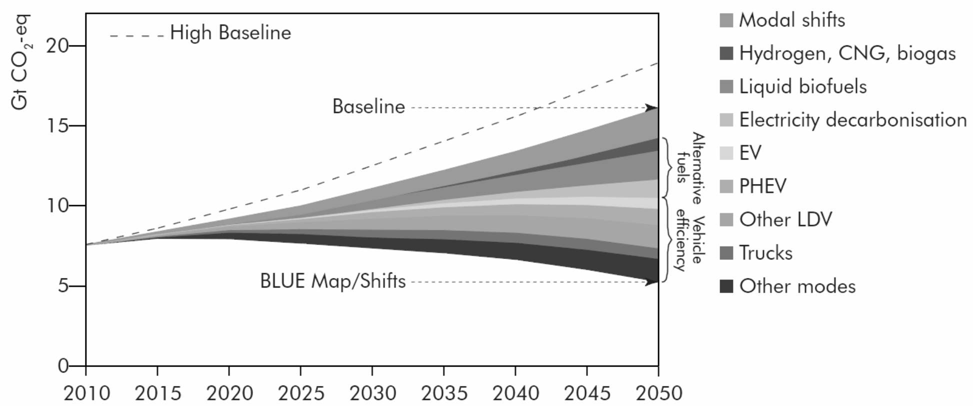


Figure 1: IEA prediction of GHG emissions reduction (IEA, 2010). Energy Technology perspectives © OECD/IEA, 2010

Results of recent studies suggest that there is a big potential for improvement of internal combustion engine (ICE) technologies (Berggren and Magnusson, 2012; FURORE, 2003; Kobayashi et al., 2009; Taylor, 2008). It is well known that about 30% of fuel energy introduced to ICE is wasted with engine exhaust gases (Berggren and Magnusson, 2012). Its utilization can lead to a significant improvement of ICE energy efficiency.

Reformer-ICE system

One of the ways to recover an engine's waste heat is by using the energy of the exhaust gases to promote endothermic reaction of alcohol steam reforming – ASR (Chakravarthy, 2010; Tartakovsky et al., 2011a). In principle, any renewable fuel may be used, not only alcohol. ICE is fed by the gaseous products of ASR, 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 more efficiently burned in the engine compared with the original fuel. This approach, called thermo-chemical recuperation (TCR), is considered nowadays as one of the possible methods of increasing powertrain efficiency and reducing emissions (Chakravarthy, 2010).

Most studies published on TCR are focused on gas turbine applications (Carapellucci and Milazzo, 2005; Carapellucci, 2009; Cocco et al., 2006; Harvey et al., 1995; Mohamed, 2003; Verkhivker and Kravchenko, 2004). Ivanic et al. (2005) studied a partial fuel reforming for ICE.

Computational analysis of a spark ignition (SI) engine performance was performed by Galloni and Minutillo (2007) for partial gasoline replacement by a reformate gas. In their work the reformate gas was produced by exothermic partial oxidation of gasoline rather than bio-fuel. Some efforts have been made to feed ICE with methanol reforming products (Brinkman and Stebar, 1985). The 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.). The catalytic reformer, if used in the motor vehicle, should operate efficiently in a wide range of fuel flow rates and exhaust gas temperatures because of engine load and speed changes. Low initial temperatures during the engine cold start and warm-up result in a non-efficient operation of the reformer. The requirement of addressing any momentary change in engine load leads to a serious complication of the fuel supply and engine control systems. 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 in the work (Brinkman and Stebar, 1985). 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. 2) having an additional energy source which provides a basis for overcoming these drawbacks.

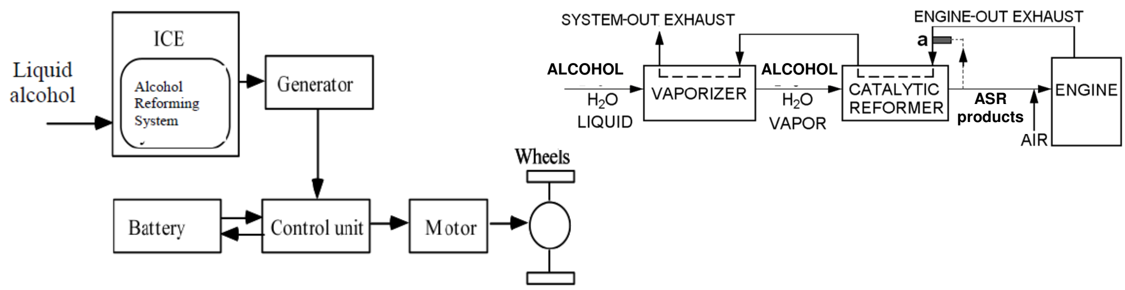


Figure 2: Hybrid propulsion system with a reformer-ICE.

Energy analysis of alcohol reforming

The thermodynamics of alcohol steam reforming aimed at hydrogen production for fuel cell applications has been widely discussed in the literature. Alcohols that are mainly considered for this purpose are ethanol (Vadya and Rodrigues, 2006; Wang and Wang, 2008; and others) and methanol (Zhou et al., 2009; Mingheng et al., 2012; and others). 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):

$CH_3OH \leftrightarrow 2H_2 + CO$ $\quad\Delta H_I$=91 kJ/mol (1)

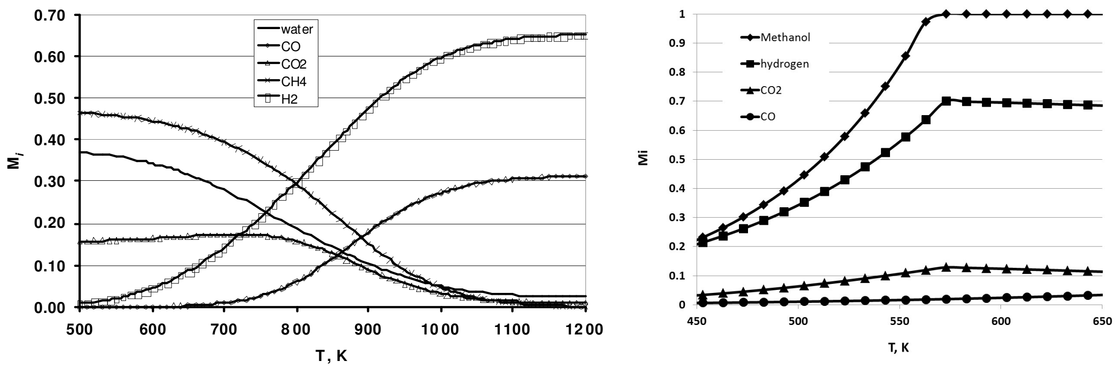
$CO + H_2O \leftrightarrow H_2 + CO_2$ $\quad\Delta H_{II}$=-41 kJ/mol (2)

$CH_3OH + H_2O \leftrightarrow CO_2 + 3H_2$ $\quad\Delta H_{III}$=50 kJ/mol (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 overall 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 CO_2 and H_2 is undesirable, because CO_2 is a diluent gas and does not carry energy. Therefore, for ICE fuelling, realization of the reaction (1) would be preferable with negligible WGS reaction extent. In ICE the exhaust heat is used to promote on-board reforming of alcohol or other hydrocarbon fuel into a mixture of hydrogen and carbon monoxide with small amounts of contaminants (carbon dioxide, methane, soot etc.). Because this gas 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 CO_2 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. One important parameter that should be used in reformer optimization is the energy efficiency of the ASR process (Tartakovsky et al., 2011b), 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):

$$\eta = (H_{out} - H_{in}) / H_d \qquad (4)$$

Simulation of alcohol steam reforming was performed for ethanol and methanol by using the Equilibrium Reactor and Gibbs Reactor models of the CHEMCAD software package. For methanol the CHEMCAD calculation results were empirically corrected based on the available experimental data to account for the non-equilibrium reforming behaviour. Molar fractions, M_i, of ASR products were calculated at atmospheric pressure for various water/alcohol (W/A) ratios and different reaction temperatures. Examples of the obtained results are shown in Fig. 3.

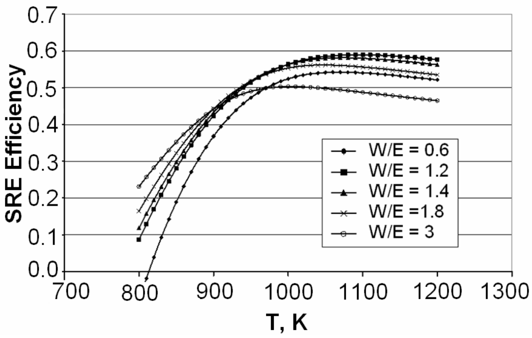


Ethanol reforming, W/A=1.2 Methanol reforming, W/A=0.5

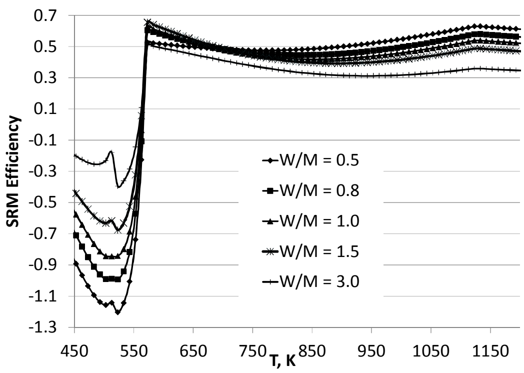
Figure 3: Alcohol steam reforming products – example of simulation results.

For ethanol reforming hydrogen yield approaches maximal value of $M_{H2} \approx$ 65 % at W/A=1.2 and T=1100K. If methanol is used as a primary fuel, the maximal hydrogen yield of 70% can be achieved at W/A=0.5 and $T \approx$ 570K. The larger hydrogen yield is explained by the higher H:C ratio of methanol compared with ethanol. Much more significant benefit of methanol over ethanol is in the substantially lower reforming temperature: about 570K compared with 1100K for ethanol.

Fig. 4 shows the energy efficiency of ASR for ethanol and methanol as a function of the W/A ratio and reaction temperature. Simulation results show that the energy efficiency of methanol steam reforming approaches maximal value of 0.66 at W/A=1.3 and reaction temperature of approximately 570K. The maximal energy efficiency of ethanol steam reforming is somewhat lower. It was found that for ethanol η achieved a maximum of approximately 0.59 at W/A=1.2 and $T \approx$ 1100K. The difference between the maximal achievable values of energy efficiency for the compared fuels is not significant, however again: for methanol it can be achieved at much lower temperature. This makes methanol the preferred option for realization of the TCR concept.



(a)



(b)

Figure 4: Energy efficiency of ASR. (a) – ethanol; (b) – methanol.

Analysis of the ICE-reformer system performance

A theoretical prediction of ICE performance and total efficiency of the ICE-reformer system was made for the example of ethanol reforming. Modelling of ICE performance was carried out by using GT-Power software. The simulated engine size and main parameters were selected while taking into consideration that the engine is a part of a series hybrid propulsion system and the prevention of too high in-cylinder maximal pressure under moderate engine speed. Optimization of the engine size and operation regime was not performed. The simulated engine was a naturally aspirated, direct injection (DI), SI engine. ICE performance was modelled and analysed for the engine fuelling by gasoline, liquid dehydrated ethanol and ASR products. Detailed description of the engine used in calculations and simulation methodology appears in (Tartakovsky et al., 2011a). The main results are shown in Table 1.

Table 1: ICE performance and pollutants emission – simulation results

Fuel type	Energy efficiency	CO emission	NO_x emission	CO_2 emission
Gasoline	100%	100%	100%	100%
Liquid ethanol	104%	29%	13%	96%
ASR products	113%	10%	19%	88%

As can be seen from the Table for the example of ethanol reforming, application of TCR concept makes possible energy efficiency improvement by up to 13% together with a significant reduction of pollutant emissions. ICE operation with ASR products resulted in a significant reduction of CO emissions: by a factor of 2.9 compared with ethanol and by the order of magnitude – compared with gasoline. NO_x emissions of the SI engine fuelled by ASR products were decreased approximately by a factor of 5 compared with the engine feeding by gasoline. They still remain slightly higher compared with liquid ethanol. This fact is explained by very high burning velocity of hydrogen rich ASR products. However, appropriate optimization of the engine operation regime (e.g. mixture leaning together with ignition advance optimization, etc.) will make possible further reduction of NO_x emissions. ICE feeding with ASR products allows also reduction of GHG CO_2 emission by 12% and 8% compared with gasoline and ethanol, respectively.

Conclusions

Thermo-chemical recuperation is considered nowadays as one of the promising methods of powertrain efficiency increase and emissions reduction. An on-board reformer cannot work efficiently in a wide range of engine operation regimes typical for a road vehicle, especially at transient modes and cold-start conditions. In case of a hybrid propulsion system, which always has an additional energy source, these shortcomings can be easily overcome.

Alcohol reforming with aid of exhaust gas energy allows on-board production of a hydrogen rich gaseous fuel for ICE that contains up to 64-70 molar per cent of hydrogen. The main benefit of methanol over ethanol is in the significantly lower reforming temperature: about 570K compared with 1100K for ethanol. Simulation results show that the energy efficiency of methanol steam reforming approaches a maximal value of 0.66 at *W/A*=1.3 and the reaction temperature of approximately 570K.

Application of TCR concept makes possible energy efficiency improvement by up to 13% together with a significant reduction of pollutant emissions. CO emissions can be reduced by a factor of 2.9 compared with ethanol and by the order of magnitude – compared with gasoline. NO_x emissions of the SI engine fuelled by ASR products may be decreased approximately by a factor of 5 compared with the engine feeding by gasoline. ICE operation with ASR products allows also reduction of GHG CO_2 emission by 12% and 8% compared with gasoline and ethanol, respectively.

Acknowledgement

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