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Thermo-Chemical Recuperation as an Efficient Way of Engine's Waste Heat Recovery

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Abstract. It is known that about 30% of fuel energy introduced to an internal combustion engine (ICE) is wasted with engine exhaust gases. One of the promising ways of waste heat recovery is thermo-chemical recuperation (TCR). For the purpose of TCR realization, in principle any fuel may be used. However, utilization of renewable bio-alcohols, especially ethanol or methanol is the most favorable. The advantages of TCR over turbocharging are in the fact that its energy transfer is not limited by isentropic expansion and that the reforming process improves the fuel properties. A comprehensive theoretical analysis of the ICE with TCR was carried out using the developed model for simulation of the joint operation of ICE with alcohol reformer, when the ICE is fed by the alcohol reforming products and the energy of the exhaust gases is utilized to sustain endothermic reforming reactions. Simulation results show that it is possible to sustain endothermic reforming reactions with a reasonable reactor size. Modeling results point out a possibility of engine's efficiency improvement by up to 13% in comparison with ICE feeding by gasoline together with achievement of zero-impact pollutant emissions.

Introduction

Improvement of the vehicles energy efficiency is one of society's most important instruments for mitigating climate change. Road transportation is responsible for about three quarters of total energy consumption in the transportation segment [1]. Energy consumption of light-duty vehicles accounted for the major share, with about 50-60%. Nowadays, road transportation is almost entirely dependent on crude oil. Transport contribution to the GHG emissions will substantially increase in the future, unless special measures will be undertaken. 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% towards 2050 in comparison with the emissions level in 2000 [2]. Expert assessments show that 80% of the projected GHG emission reduction can be reached by improvement of vehicle efficiency and introduction of alternative fuels [3]. The latter would enhance also the security of energy supply. Therefore, in order to meet GHG emission targets, as well as to decrease oil dependency, overall energy consumption of road vehicles must be reduced significantly. The major challenge in reaching this goal is that the necessary reductions in the carbon emissions by vehicles must be achieved without disruptions in transportation patterns and population mobility.

Waste heat recovery

It is known that about 30% of fuel energy introduced to ICE is wasted with engine exhaust gases. Utilization of this energy may provide substantial improvement of engine efficiency. Turbocharging is a widely applied and well known method of the waste heat recovery (WHR). However, at the turbine exit of a conventional turbocharger, a high exergy of exhaust gas is still available. Utilization of the two-stage turbocharging architecture [4] may contribute to further WHR improvement. For some usage patterns the turbo-compounding approach that applies an additional power turbine coupled with the electric generator may be an attractive option [5]. Energy efficiency improvement by turbo-compounding is assessed by experts at about 2 %. Higher amounts of the waste exhaust energy can be utilized in a Rankine cycle, where exhaust heat feeds into a steam generator to produce a steam, which is used through the steam turbine/generator system to convert the recovered exhaust waste heat into electrical power [6]. The latter may be used to assist the engine, charge the battery or cover the onboard electrical power demand. It was demonstrated that up to 50% of the exhaust gas exergy can be recovered when a WHR system based on the Rankine cycle is employed. This means that engine efficiency improvement of about 10 percent may be achieved [6]. Several automakers have announced R&D activities in different thermoelectric devices. The latter rely on the Seebeck effect and can directly convert part of the exhaust heat to electric power, without the use of mechanically moving parts. They provide some additional benefits such as noise and vibrations absence, sometimes no moving fluids and a high reliability. Nonetheless, significant system design challenges, such as low conversion efficiency with current technology and the relatively high costs of the thermoelectric semiconductor materials, should be overcome during development of the thermoelectric technology. Latest advances in the semiconductor materials have paved the road to further development that could permit the improvement of powertrain efficiency by 5–10 percent [7].

Thermo-chemical recuperation

Another way to recover engine's waste heat is by using the energy of exhaust gases to promote endothermic reactions of fuel reforming. This method is frequently called thermo-chemical recuperation (TCR) [8]. Fig. 1 shows a scheme of ICE with TCR.

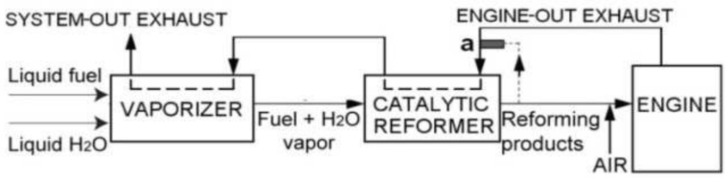

Fig. 1. Internal combustion engine with thermo-chemical recuperation

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 because of the high hydrogen content in the fuel. 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 allows faster combustion and use of higher compression ratio compared with the primary liquid fuel, thus resulting in higher engine thermal efficiency. The TCR approach is considered nowadays as one of the promising methods of powertrain efficiency increase and emissions mitigation.

The idea of TCR through alcohol decomposition or reforming has been investigated in the last few decades. Pettersson and Sjostrom [9] reviewed most of the research efforts in the field up to the early 90's. The main problems reported in these preceding studies were backfire, coke formation on the reformer, cold start difficulties, lower maximum power due to reduced air charging, formaldehyde formation (in the cases of liquid methanol burning) and pre-ignition. Latest studies accomplished by researchers from MONSANTO in cooperation with MIT and AVL [10] overcame some of these drawbacks by feeding the ICE with low temperature ethanol reformate consisted of equal molar fractions of hydrogen, CO and methane. In this study we consider a hybrid direct injection (DI) ICE-alcohol steam reforming system (Fig. 2) as another way of solving these problems.

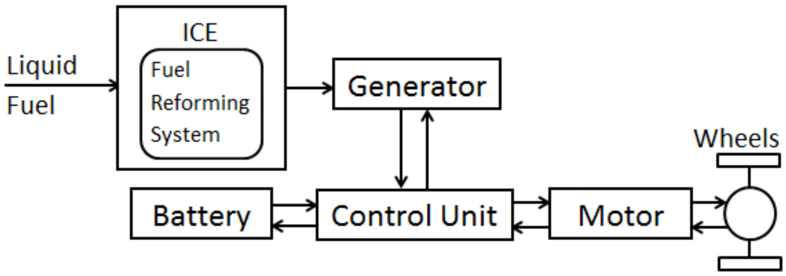

Fig. 2. Hybrid propulsion system with on-board fuel reforming

In this concept a battery of the hybrid system can be used as an energy source for cold start. Steam reforming of alcohol is less sensitive to coke formation than alcohol decomposition. The DI method can allow increase in the ICE maximum power output, prevent volumetric efficiency deterioration and deal with pre-ignition problems. A detailed analysis of this concept and its benefits is provided in [11].

Modeling ICE with TCR

It is clear from the scheme in Fig. 1 that the engine performance depends on the composition of the reforming products and the reforming products are affected by the exhaust gas temperature, flow rate and composition. Due to the tight interrelations between these two parts of the considered ICE-reformer system, it is desirable to have a single model that simulates their joint operation and takes into account their mutual dependence.

Such a model can be used for determining the required properties of the reformer and its design. It can provide a tool for optimizing the design and operation parameters of the ICE-reformer system. Further on, this model can be useful in studying the complicated transient behavior of the system. The importance of the model is that it provides a rather simplified way of exploring any ICE-reformer system by using the commercial engine simulation software, and thus can help other research groups working on other TCR schemes.

The model simulating joint operation and mutual effects of an engine and a reformer as interdependent parts of the whole system of ICE with TCR was developed and validated. Its detailed description appears in [12]. In this paper main features of the model and its capabilities are provided.

The model was developed based on the GT-Power software for the case of methanol as a liquid fuel that undergoes the steam reforming process in the reactor. However, the developed approach may be applied also with other engine simulation tools, such as WAVE of Ricardo, FIRE of AVL, etc. In the developed simulation tool a 1-D homogeneous reformer model (i.e., ignoring interphase and intraphase concentration and temperature gradients) of a packed bed reactor (PBR) is considered. This type of reactor is very common and provides a high flexibility in selection of a catalyst type and pellets size. Radial gradients are assumed to be negligible. For simplicity a counter-current tube-in-tube heat exchanger-reactor contained of 100 tubes was created. Fig. 3 shows an example of a small scale reformer model as it was built in the GT-Power. The reformer is divided to a number of mixed sections. Each section has uniform fluid properties. Since there is no available experimental data that suggest numeric values of the coefficients in the Wiebe model adjusted to the gaseous fuel compositions considered in the current work, an approach suggested in [13] was applied. Actual burning velocities of the considered fuels inside a cylinder were assumed to be proportional to the appropriate laminar flame velocities. Laminar flame velocity for each of the considered gaseous fuel compositions was estimated based on the published experimental data.

Woschni correlation for an engine without swirl was used for calculation of the in-cylinder heat transfer.

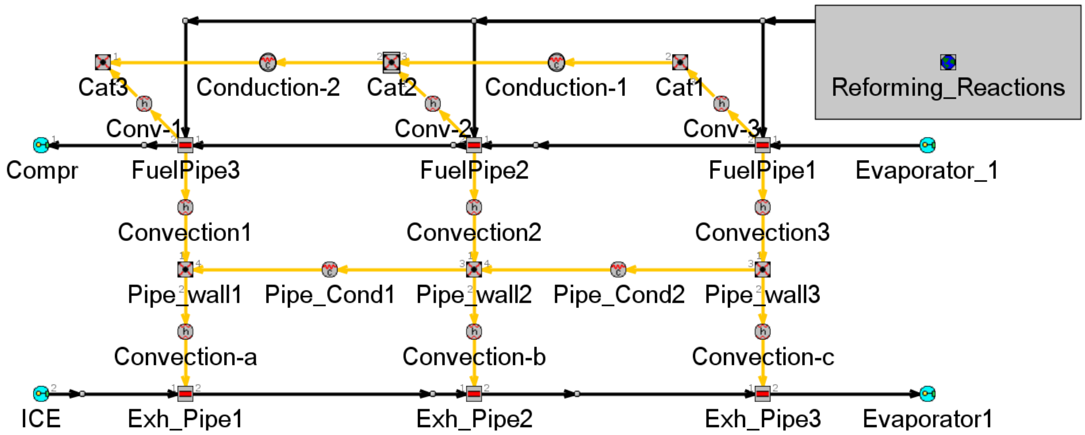

Fig. 3. Alcohol reformer as it was modelled in GT-Power

The developed simulation tool facilitates studying the combined effects of reformer design and engine operation parameters on the performance of the whole ICE-reformer system, optimization of the heat-exchange process in the reformer, study of pressure effects, investigation and understanding processes inside this complex system during various transient events, etc.

Fuels suitable for ICE with TCR

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. 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. In cases where 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 usually overcome by combusting an additional primary fuel and thus reducing the energy efficiency improvement. In principle, any fuel may be used in ICE with TCR. However, alcohols' reforming is most frequently considered with a main focus on methanol and ethanol as possible primary fuels.

Comparative performance analysis

The developed simulation capabilities were used for the performance analysis of ICE with TCR in comparison with an engine fed by gasoline and primary liquid alcohols ethanol and methanol. Feeding ICE-reformer system by the reforming products of two different alcohols: ethanol and methanol was considered. Effects of the steam reforming of methanol (SRM), ethanol (SRE) and the low-temperature ethanol reforming (LTER) methods on the system’s energy efficiency and pollutants formation were analyzed. Main parameters of the engine used in the performance modelling are shown in Table 1. It is a naturally aspirated, direct injection, SI engine.

Table 1. Main parameters of the simulated engine.

Cylinder bore [mm]	Piston stroke [mm]	Cylinders number	Compression ratio	Rated speed [rpm]	Rated brake power [kW]
90	90	4	10	4000	75

The results of energy efficiency comparison are shown in Fig. 4. ICE with TCR powerplant that applies steam reforming of 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. Efficiency of the engine fed by the low-temperature ethanol reformate has become worse not only in comparison with the reference liquid fuel – ethanol but even in comparison with gasoline. This is explained by the lower burning velocity of this reformate compared with the steam reforming 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 reformate volume compared with liquid primary fuels.

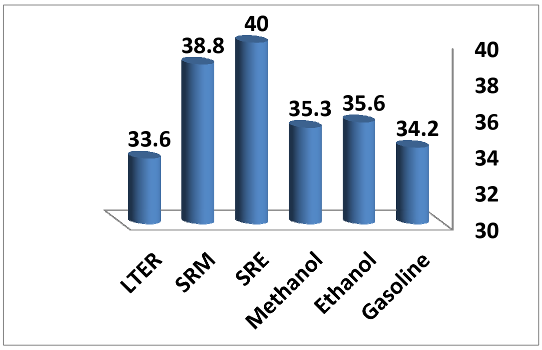

Fig. 4. Energy efficiency comparison of the ICE with TCR powerplant and SI engine fed by liquid fuels, %.

A comparison of engine NO_x emissions for the considered fuels is shown in Fig. 5. Engine feeding by ethanol steam reforming products 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 methanol steam reforming products 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 were lower by factors of 4.5 and 29, respectively, in comparison with the case of gasoline. The low-temperature ethanol reformate did not allow such a substantial decrease of NO_x emissions. They dropped down only by a factor of 1.45 compared with gasoline.

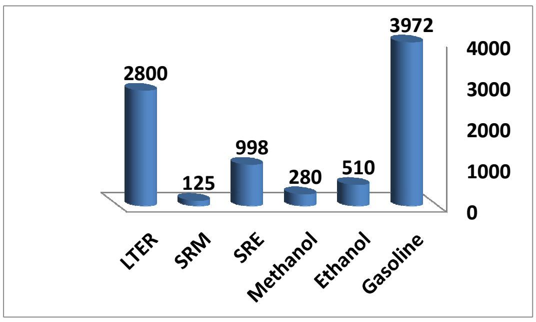

Fig. 5. Comparison of NO_x emissions, ppm.

Summary

Thermo-chemical recuperation is one of the promising ways of engines' waste heat recovery. The advantages of TCR over turbocharging are in the fact that its energy transfer is not limited by isentropic expansion and that the reforming process improves the fuel properties. The reforming mixture has higher octane number compared with a primary fuel. Therefore, the thermal efficiency can be further improved by increasing the compression ratio. It is desirable to have a single model that simulates joint operation of ICE and reformer, and takes into account their mutual dependence. Such a model was developed and can be used for determining the required properties of the reformer and its design, as well as for study and understanding processes inside this complex system during various transient events. Modeling results showed that efficiency of the reformer-engine powerplant fed by SRE and SRM products increases by 17% and 13%, respectively in comparison with the case of the engine feeding by gasoline. The lowest NO_x emissions are obtained with the engine feeding by SRM products. These emissions are lower by a factor of 29 compared with gasoline.

Acknowledgements

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