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Energy efficiency of a direct-injection internal combustion engine with high-pressure methanol steam reforming

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ABSTRACT

This article discusses the concept of a direct-injection ICE (internal combustion engine) with thermo-chemical recuperation realized through SRM (steam reforming of methanol). It is shown that the energy required to compress the reformate gas prior to its injection into the cylinder is substantial and has to be accounted for. Results of the analysis prove that the method of reformate direct-injection is unviable when the reforming is carried-out under atmospheric pressure. To reduce the energy penalty resulted from the gas compression, it is suggested to implement a high-pressure reforming process. Effects of the injection timing and the injector's flow area on the ICE-SRM system's fuel conversion efficiency are studied. The significance of cooling the reforming products prior to their injection into the engine-cylinder is demonstrated. We show that a direct-injection ICE with high-pressure SRM is feasible and provides a potential for significant efficiency improvement. Development of injectors with greater flow area shall contribute to further efficiency improvements.

1. Introduction

It is well known that in an ICE (internal combustion engine) about 30% of the energy introduced with the fuel is wasted along with the hot exhaust gases [1]. Utilizing a part of this energy, also known as WHR (waste heat recovery), can lead to a significant increase in the overall ICE efficiency. Several ways of WHR considered nowadays are: turbocharging [2], turbo-compounding [3], Rankine cycle [4], thermo-electric [5], cabin cooling [6], in-cylinder WHR [7] and others. The most mature and widely used method of waste heat recovery is the well-known turbocharging [8]. The hot exhaust gases can also be used to sustain endothermic reactions of fuel reforming. This method is often referred to as TCR (thermochemical recuperation) [9]. TCR has two main advantages over turbocharging. Firstly, the amount of energy that might be utilized from the exhaust gases is not limited by isentropic expansion. Secondly, the gaseous mixture of the reforming products (reformate) usually have high hydrogen content resulting in increased flame velocity, higher octane number,wider flammability limits and reduced combustion irreversibility [10]. Thus, the TCR contribution to the ICE efficiency improvement is not only due to the increased LHV (lower heating value) of the fuel, but also owing to lean operating possibilities, getting closer to the theoretical Otto cycle and a possibility of increasing the engine's CR (compression ratio). Bio-alcohols, such as methanol and ethanol, are excellent candidates for TCR since they can be reformed at relatively low temperatures to yield high hydrogen-content reformate. Commonly investigated reforming schemes are methanol decomposition – MD (1), methanol steam reforming - SRM (2), and low-temperature ethanol reforming (3).

$$CH_3OH_{(g)} \rightarrow CO + 2H_2 \quad \Delta H = 90\ kJ/mol \tag{1}$$

$$CH_3OH_{(g)} + H_2O_{(g)} \rightarrow CO_2 + 3H_2 \quad \Delta H = 50\ kJ/mol \tag{2}$$

$$C_2H_5OH_{(g)} \rightarrow CH_4 + CO + H_2 \quad \Delta H = 50\ kJ/mol \tag{3}$$

In our study we focus on methanol because it can be reformed at low temperature (~573K) and produced from abundant and widely available sources such as coal and natural gas, as well as from renewable sources such as bio-mass. Hence, it is considered to be a promising alternative fuel for ICE's [11]. Usually the fuel reforming is carried out under atmospheric pressure, but it can also be executed at elevated pressures. Peppley [12] investigated the possibility of onboard high-pressure SRM for a proton-exchange-membrane fuel cell vehicle.

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Nomenclature

Symbols

BTE	brake thermal efficiency
C_D	flow discharge coefficient
C_i^T	concentration of active site i, mol/m^2
d_R	injector reference flow diameter, mm
ΔH	enthalpy of reaction, kJ/mol
K_i	equilibrium constant of reaction i
k_i	rate constant of reaction i, m^2/(s·mol)
LHV	lower heating value, MJ/kg
$\dot{m}$	mass flow rate into the cylinder mg/s
$\dot{m}_{CH_3OH}$	methanol mass flow rate, kg/s
P_b	engine brake power, kW
P_{comp}	compressor power consumption, kW
p	static outlet pressure, Pa
p_o	total inlet pressure, Pa
p_i	partial pressure of species i, bar
R	gas constant, J/(kg·K)
r_i	rate of reaction i, mol/(s·m^2)
S/M	steam to methanol molar ratio
T_o	upstream stagnation temperature, K
W/F	ratio of catalyst load to initial methanol flow rate, kg·s/mol

Greek symbols

γ	specific heat ratio
ρ_o	upstream stagnation density, kg/m^3

Subscripts

D	methanol decomposition
NC	without compression power consideration
R	steam reforming of methanol
W	water gas shift
WC	with compression power consideration

Superscripts

*	ratio of equilibrium or rate constants
(i)	adsorption site i

Acronyms

BTDC	before top dead center
CNG	compressed natural gas
CR	compression ratio
DI	direct injection
ICE	internal combustion engine
IRFD	injector reference flow diameter
IVC	inlet valve close
MD	methanol decomposition
PBR	packed bed reactor
SOI	start of injection
SRM	steam reforming of methanol
TCR	thermo-chemical recuperation
TDC	top dead center
WGS	water gas shift
WHR	waste heat recovery
WOT	wide open throttle

The idea of TCR is not new. In the 1980s various research groups studied TCR through methanol decomposition [13] and had even built cars [14] reporting up to 40% increase in the BTE (brake thermal efficiency) compared to gasoline-fed cars. In these studies reformate fuel was supplied to ICE through fumigation. The main problems that were reported are: cold start, pre-ignition, backfire, knock and coke formation on the catalyst surface [13].

In the last years TCR has regained an interest due to the raising environmental awareness and soaring oil prices [15]. Low-temperature ethanol reforming, which yields equal molar parts of CO, CH_4 and H_2, has been thoroughly investigated [16]. It was reported that 50% fuel reforming lead to a significant improvement (10%–17%) in BTE at medium and light loads over the E85 reference fuel. In that study, a dual port fuel injection system was used: one for the reformate supply, and another one - for the liquid E85 injection. Tartakovsky et al. [17] suggested using the ICE-reformer system as part of a hybrid propulsion scheme, where an additional energy source, e.g. a battery, is used for startup, thus resolving the cold start problem and improving the transient response of the propulsion system. The pre-ignition problems of ICE with TCR were solved by some authors [16] through limiting the hydrogen content in the induced fuel by partial fuel reforming at light and medium loads, and using the liquid unreformed fuel at high loads. Even if the pre-ignition problems of ICE operating with stoichiometric air–hydrogen mixture and fuel supply to intake manifold or port fuel injection would be resolved, its maximal power output still will be lower by about 17% compared to a same-size gasoline engine. The latter is a result of the high partial volume of hydrogen in the mixture and absence of the charge cooling due to the liquid fuel evaporation in the intake manifold [18].

DI (Direct injection) as the fuel supply method can solve the described above problems. Researchers from the Argonne National Lab found that for a hydrogen-fueled engine, DI is the most promising method of achieving high BTE, power density comparable to gasoline engines and resolving the pre-ignition and backfire problems [19]. They reported on a high-efficiency low-NO_x turbocharged H_2-ICE with injection pressure of 100 bar [20]. In various CNG (compressed natural gas) [21] and hydrogen [20] DI-ICE studies, the injection pressures varied from 20 to 100 bar. In the mentioned above studies high injection pressure was used for several reasons. The first - is to allow late injection during the compression stroke and thus enable mixture stratification. The second reason is a possibility of limiting the compression work increase caused by rise of the partial volume of gaseous fuel in the air-fuel mixture compared to the liquid-fuel counterpart. Retarded fuel injection may reduce this negative influence, but requires high injection pressure to overcome the pressure build-up in the cylinder. Other benefits of high-pressure injection are increased fuel penetration into the densely-charged cylinder and chocked flow through the injector that simplifies the fuel flow-rate control. In the mentioned above works the hydrogen\CNG was stored onboard in pressurized vessels that were pressurized outside a vehicle. Hence, the energy required to compress the gas to the high pressure was obviously not considered in the overall ICE efficiency analysis.

Considering the described above advantages of DI, applying it in an ICE with TCR was suggested [22]. This would allow preventing the backfire, pre-ignition and reduced maximal power problems without a need to limit hydrogen content of the reformate gas or to inject a liquid non-reformed fuel at high engine loads. A potential of significant improvement in efficiency of a DI-ICE with TCR over a gasoline counterpart was demonstrated. However, the analysis did not include consideration of the energy required for reformate-gas compression. In contrast to the engines fed by a gaseous fuel from the compressed-gas vessels, in the case of TCR, when the gaseous