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

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ABSTRACT

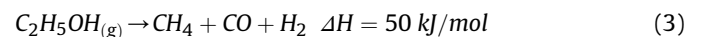
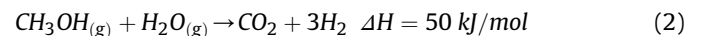
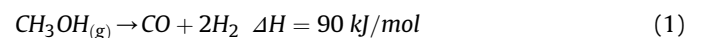
This article discusses the concept of a direct-injection ICE (internal combustion engine) with thermo-chemical recuperation realized through SRM (steam reforming of methanol). It is shown that the energy required to compress the reformat gas prior to its injection into the cylinder is substantial and has to be accounted for. Results of the analysis prove that the method of reformat 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.

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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 (reformat) 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 reformat. Commonly investigated reforming schemes are methanol decomposition – MD (1), methanol steam reforming - SRM (2), and low-temperature ethanol reforming (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, CH₄ and H₂, 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 H₂-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

reformate-fuel is produced onboard, the energy required to compress the gas prior to its injection to the engine's cylinder has to be taken into account.

The main goal of the reported study is to analyze the concept of ICE with TCR and direct reformate injection, and to discuss a method that might allow substantial improvement of the efficiency of a DI-engine with TCR.

2. Model description

For the purpose of a comprehensive analysis of the ICE-TCR system, a model of a DI-ICE with a chemical reformer was devel-

2.1. Reformer model

The reformer was modeled as 1-D, homogenous, CuO/ZnO/Al₂O₃-catalyst, counter-current packed-bed reactor (PBR). Intra-phase and interphase concentration and temperature gradients were not considered. Radial gradients within the PBR were assumed to be negligible. The above approximations are commonly used and can give good simulation results under the operating conditions considered in this work [25]. Reaction kinetics was modeled using the rate expressions suggested by Peppley [12] based on his development of a Langmuir–Hinshelwood mechanistic model:

$$r_R = \frac{k_R K_{CH_3O}^* \left(\frac{p_{CH_3OH}}{p_{H_2}^{0.5}} \right) \left(1 - p_{H_2}^3 p_{CO_2} / K_R p_{CH_3OH} p_{H_2O} \right) C_{S_1}^T C_{1a}^T}{\left(1 + K_{CH_3O}^* \left(\frac{p_{CH_3OH}}{p_{H_2}^{0.5}} \right) + K_{HCOO}^* p_{CO_2} p_{H_2}^{0.5} + K_{OH}^* \left(\frac{p_{H_2O}}{p_{H_2}^{0.5}} \right) \right) \left(1 + K_{H(1a)}^{0.5} p_{H_2}^{0.5} \right)} \quad (4)$$

$$r_W = \frac{k_W K_{OH}^* \left(\frac{p_{CO} p_{H_2O}}{p_{H_2}^{0.5}} \right) \left(1 - p_{H_2} p_{CO_2} / K_W p_{CO} p_{H_2O} \right) C_{S_1}^T}{\left(1 + K_{CH_3O}^* \left(\frac{p_{CH_3OH}}{p_{H_2}^{0.5}} \right) + K_{HCOO}^* p_{CO_2} p_{H_2}^{0.5} + K_{OH}^* \left(\frac{p_{H_2O}}{p_{H_2}^{0.5}} \right) \right)^2} \quad (5)$$

$$r_D = \frac{k_D K_{CH_3O}^* \left(\frac{p_{CH_3OH}}{p_{H_2}^{0.5}} \right) \left(1 - p_{H_2}^2 p_{CO} / K_D p_{CH_3OH} \right) C_{S_2}^T C_{2a}^T}{\left(1 + K_{CH_3O}^* \left(\frac{p_{CH_3OH}}{p_{H_2}^{0.5}} \right) + K_{OH}^* \left(\frac{p_{H_2O}}{p_{H_2}^{0.5}} \right) \right) \left(1 + K_{H(2a)}^{0.5} p_{H_2}^{0.5} \right)} \quad (6)$$

oped and applied. In this model, an ICE with TCR utilizing steam reforming of methanol is considered. A flow chart of the ICE-SRM system is shown in Fig. 1.

This system is comprised of two main parts that have mutual effect on each other. The hot exhaust gases leaving the ICE are being utilized to sustain the endothermic chemical reactions in the reformer and the gaseous reformate leaving the reformer is used as a fuel for the ICE. Due to the mutual effects the ICE and the reformer have on each other, the developed model considers joint operation of the engine and the reformer. Out of the two main parts of the ICE-SRM system, the ICE is the more complex one. Therefore, a decision was made to use validated engine-development software, such as GT-Power, and to model a reformer within this software.

Heat transfer architecture of the reforming system is an aspect that has to be taken into account. For example, the hot exhaust gases leaving the engine can flow first to the reformer and then to the evaporator/super-heater as in Ref. [23] or in the opposite direction as in Ref. [24]. In this study we considered the latter case where the exhaust gases are first utilized to evaporate the water-methanol mixture and then enter the reformer. This arrangement was chosen to meet the high energy requirement of the evaporation stage and to diminish the problem of catalyst over-heating. This configuration also has drawbacks, but in this study only one possible design of the reforming system was considered. Heat transfer optimization in the reforming system is not discussed herein.

where: r_R, r_W, r_D are reaction rate expressions of SRM, WGS (water-gas-shift) and MD, respectively; k_R, k_W and k_D are reaction rate constants of SRM, WGS and MD, respectively (calculated by Arrhenius expression); K_R, K_W and K_D are equilibrium constants of the SRM, WGS and MD, respectively. The expression for calculation of the latter constants was taken from Ref. [26]. Other equilibrium constants (i.e. K_i) were calculated using van't Hoff equation; C_i^T - active site concentration for each type of active site on the catalyst; p_i - the partial pressure of species i . Further information regarding the constants can be found in Ref. [12].

To avoid division by 0 at the initial conditions, small hydrogen fraction (10^{-18}) was supplemented to the calculated hydrogen fraction. Therefore, the partial pressure of hydrogen was never zero. When simulating ICE-TCR-system performance at steady-state conditions, the thermal mass of the components could be reduced to achieve faster thermal conversion. When the reforming process is considered, the limiting regime in terms of methanol conversion is the engine rated power. Thus, simulations were performed for the latter operating mode. At these conditions the high flow rate through the reformer increased the Péclet number to a value where the conductive heat transfer along the reformer's axis became to be negligible. A segment of the reformer model, as it was built in the GT-Power software, is shown in Fig. 2.

The heat transfer coefficients between the reforming gases and the reformer wall (Convection 1–3 in Fig. 2) were taken from Ref.

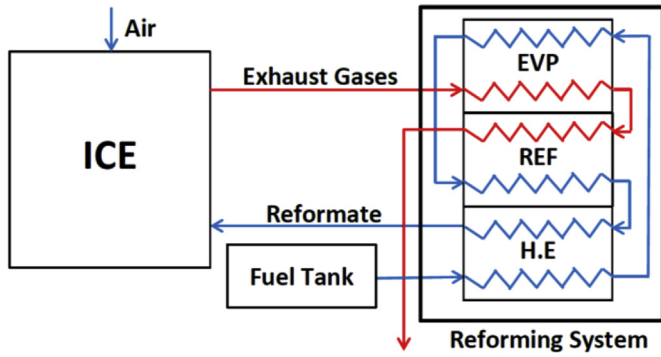


Fig. 1. Flow chart of the ICE-SRM system. EVP-evaporator & super-heater, H.E-heat exchanger, REF-reformer.

[25]. The convection coefficient for the heat transfer between the reformer wall and the exhaust gases was taken from Ref. [27].

2.2. Engine model

The engine model applied in these simulations is similar to the one described in Ref. [28], where it is depicted in further details. Main parameters of the simulated engine are given in Table 1.

The in-cylinder heat transfer was calculated using Woschni correlation for an engine without swirl. Combustion was simulated using Wiebe model. Because values of Wiebe coefficients for the varying compositions of the reformat fuel were missing, it was assumed that combustion duration is proportional to the laminar burning velocity of the fuel. The laminar burning velocities of various reformat mixtures were estimated using published experimental data [29–31] and results of the measurements carried-out in our laboratory.

After leaving the reformer, the reformat gas enters a heat exchanger where it is cooled-down while heating the cold

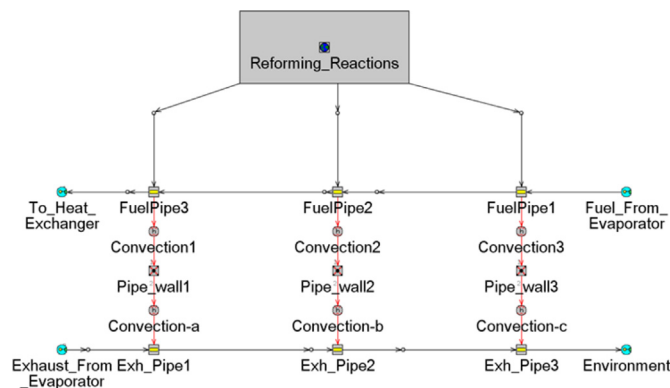


Fig. 2. Segment of the reformer model.

Table 1
Main parameters of the simulated engine.

Cylinder bore	90 mm
Piston Stroke	90 mm
Number of Cylinders	4
Compression ratio	10:1
Rated Speed	4000 rpm
Rated Brake Power	75 kW
BMEP	9.8 bar
IVC	120 CAD BTDC

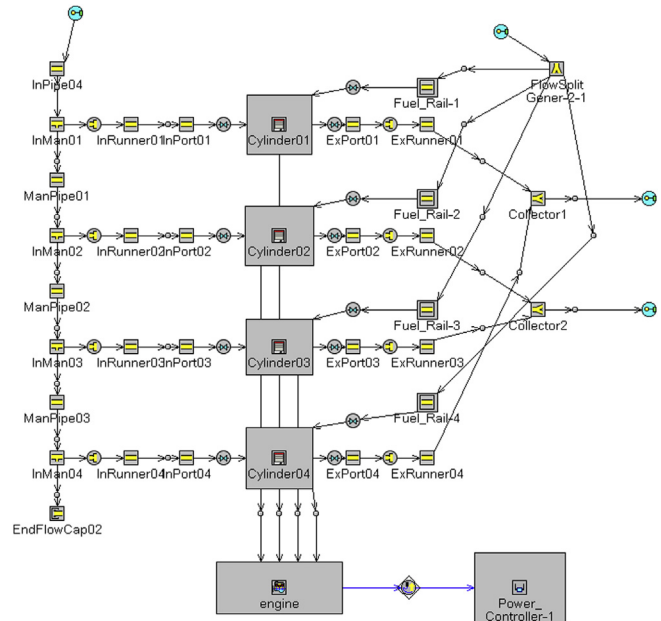


Fig. 3. Engine model in the GT-Power software.

methanol-water mixture – Fig. 1. Then, the cooled reformat is injected into the cylinder through the fuel injector. A PID controller regulates the injectors' opening duration to maintain the desired power value. The injectors and PID controller are shown in the GT-Power model of the engine (Fig. 3).

Throughout this paper brake thermal efficiency (BTE) values were calculated using eq. (7):

$$BTE_{WC} = \frac{P_b - P_{comp}}{\dot{m}_{CH_3OH} \cdot LHV_{CH_3OH}}; BTE_{NC} = \frac{P_b}{\dot{m}_{CH_3OH} \cdot LHV_{CH_3OH}} \quad (7)$$

Where: BTE_{WC} - BTE considering the compression power requirement; BTE_{NC} - BTE without considering the compression power requirement; P_b - engine brake power; P_{comp} - compressor power consumption (calculated assuming ideal gas and isentropic efficiency of 0.7); \dot{m}_{CH_3OH} - methanol mass flow rate; LHV_{CH_3OH} - liquid methanol lower heating value (19.9 MJ/kg).

2.3. Steam-to-Methanol ratio considerations

Steam-to-methanol (S/M) ratio is defined as the molar ratio of H_2O to CH_3OH at the entry to the reformer. Low S/M ratios are advantageous in terms of the higher heating value of SRM products and lower heat amount that is required for water evaporation and heating. The main drawback of low S/M ratios, especially those lower than 1, is an increased tendency of coke formation and deactivation of the catalyst [32]. Therefore, in this work S/M ratio of 1 was used. Obviously, if the coke formation problems would be resolved as suggested in Ref. [33], the MD process will be superior to SRM.

3. Model validation

The chemical model of the reformer is based on reaction kinetics developed and presented by Peppley in Ref. [12]. To validate our model of the reformer, we have reconstructed the experimental conditions of Peppley's experiments and changed, exactly as Peppley did, the catalyst surface area, so the prediction results would account for catalyst deactivation due to coke formation. The

Table 2
Comparison of the model predictions with experiments of Peppley [12].

Experimental run	Temperature [K]	Pressure [bar]	W/F [kg·s/mol]	S/M ratio	Experimental Methanol Conversion [12]	Predicted Methanol conversion
1	513	1.01	3.14	1	0.13 ± 0.01	0.13
	513	1.01	3.65	1	0.14 ± 0.01	0.14
	513	1.01	4.25	1	0.15 ± 0.01	0.16
	513	1.01	6.35	1	0.21 ± 0.01	0.21
	533	1.01	5.38	1	0.35 ± 0.02	0.34
	533	1.01	1.37	1	0.13 ± 0.01	0.13
2	533	1	83	1	0.98 ± 0.02	0.98
	533	39	83	1	0.85 ± 0.02	0.79

Table 3
Comparison of the model predictions with experiments of Agrell [34].

Temperature [K]	Pressure [bar]	W/F [kg·s/mol]	S/M ratio	Experimental Methanol Conversion [34]	Predicted Methanol conversion
533	1.01	24	1.3	1	0.97
533	1.01	15.4	1.3	0.95	0.91
533	1.01	9.1	1.3	0.85	0.80
598	1.01	6.03	1.3	1	1
578	1.01	6.03	1.3	0.95	0.99
556	1.01	6.03	1.3	0.88	0.89
543	1.01	6.03	1.3	0.75	0.77

validation runs were designed to check whether the model accurately predicts methanol conversion in conditions of varying pressure, temperature and W/F ratio (W – catalyst load; F – methanol flow-rate at the entry to the reformer). The predicted and experimental results are shown in Table 2.

The results of experimental Run 1 show that the model predicts well values of methanol conversion as a function of reforming temperature and W/F ratio variations. All the prediction results are within the range of the experiments error. The prediction of methanol conversion dependence on pressure variation (Run 2) gives an error of 7%, which is less accurate compared with the Run 1 predictions, but still acceptable.

In his work Peppley performed mainly differential rate experiments [12]. The experimental data on integral reactor measurements at high conversion and pressure is limited. To further validate our reformer model for high methanol conversion and temperature values, as well as different type of CuO/ZnO/Al₂O₃

catalyst, we also used experimental results obtained by Agrell [34]. Table 3 shows a comparison of the simulation results with data experimentally measured by Agrell [34].

Table 3 shows that the developed model provides acceptably accurate prediction in terms of methanol conversion for various temperatures, W/F and S/M ratios, at different catalyst formulations, and experimental setups. The maximal error of the methanol conversion prediction does not exceed 7%, while the average error is 3%.

To check the influence of an error in the methanol conversion prediction on the obtained BTE_{NC} values, a sensitivity analysis was performed (for $P_b = 75$ kW, $n = 4000$ rpm, injection pressure 111 bar, injector reference flow diameter 1.74 mm and injection temperature 373K). The obtained results indicate that changing the methanol conversion value within the relevant range (0.95–0.7) has a minor effect on the engine BTE_{NC}, not exceeding 0.5%. Thus, we can conclude that the prediction error of methanol conversion does not lead to a significant error in the calculation of engine efficiency.

With regard to the engine model, GT-Power is extensively validated commercial software, which is widely used worldwide in engines development. Therefore, it was not necessary to validate the model of the engine.

4. Results and discussion

4.1. Energy penalty of gaseous fuel compression

In the case of onboard fuel reforming, the energy necessary for compression must be taken into account. Even though isothermal compression consumes less power than adiabatic isentropic compression, in many applications, including automotive, it is more common to refer to adiabatic isentropic compression since there is not enough time for substantial heat transfer from the compressed gas during the compression process. Better efficiency may be achieved by subdivision of the compression process into multiple stages and gas intercooling between the stages. Of course, the latter approach has drawbacks of weight and volume increase together with design complication. Fig. 4 shows the energy required for compression of various gaseous fuels (as a fraction of the fuel's lower heating value – LHV) vs. compression ratio. This calculation

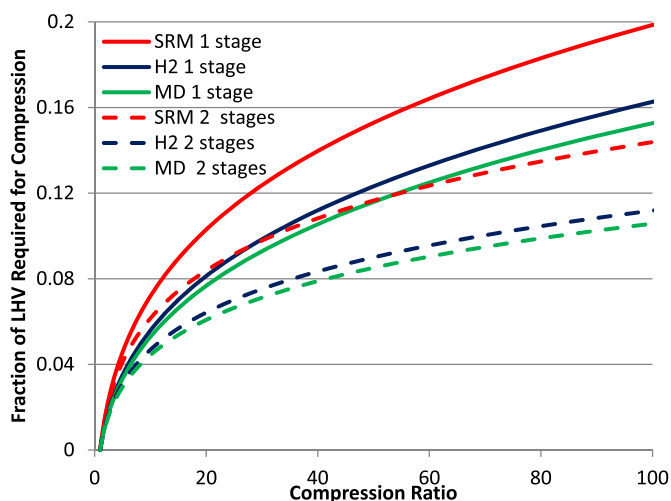


Fig. 4. Fraction of the gaseous fuel LHV required for 1- and 2-stage gas compression (SRM: 75% H₂, 25% CO₂; MD: 67% H₂, 33% CO). Temperature at the start of compression is 350K.

was performed assuming ideal gas and typical compressor isentropic efficiency of 70% [35].

The energy required for compression of SRM products is higher than that of hydrogen and MD products in terms of LHV percentage because of the diluent CO₂ fraction which is compressed, but does not contribute to the LHV of the gaseous fuel. Compression of the considered SRM mixture with a pressure ratio of 10 would consume about 7.2% of the mixture's LHV, which represent 18% of the ICE power generation for BTE_{NC} of 0.4. For hydrogen and MD mixtures the power consumption is slightly lower, but still results in an intolerable fraction of the engine's power that should be invested to gas compression. The compression ratio also dictates the compressor types and number of stages needed, whereas high compression ratios would probably require larger and heavier equipment. Therefore, if the onboard fuel reforming is done under atmospheric pressure, high pressure DI would not be advantageous.

It is clear that the injection pressure, fuel supply strategy and injector design are mutually interrelated. The compressible flow equations for un-choked (8) and choked (9) mass flow [36] reveal a possibility to deliver adequate fuel quantities even at pressures lower than 20 bar.

$$\dot{m} = C_D \frac{\pi d_R^2}{4} \rho_o \left(\frac{p}{p_o} \right)^{1/\gamma} \sqrt{\gamma R T_o} \left\{ \frac{2\gamma}{\gamma-1} \left[1 - \left(\frac{p}{p_o} \right)^{\frac{\gamma-1}{\gamma}} \right] \right\}^{0.5} \quad (8)$$

$$\dot{m}_{ch} = C_D \frac{\pi d_R^2}{4} \rho_o \sqrt{\gamma R T_o} \left\{ \frac{2}{\gamma+1} \right\}^{\frac{\gamma+1}{2(\gamma-1)}} \quad (9)$$

Where: \dot{m} -mass flow rate into the cylinder; C_D -flow discharge coefficient; d_R - the injector's reference flow diameter – IRFD. The latter represents the diameter of the injector flow area, if it would have a circular cross-section; ρ_o - upstream stagnation density; p - static outlet pressure p_o - total inlet pressure; R - gas constant; T_o - upstream stagnation temperature; γ - specific heat ratio.

This could be done by increasing the IRFD so the injectors would be able to deliver a large amount of fuel in a short time early in the compression stroke. There are several obstacles that prevent implementation of this strategy. First, the cylinder head is normally crowded, thus making difficult placing a big injector. Second, the injector would have to withstand high forces resulting from great in-cylinder combustion pressures and large injector diameter. An additional shortcoming of the low-pressure fuel injection is that the fuel is delivered to the cylinder early in the compression stroke and then is compressed prior to the combustion. This results in an increase of the compression work with a subsequent reduction of BTE. The later the injection, the smaller is the negative compression work.

4.2. Effects of fuel direct injection strategy

To quantify benefits and drawbacks of the direct-injection method, an analysis was performed of effects and mutual relationship of various fuel direct-injection strategies. Influence of injection pressure, injection timing, IRFD and injection temperature on efficiency of the ICE-reformer system was examined.

4.2.1. Effects of IRFD and injection timing

The injection pressure required for operating the engine at its rated power for different IRFD and start of injection (SOI) values is shown in Fig. 5. The flow discharge coefficient, C_D , was conservatively set to 0.7 based on the published experimental data for CNG-DI engine [37]. Duration of the injector's opening and closing events was assumed to be 1 crank angle degree (CAD). Mixture

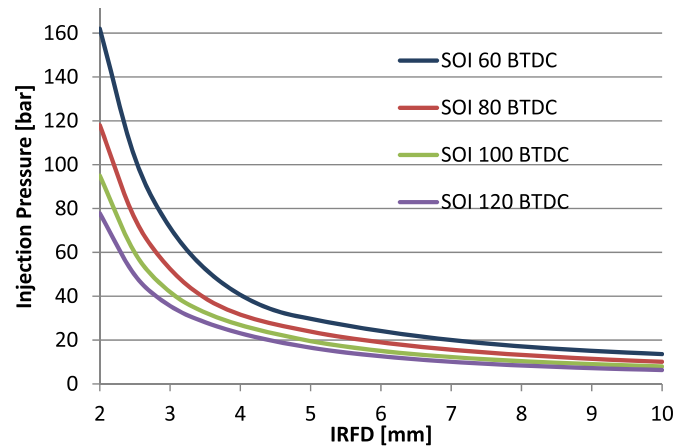


Fig. 5. The effect of IRFD and SOI values on the necessary injection pressure. SRM mixture (75% H₂, 25% CO₂), $P_b = 75$ kW, $n = 4000$ rpm, $C_D = 0.7$, $T_o = 350$ K.

formation and stratification were not considered. Taking into account that charge stratification effects were not considered in this work and based on the available data for DI-hydrogen ICE [38], we have limited the injection timing in such a way that end of injection could not be retarded beyond 10 CAD before top dead center (BTDC).

As anticipated, increasing the IRFD significantly reduces the required injection pressure. Retarding the SOI timing from 120 to 60 CAD BTDC roughly doubled the required injection pressure. Fig. 6 shows the ICE's BTE as a function of the IRFD and the SOI. The solid and the dashed lines in Fig. 6 represent BTE_{NC} and BTE_{WC} values, respectively.

When the compression work was not taken into account, retarded injection and small IRFD lead to BTE increase, because the fuel entered the cylinder later in the compression stroke, thus reducing the negative compression work of the piston. Of course, retarded fuel injection would require higher injection pressure. When energy investment for gaseous fuel compression is considered, increase of the IRFD and injection advancement has a positive effect on the BTE. Results presented in Figs. 5 and 6 show that gaseous fuel compression to high pressures in order to enable late

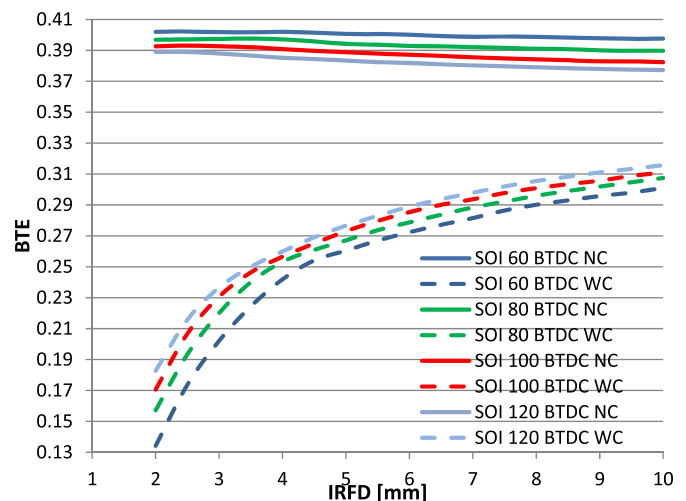


Fig. 6. Dependence of BTE on IRFD and SOI values. SRM mixture (75% H₂, 25% CO₂), $P_b = 75$ kW, $n = 4000$ rpm, $T_o = 350$ K, pressure prior to compression 1 bar.

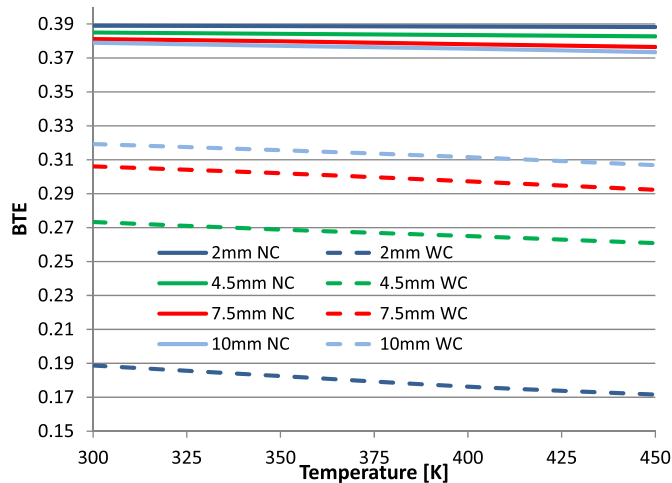


Fig. 7. The effect of injection temperature and IRFD on the BTE. SOI = 120 CAD BTDC, $P_b = 75$ kW, $n = 4000$ rpm, SRM mixture (75% H_2 , 25% CO_2), pressure prior to compression 1 bar. Solid lines – BTE_{NC} , dashed lines – BTE_{WC} .

injection would be unprofitable. This result is in a good agreement with data of [39], where computational study of a small engine operated with hydrogen stored at atmospheric pressure in liquid organic hydrogen carriers, was conducted.

4.2.2. Effects of fuel cooling

It follows from eq. (8) and (9) that the temperature is another factor that affects the fuel mass flow-rate into the cylinder. Since the density (ρ_0) is virtually inversely related to the temperature, the mass flow rate is inversely related to the square root of the temperature. This factor is an issue because reforming is carried out under high temperatures (about 570K). Therefore, the reformat gas should be cooled prior to compression (if necessary) and injection. This should be done to reduce power consumption of the compressor and the required injection pressure. An efficient way of the reformat cooling is by applying a heat-exchanger that heats the liquid fuel prior to its evaporation (as shown in Fig. 1). In order to understand influence of the injection temperature on the BTE, simulations of the engine at the rated power and different reformat temperatures were performed. The results are shown in Fig. 7

To compensate for the fuel temperature rise and to keep the same brake power, higher injection pressures were applied for the higher fuel temperatures – see eq. (8) and (9). This is the factor that leads to lower BTE_{WC} for the higher reformat temperature – Fig. 7. Nevertheless, there is also a slight decrease in BTE_{NC} . This is a result of increased compression work of the engine's piston when the reformat fuel enters the cylinder at higher temperatures. The results presented in Fig. 7 show relative BTE_{WC} improvement of 3–6% when the reformat fuel is cooled from 450K to 350K. The results of the simulations discussed above allow us to conclude that when the reforming process is performed under atmospheric pressure, DI method in ICE with TCR would be unviable. This remains true even if the reformat is cooled to 350K and the IRFD is enlarged to 10 mm (in this case $BTE_{WC} = 0.32$ compared with $BTE_{gasoline} = 0.34$ for the considered engine), and definitely – for the known DI-injector prototypes (developed for H_2 - and CNG-engines) with IRFD values lower than 2 mm ($BTE_{WC} = 0.18$).

However, if instead of energy consuming gas compression it would be possible to compress a liquid rather than a gas, thus the energy required for the process will be reduced by orders of magnitude.

4.3. A concept of ICE with high-pressure SRM

It is possible to tremendously reduce the energy required for fuel compression in a DI-ICE with TCR by compressing the liquid methanol-water mixture prior to its evaporation. This, together with increasing the IRFD above 3 mm can totally eliminate the need for gas compression prior to its injection to the cylinder. To realize this idea, high-pressure methanol reforming has to be applied.

Available literature data prove the feasibility of high-pressure SRM [12]. Obviously, the high-pressure reforming system has to be more robust (i.e. weigh more), in order to withstand the high pressures. A problem of the equilibrium shift to lower methanol conversion values at higher pressures is proven to be not severe. Peppley's experiments [12] showed that at 39 bar and 533K methanol conversion reaches 85%. In that study the temperature of 533K was not exceeded to prevent catalyst sintering. However, it is known that some $CuO/ZnO/Al_2O_3$ catalysts can successfully function at temperatures above 573K [34]. When the reforming temperature is increased to 573K, the equilibrium of methanol conversion is well above 90% even at the pressure of 40 bar. Thus, it seems that methanol conversion value at high pressures does not pose a serious problem. Moreover, we showed in previous calculations [28] that full methanol conversion should not be a prerequisite in the system design. Even though the tendency for carbon formation increases with pressure, no increase in catalyst fouling was experimentally observed for pressures as high as 40 bar at steam-to-methanol ratios greater than unity [40].

Figs. 8 and 9 show simulation results of a DI-ICE with high-pressure SRM obtained using the model described in Section 2. The simulations were performed for the rated power and speed (75 kW and 4000 rpm, respectively).

Fig. 8 shows the BTE_{WC} and methanol conversion as a function of reforming pressure for two different IRFD values. The small IRFD (1.74 mm) was chosen to match the existing injector prototype described in Ref. [37], where a fuel delivery system for a CNG DI-engine was reported. The large IRFD (3.84 mm) was chosen to achieve the rated power with injection pressure as low as 25 bar. This IRFD is larger than in the existing prototypes developed for various compressed-hydrogen and CNG DI-engines. The results shown in Fig. 8 demonstrate the significance of developing larger-IRFD injectors for the DI-ICE-TCR applications. As anticipated,

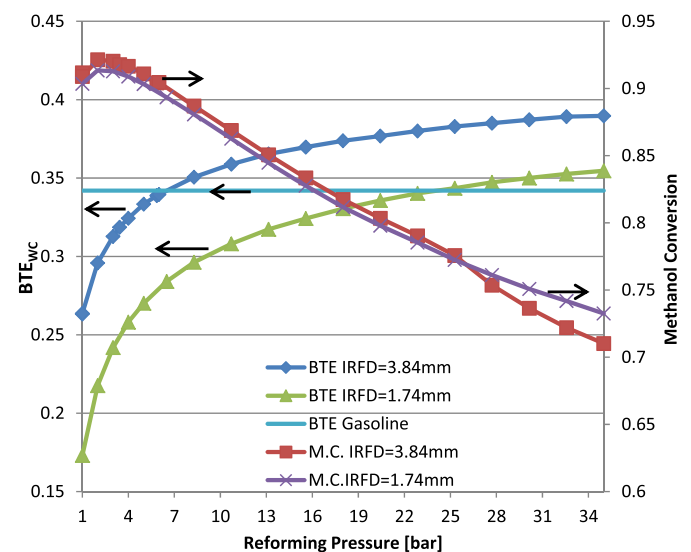


Fig. 8. Dependence of BTE_{WC} and methanol conversion (M.C.) on reforming pressure. $P_b = 75$ kW, $n = 4000$ rpm, WOT, $\lambda = 1.2$, reformer heat transfer area = 1.78 m².

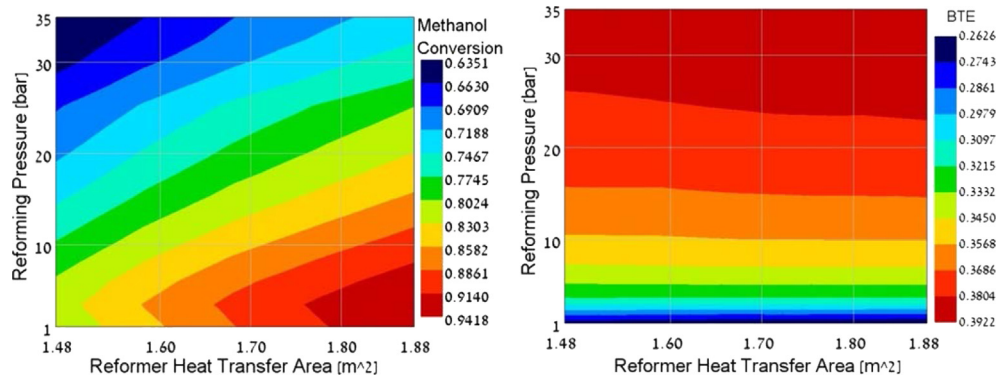


Fig. 9. Methanol conversion and BTE_{WC} as a function of the reformer heat transfer area and reforming pressure. $P_b = 75$ kW, $n = 4000$ rpm, WOT, $\lambda = 1.2$.

increasing the reforming pressure resulted in a great BTE_{WC} improvement with a steep incline in the low-pressure region. At low-reforming pressures (less than 4 bar), a slight increase (up to 1%) in methanol conversion was observed with rise of the reforming pressure. This is explained by a slight growth of the reforming temperature that resulted from the reformate-density increase with pressure rise. This, in turn caused a reduction of flow velocity that increased the residence time of the reformate gas in the reformer and hence - its temperature. At these low pressures the significance of the equilibrium shift due to the pressure change is still smaller than that cause by the temperature rise. Further increase in the reforming pressure causes significant reduction in methanol conversion, which is a result of the reaction rates reduction as the reforming products approach to equilibrium composition. As expected, no substantial dependence of methanol conversion on the IRFD was observed (Fig. 8). Change of the IRFD by a factor of 2.2 resulted in methanol conversion change that did not exceed 2% and was in a range of the prediction accuracy. The BTE_{WC} of the whole ICE-with-TCR system increases with the reforming pressure rise despite a reduction in methanol conversion. The observed BTE_{WC} behavior is explained by dominant impact of decreasing the energy required for gas compression with the reforming pressure rise. This positive effect overcomes the opposite influence of fuel-LHV reduction and lower hydrogen content that resulted from the methanol conversion reduction. The latter phenomenon is well-illustrated in Fig. 9.

As seen in Fig. 8, applying the high-pressure SRM of 26 bar or higher together with DI injector of IRFD = 3.84 mm provides engine efficiency improvement of 12–14% compared with the gasoline-fed counterpart. It should be noted that the rated-power operating mode considered in this work is the most problematic working regime for the ICE-SRM system. At partial loads the expected improvement in engine's efficiency will be substantially higher [13]. This is due to the lean-operating possibilities enabled by the high hydrogen content in the reforming products.

Fig. 9 shows that the increase in methanol conversion has relatively small contribution to the BTE_{WC} increase compared to influence of the reforming pressure. Nevertheless moderate influence of methanol conversion on BTE_{WC} , it is important to note that methanol conversion value affects reformate composition. Therefore, high conversion ratios are important to reduce the negative effects of methanol combustion on pollutants formation, enable lean engine operating and higher compression ratios.

5. Conclusions

This work examined the concept of direct-injection ICE with TCR. It was found that compressing the reformate-gas to high

pressures that enable late fuel injection is not energetically efficient. We proved that DI-ICE with TCR is unviable, if reforming is carried out at atmospheric pressure.

It is possible to tremendously reduce the energy required for fuel compression in a DI-ICE with TCR by compressing the liquid methanol-water mixture prior to its evaporation. This can be done by applying high-pressure methanol reforming. Available literature data prove the feasibility of high-pressure SRM. Computational analysis performed in this work shows a possibility of engine's efficiency improvement by 12–14% compared with a DI-gasoline-fueled counterpart by applying a DI-ICE with TCR and high-pressure methanol reforming. Applying direct-injection concept for ICE with TCR would allow mitigation of the backfire, pre-ignition and reduced maximal power problems that prevented this promising method of waste heat recovery from further development. Increasing the DI-injector size in an ICE with TCR would allow further BTE improvement as well as a reduction of the required reforming pressure.

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