

A Polygeneration Process Concept for Methane fueled HCCI- Piston Engines

Modeling of syngas cleanup and exergy losses

Robert Hegner* and Burak Atakan

Thermodynamics and CENIDE, IVG, Mechanical and Process Engineering, Faculty of Engineering, University of Duisburg-Essen, Lotharstr. 1, D-47057 Duisburg, Germany

Abstract

This modeling study addresses the question, whether HCCI piston engines can be used as chemical reactors in a polygeneration processes. In this context, the combustion engine is used to produce synthesis gas by partial oxidation and the further process assures the purification of the syngas. Some aspects were addressed during the development of the process, regarding separation units, pressure rise rates during ignition and integration of the energy of the exhaust gas. The results were compared, by calculating rational efficiencies and exergy losses of the overall process for different amounts of recirculated exhaust gas. The purity of the produced syngas could be elevated starting at 38% without purification, to 95% with the proposed polygeneration concept. The rational efficiency was found to be comparably high, at around 76-85%.

1. Introduction

Due to efforts to reduce the amount of CO₂ exhausted in energy conversion by combusting fossil fuels, the amount of energy conversion from so called renewable energy sources increases strongly in different regions of the world, including Europe and especially Germany. The intrinsic problem of the strongly fluctuating power from wind and solar energy conversion is well known and the electrical power production is also not following the power demand within a society. Thus, flexibility in energy conversion and possibilities for energy storage get into the focus of many societies. The question addressed in this paper is, whether combustion processes or more generally high temperature processes within piston engines might be helpful in gaining flexibility in energy conversion, using piston engines as polygenerating chemical reactors.

Generally polygeneration is discussed in terms of coupling processes, without changing the processes themselves [1]. The proposed polygeneration process would be a coupling of a chemical reactor and a piston engine in one. In order to maximize the flexibility, polygeneration systems often intend to provide a well-adjusted combination of various outputs. A motor polygeneration process would be able to provide mechanical work, heat and a wide range of chemicals, ranging from syngas to different unsaturated or partially oxidized hydrocarbons. The work output of polygeneration engines is usually small, compared to conventional combustion engines, since part of the fuel energy is converted to heat or it is stored in chemical form in the exhaust gas. This makes polygeneration processes suitable for adapting the electrical power production easily to the power demand, especially in periods where the power demand is small e.g. at night.

The present modeling study is focused on the production and

cleanup of synthesis gas in homogeneous charge-compression-ignition (HCCI) engines. Regarding the production of synthesis gas in engines, some investigations are available, mainly by Karim and coworkers [2] but also from other authors [3][4]. A merely thermodynamic analysis for syngas production was performed for gas turbines recently and appeared to be promising [5]. However, investigating the mere production of syngas has its limits because the product gas would contain several impurities, which need to be removed. Only when the process and product syngas meetsome requirements regarding purityand technical feasibility, the polygeneration process would be able to compete with conventional syngas production systems like steam reforming. Thus, an overall process concept is designed, that includes the central polygenerating engine, as well as necessary auxiliary units, like preheaters or separation units.

In order to identify optimal operation points, a parameter study is then conducted for the process. Available energy (or exergy) and its losses is a concept to judge such polygeneration processes, which are usually designed to have low exergy losses. The higher the exergy losses of a process are, the more it deviates from a thermodynamically ideal process. The overall exergy loss of such a process is calculated here using chemical elementary reaction mechanisms together with the second law of thermodynamics. Methane was investigated as the fuel and oxygen as oxidizer, in order to obtain high syngas purities. It turns out, that the needed initial temperature with typical engine speeds and compression ratios are quite high in order to obtain chemical conversion. Therefore fresh gas preheating in combination with exhaust gas recirculation is evaluated to elevate the inlet temperatures and to reduce peak pressures during ignition. A single-zone HCCI model is

* Corresponding author: robert.hegner@uni-due.de

2. Theoretical Background and Modeling

In order to describe and simulate the processes inside the engine, time dependent chemical kinetics simulations were performed. The simulation consists of a compression and expansion stroke, starting at the bottom dead center with closed valves. All concentration changes due to chemical reactions during the engine cycle were accounted by elementary reaction kinetics mechanisms. The crucial point in these kinds of processes is to produce sufficiently high radical concentrations after compression which finally lead to ignition. The calculations were performed using the framework of the reactor model implemented in Cantera [6] within Python. Here a homogeneous gas mixture within the reactor is assumed for each state, thus, we are concentrating on the main chemical processes and neglecting all complications due to transport processes. The reaction mechanism and the thermodynamics database were taken from the USC mechanism II [7]. The oxidizer was assumed to be pure oxygen.

Intake Pressure p_0	101,3 kPa
Compression Ratio ε	16,5
Engine Speed N	3000 rpm
Displacement V_D	3.996 l

Table 1

In order to simulate the process including the chemical reaction kinetics, further information and some assumptions about the simulated engine and operation conditions are necessary, which are given in Table 1. In order to simulate compression and expansion the piston speed, and thus the volume, at any time has to be known. In order to calculate this, the following equation [8] is used:

$$u(\varphi) = \tilde{u} * \frac{\pi}{2} * \sin(\theta) * \left(1 + \frac{\cos(\theta)}{C^2 - \sin^2(\theta)^{\frac{1}{2}}} \right) \quad (1)$$

with the mean piston speed \tilde{u} , the crank angle θ and the constant $C = 3.5$. The cycle period is now simulated as a function of time; the change of composition due to chemical reaction kinetics is calculated while volume and internal energy are changing due to the transferred work and heat. The time dependent temperature, pressure and composition inside the engine are calculated numerically by Cantera from reaction kinetics and thermodynamics, with the given volume and total energy. The total energy is calculated from the internal energy of the previous time step and the work and heat transferred in each time step. Heat losses are calculated using the Woschni-equation [9]. Finally, when the cycle is completed, the exhaust gas composition, entropy generation and total work transferred is evaluated.

The total work is then calculated from integrating pressure and volume ($-pdV$) along the cycle. However the work output alone is not sufficient to evaluate polygeneration processes, since a lower work output is intended in favor of a thermodynamically ideal conversion of the fuel to the desired product species. This contrasts conventional piston engines, where the exhaust gas is rarely utilized in further processes, since the exhaust gas species are usually already fully

oxidized and not of interest for chemical processes. But the exhaust gases of polygeneration engines contain high amounts of chemically useful species and unconverted (available) energy. In order to consider this amount of energy and to evaluate the process, the concept of exergy was used. Unlike energy, which is just converted to other kinds of energy, exergy can be actually destroyed. This exergy loss is caused by irreversibilities and can be used to evaluate how well the fuel exergy is converted to work or conserved in the exhaust gas. The losses in exergy E_v are dependent on the ambient temperature T_{sur} , here assumed to be 298 K and the irreversible entropy generation S_{irr} of the engine cycle:

$$E_v = T_{sur} S_{irr} \quad (2)$$

By calculating the entropy generation of a unit, its exergy loss is determined according to Eq. (2).

The engine isn't the only unit in the process. In order to evaluate the overall process concept, the exergy losses of all units are summed up and the rational efficiency is then calculated by the following equation:

$$\eta_{rat} = \frac{E_{out}}{E_{in}} = 1 - \frac{E_v}{E_{in}} \quad (3)$$

where the molar fuel exergy $e_{in} = 0.8365 \text{ MJ/mol}$ was taken from [10]. The entropy production of a unit is calculated by the second law or thermodynamics for open, steady systems:

$$S_{irr} = \sum m_{out} * s_{out} - \sum m_{in} * s_{in} - \frac{Q}{T_{ref}} \quad (4)$$

Two cases were analyzed regarding the reference temperatures T_{ref} : The first case is that the transferred heat of the respective unit Q is used in other processes, according to the polygeneration concept. In this case, the reference temperature is set to 100K below the mean temperature of heat exchange T_{mean} :

$$T_{mean} = \frac{h_{out} - h_{in}}{s_{out} - s_{in}} \quad (5)$$

The second case is that the heat is not used and therefore lost to the surroundings. Here the T_{ref} is set to the ambient temperature of 298K.

With the calculations and modeling described in this section, the exhaust gas composition and exergy losses of individual units are calculated. The next section describes the difficulties and considerations of merging the engine and several auxiliary units into a functioning and flexible polygeneration process concept.

3. Process Concepts

The main purpose of the process concept is to enable the purification of the synthesis gas, generated by the engine. Therefore the syngas purity is the main design variable. However, focusing solely on purification units would not only lead to misleading exergy losses, but would also result in a process concept with huge technical difficulties, as will be explained. This means that the development of a process concept needs to address two major problems: first defining the impurities and identify means to separate them, and secondly including these separation units in a functioning concept and resolving the resulting technical difficulties.

3.1 Separation Units

Prior to choosing suitable separation units, the impurities need to be specified. Table 2 shows a typical exhaust gas composition of a polygeneration engine, operating with methane and air at an equivalence ratio $\Phi = 2$. The equivalence ratio Φ is defined as the amount of oxidizer that would be necessary for stoichiometric combustion, divided by the amount of oxidizer in the actual combustion case.

N ₂	51.10%
H ₂	23.20%
H ₂ O	9.30%
CO	14.90%
CO ₂	1.50%

Table 2

The resulting syngas purity would be around 38%, with nitrogen as the main impurity and lower amounts of water and carbon dioxide. The removal of water can be easily accomplished by condensers, although restricted by the vapor pressure. Nitrogen separation is commonly done prior to combustion in air separation units (ASU). These are cryogenic rectification columns with comparably high work demands and high exergy losses. Some groups already investigated ASU's and agreed on some key figures, regarding molar exergy loss $e_v = 4.95 \pm 0.7 \text{ MJ/kmol}_{Air}$ and work demand $w = 6.9 \pm 0.7 \text{ MJ/kmol}_{Air}$ [11,12] CO_2 removal is conducted in chemical absorption units with various solvents on amine basis for instance. The solvent is usually regenerated by desorption of the dissolved CO_2 with steam. Regarding the exergy loss and the steam consumption in CO_2 -absorption there are some publications as well. The specific exergy losses around $e_v = 1.82 \pm 0.4 \text{ MJ/kg}_{CO_2}$ and the steam consumption $m_{steam} = 1.9 \pm 0.1 \text{ kg}_{steam}/\text{kg}_{CO_2}$ [13], [14]. These publications also state some restrictions regarding temperature: The inlet temperature of the exhaust gas should not be higher than 423K in order to prevent solvent vaporization and the outlet temperature of the purified exhaust gas is around 323K. The required steam temperature is usually around 393K dependent on the pressure in the desorption column. With this, all necessary separation units (ASU, CO_2 -absorption and condenser) can be described quantitatively and the focus is now set on coupling them with the HCCI engine.

3.2 Pressure Rise Rate

The pre-combustive removal of nitrogen results in the combustion with oxygen inside the engine. This holds some problems since especially in HCCI engines this may cause severe damage to the engine, since the pressure rise rates (PRR) are too high for the engine to withstand them a long time. This is shown among others in Fig.1. This diagram depicts calculations with a multi-zone model similar to the one of [15] and shows the pressure inside the engine at different crank angles. The curve for the combustion with pure oxygen at an equivalence ratio of $\Phi = 2$ shows the highest peak

pressure and a PRR of around 20bar/CA, which is far too high. In order to reduce the PRR a buffer gas should be mixed with the fresh gas methane-oxygen-mixture.

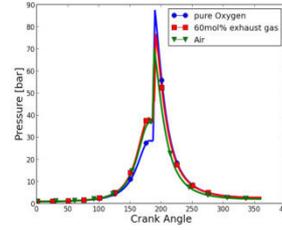


Fig.1 Multi-zone model pressure profiles for $\Phi = 2$

This buffer gas should consist of species already listed in Table 2 (except nitrogen), to avoid additional downstream separation units. Therefore pure CO_2 or H_2O would be possible buffer gases. But recirculation of the exhaust gas, which contains mainly H_2 , CO , H_2O and CO_2 would be a promising opportunity too and offers much more advantages than using steam or separated carbon dioxide as buffer gas, as it is explained in the following section. Most of the exhaust gas species are more or less inert, (with hydrogen as the only exception, as discussed later) which makes it suitable as buffer gas, as also shown in Fig.1. Here a mixture of 60mol% exhaust gas and 40mol% fresh gas is compared to the usual combustion with air, both with an equivalence ratio of $\Phi = 2$. This specific composition was chosen, since the nitrogen content in the methane-air mixture would also be around 60mol%. The graphs show that although the peak pressure of the exhaust gas recirculation is slightly higher, due to the hydrogen content, the pressure rise rate is comparable to that of combustion with air at around 10bar/CA and therefore successfully reduced, compared to the combustion with pure oxygen.

3.3 Fresh Gas Preheating

The usage of exhaust gas recirculation holds another advantage, with respect to HCCI engines. Since HCCI engines depend on auto-ignition and conventional Otto fuels are hardly ignitable, a preheating of the fresh gas is usually unavoidable. Unfortunately most methane reactions have especially high activation energies, which necessitate high temperatures at the end of the compression stroke to overcome these barriers, thus, also leads to comparably high initial temperatures of the fresh gas mixture. So besides reducing the pressure rise rates, the recirculation of exhaust gas can contribute to the preheating of the fresh gas and therefore enable ignition. In order to identify how much exhaust gas is needed, an exhaust gas ratio (EGR) is defined as the molar content of exhaust gas in the inlet mixture:

$$EGR = \frac{n_{EG}}{n_{FG} + n_{EG}} \quad (6)$$

where n_{EG} and n_{FG} are the molar amounts of exhaust gas and fresh gas respectively. Fig.2 shows the fuel conversion dependent on this exhaust gas ratio assuming a fresh gas temperature of 298K and an exhaust gas temperature of 940K for an equivalence ratio of $\Phi = 3$.

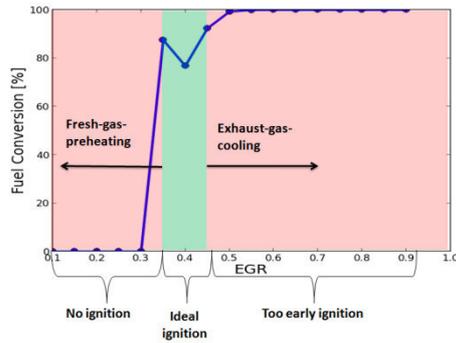


Fig.2 Fuel conversion dependent on EGR for $\Phi = 3$
 This diagram is divided in 3 zones. For EGR lower than 40mol% the conversion is 0. Here the content of exhaust gas would not be sufficient to elevate the mixture temperature to the required value for ignition. For EGR above 40mol%, the conversion would be nearly 100%. However, the high exhaust gas content would increase the temperature to a level, where the ignition would already take place in the compression stroke, which would again increase the pressure rise rate. These both effects result in a very small operation range around an EGR of 40mol%. This would lead to huge restrictions with regards to flexibility. In order to extend the range of operation, two process concepts were developed, according to the different EGR-zones Fig.2.

At low EGR's the fresh gas needs to be preheated additionally, before the mixing with exhaust gas. In this way, the temperature is increased to enable the ignition. Fig.3 shows the process scheme for this case:

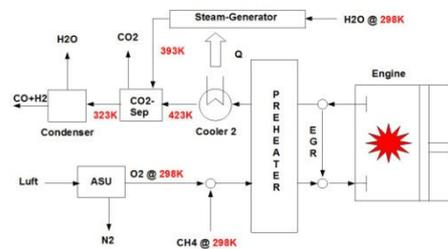


Fig.3 Process concept for EGR < 40 mol%

Here, air is separated by the ASU and the oxygen is then mixed with methane. This fresh gas mixture passes a preheater where heat is supplied by that part of the exhaust gas which is not recirculated. Then, the fresh gas is mixed with exhaust gas, and supplied to the engine. The engine compresses the mixture until a partial oxidation takes place and work is generated during the expansion stroke. A part of the exhaust gas is then recirculated, while the remaining gas is first lead through the preheater and then trough cooler 2, where the temperature is reduced to 423K. The heat released from cooler 2 is used to generate steam for the CO_2 -separation unit, which the exhaust gas passes after exiting the cooler 2. Now the only remaining impurity is water, which is condensed after the CO_2 removal, leaving processible syngas.

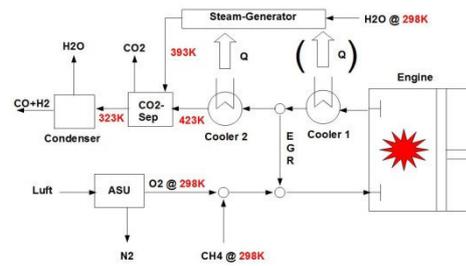


Fig.4 Process concept for EGR > 40 mol%

The process concept for EGR's higher than 40mol% is shown in Fig.4. In this case, the mixture temperature is too high and needs to be reduced. This is done by intercooling the exhaust gas in cooler 1 before it is recirculated. The heat is then either used as output stream of the polygeneration process or to assist the cooler 2 in steam generation. The remaining process was mostly already described in the previous paragraph.

These both process concepts can greatly increase the flexibility of the polygeneration process, since now, the whole range of exhaust gas ratios is applicable and parameter studies can be performed on a broad basis.

4. Results and Discussion

In order to identify, which exhaust gas ratios are suitable for polygeneration, the EGR was varied, while the synthesis gas purity should be hold on a constant, high level, since this is the purpose of both process concepts. By calculating the rational efficiency of the process, reasonable conclusions can be drawn, on which EGR's are most promising.

Therefore Fig.5 shows the calculated molar purity of the produced syngas for the respective EGR's.

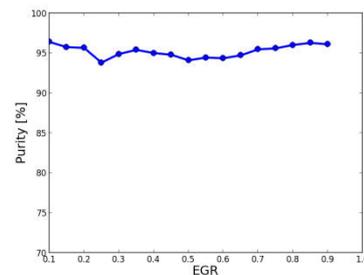


Fig.5 Syngas purity at different exhaust gas ratios

The syngas purity is maintained quite constant by the process at around 95%. Among the remaining impurities, 4-5% are water, which is easily condensed at lower temperatures than 298K or adsorbed using e.g. active carbon. Another 1-2% of the remaining impurities are unburned fuel, which could be avoided by increasing the equivalence ratio. However, with respect to the equivalence ratio, some considerations weren't addressed yet: Above, it was mentioned, that the hydrogen in the recirculated exhaust gas is not inert. Since hydrogen already ignites at lower temperatures than methane, it can assist in the ignition of the fuel, but in order to compensate for the oxygen lost due to the combustion of hydrogen, the fresh gas equivalence ratio

needs to be adjusted to the exhaust gas ratio. If the fresh gas equivalence ratio would be held constant at $\Phi = 3$, the increasing hydrogen content in the mixture would consume most of the oxygen, leaving high amounts of unburned fuel and a bad fuel conversion of only 11%. Therefore the fresh gas equivalence ratio is decreased with increasing EGR in order to provide sufficient oxygen to burn both, part of the hydrogen and most of the methane. The resulting fresh gas equivalence ratios are shown as solid blue line in Fig.6.

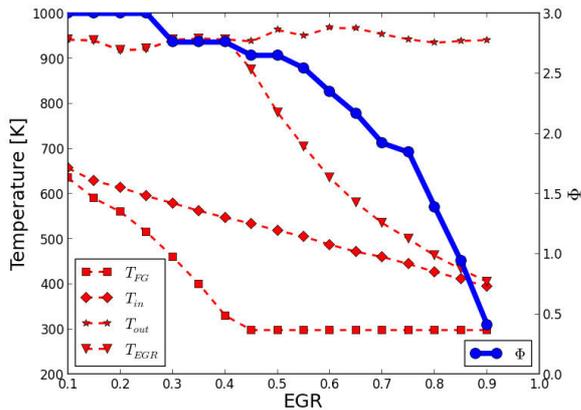


Fig.6 Fresh gas equivalence ratio and temperatures

These changes in equivalence ratio also have a huge impact on the exergy loss and rational efficiency, as it is shown in Fig.7.

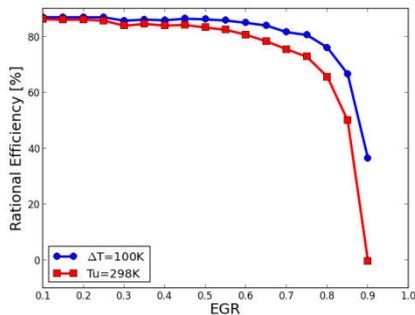


Fig.7 Rational efficiency as function of EGR

This diagram compares the rational efficiency for the two cases explained in section 2: Either the process heat is utilized at a mean temperature difference of 100K or it is lost to the surroundings. However both curves show a similar trend. At low EGR's the rational efficiency is highest, starting at around 86%. This value remains nearly constant until an EGR of 60mol%. Then the rational efficiency begins to decrease with increasing EGR, to around 76% at an EGR of 80mol%. Above this value, the efficiency drops to unacceptably low values of below 40%. An explanation of this behavior can be found in the equivalence ratio, since all further simulations were performed using the equivalence ratios in Fig.6. Comparing Fig.6 and Fig.7, some similarities are found: At high EGR's more hydrogen is present in the mixture and therefore more oxygen is necessary, as already explained. The combustion of hydrogen to water, finally results in additional entropy generation and exergy losses, which

can't be associated with the fuel exergy. Therefore, the higher the EGR gets, the more hydrogen takes part in the combustion and the less the exergy loss is directly affected by the fuel. From this reasoning some conclusions, regarding an optimal range of exhaust gas ratios, can be drawn: At EGR's below 40mol% the efficiency is highest, however lower EGR's would do a bad job in reducing the pressure rise rates during ignition. Thus, too high EGRs result in very low rational efficiencies. Therefore an EGR between 40-80mol% seems to be most promising, with rational efficiencies between 76-85%. Compared to conventional syngas production by steam reforming, which have rational efficiencies around 65% [17] this would be a huge improvement. A comparison of both cases of heat usage shows that both curves begin at nearly the same value of a rational efficiency of 86% at low EGR's. This is due to the fact, that most of the exhaust gas heat is already used in the preheater and for steam generation, which means that the exergy loss, caused by heat transfer to the surroundings is comparably small. As soon as the preheater isn't necessary anymore at an EGR of 40mol% the calculated rational efficiencies start to differ. First slightly, but the difference increases with increasing EGR, since more and more excess heat is transferred to the surroundings, especially through cooler 1. This indicates that the excess heat should be used in other processes if possible, especially at EGRs above 70mol%.

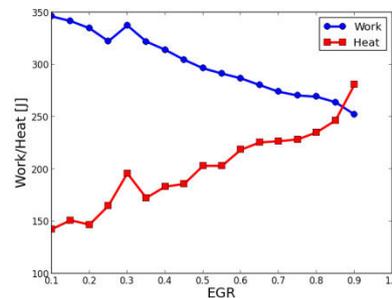


Fig.8 Work and heat output dependent on EGR

The superiority of polygeneration processes regarding flexibility can be derived from Fig.8. This figure shows the total work and heat output of the process for different EGRs. As expected, the work is reduced with increasing EGR. The higher the exhaust gas ratio is, the less fuel is fed to the engine. This results in decreasing work output, which is indeed often desired, with respect to polygeneration processes. The heat output however increases with increasing EGR. This is due to the split process concepts itself. At lower EGR the preheater and steam generator consume most of the exhaust gas energy. But as soon as the cooler 1 is introduced at EGR's over 40mol% more heat can be drawn out of the process, since the exhaust gas needs to be cooled. Thereby a simple relation needs to be kept in mind: the more exhaust gas is recirculated, the lower the temperature of this exhaust gas needs to be, in order to avoid ignition in the compression stroke. This is seen in Fig.6 where some important temperatures are displayed as dashed lines.

T_{FG} is the temperature of the fresh gas mixture, which is mixed with exhaust gas. T_{in} is the inlet temperature of the fresh gas – exhaust gas mixture into the engine. T_{out} the respective exhaust gas temperature and T_{EGR} the temperature of the intercooled and recirculated exhaust gas, leaving cooler 1. As already mentioned, T_{EGR} decreases constantly with increasing EGR, while T_{out} remains nearly constant. This means that more and more heat is provided by cooler 1 and explains the increasing heat output in Fig.8. The opposed trends for work and heat output leads to an interesting effect, where the ratio of both covers a wide area of values, ranging from 2.4 at EGR=10mol% to 1.1 at EGR=80mol%. This so called power to heat ratio is a crucial variable in cogeneration processes for instance. By the proposed polygeneration process, this variable can be easily adjusted to the desired value, which contributes to the overall high flexibility.

5. Conclusions

An HCCI engine running with methane, oxygen and recirculated exhaust gas was simulated. The engine was operated in the fuel rich regime, so that a partial oxidation of methane to synthesis gas took place. However, syngas produced by this means still contains high amounts of impurities. Therefore a process concept was developed, which enables the purification of the synthesis gas. Three major challenges arose during the development of the process concept: The purification units and their respective exergy losses and restrictions, the pressure rise rate during ignition and the preheating strategy. Information regarding purification units were taken from the literature, the latter two problems were partially solved by recirculating a part of the exhaust gas. However, recirculating exhaust gas without any pretreatment, imposes huge restrictions, since only an exhaust gas content of 40mol% results in a successful ignition during the expansion stroke. From this reasoning fresh gas and exhaust gas pretreatment is included in order to increase the range of feasible exhaust gas ratios. The results indicate that the exergy losses are highly dependent on EGR and waste heat usage. Therefore it is aimed to utilize the thermal energy of the exhaust gases in the process, especially for fresh gas preheating or to provide steam for auxiliary units. It was found, that EGR-ratios below 80mol% are most suitable with regards to methane conversion, syngas yields and exergy losses. The syngas purity was raised from 38% without purification to 95% by the proposed process concept and by adjusting the equivalence ratio to the exhaust gas content. Comparingly high rational efficiencies of up to 85% were obtained with EGR's of 40-60mol%, typical for HCCI engines. The heat and work output was found to react as desired on changes in EGR ratios.

All results indicate, that the production of synthesis gas in piston engine polygeneration processes, has several advantages, compared to conventional syngas production. It includes the possibility to cogenerate work and heat as well, with a huge flexibility towards

the desired values. This all is accomplished with low exergy losses, due to the thermodynamically nearly ideal conversion.

6. Acknowledgement

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7. References

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