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Full Length Article

Combined production of power and syngas in an internal combustion engine – Experiments and simulations in SI and HCCI mode

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ABSTRACT

In this work, an internal combustion engine is used as a reactor for partial oxidation to produce syngas together with mechanical work. Experiments were performed in a single-cylinder engine operated on methane/air. Spark-ignition (SI) and homogeneous-charge compression-ignition (HCCI) were investigated. For HCCI, 5 mol% n-heptane were added to the fuel to reduce auto-ignition temperatures. With spark ignition at $\phi = 1.56$, the product gas contained up to 8.6 mol% CO and 7.7 mol% H_2 at 71.5% exergetic efficiency, while at $\phi = 0.72$ roughly the same mechanical work was generated, but with only 42.5% exergetic efficiency. Under the richer conditions achievable in HCCI combustion, syngas content increased to 15.8 mol% CO and 17.9 mol% H_2, and the exergetic efficiency to 81.5%. A homogeneous single-zone model coupled with a detailed reaction mechanism was used to simulate the process. The experimental results and the simulation were in good agreement for operating points without frequent misfires.

1. Introduction

Flexible solutions for energy conversion and energy storage are gaining importance. In the case of internal combustion (IC) engines, flexibility can be achieved by varying the engine load. However, IC engines suffer from decreasing efficiency under part-load [1]. But the part-load efficiency could be increased by only partially oxidizing the fuel, thus simultaneously generating both a reduced amount of work and heat as well as potentially useful chemicals. This is most interesting for stationary (as opposed to automotive) applications, for example in the chemical industry where the product chemicals may be used as an input to downstream processing.

Polygeneration, i.e., the coupling of energy conversion and chemical conversion towards useful chemicals, is usually discussed in terms of a flexible combination of – otherwise unchanged – processes [2,3], such as steel production with electricity production, district heating, and methanol production [4]. In contrast, in this work we use an IC engine with fuel-rich combustion as a polygenerating chemical reactor that can produce both base chemicals and mechanical work in a single device. The process would be able to flexibly change between various ratios of mechanical work, process heat, and chemicals like syngas. Operating an engine with partial oxidation would decrease its work output compared to stoichiometric conditions. In contrast to lean combustion, a part of the fuel exergy remains in the product gas. Though not investigated here, it is even conceivable to increase the heating value of fuels through pyrolytic processes, thus to store energy. This makes this kind of polygeneration process especially suitable for adapting the electrical power production (and eventually consumption) to demand.

Co-generation of synthesis-gas and mechanical power in an IC engine was already studied in 1956 by Szezich, who used spark ignition (SI) with CH_4/air mixtures at low compression ratios [5]. Karim et al. [6] ignited mixtures of CH_4 and O_2-enriched air by a pilot injection of Diesel fuel. Yang et al. investigated HCCI combustion in rich CH_4/O_2 mixtures (also in $CH_4/O_2/CO_2$ mixtures to simulate biogas) and were successful in syngas production [7]. Morsy modeled an HCCI process with methane to find good conditions for syngas production [8] and proposed to start compression at relatively high temperatures to achieve ignition. McMillan and Lawson experimentally investigated a fuel-rich natural-gas SI process, but also modeled an HCCI process [9]. With SI, they were successful in producing syngas up to $\phi = 1.62$, the equivalence ratio ϕ being the ratio of the actual fuel/air ratio to that needed for complete combustion to fully oxidized products. In multi-cylinder engines, the syngas produced by in-cylinder fuel reforming in *one* of the cylinders has been ad-mixed to the fresh charge of the *other* cylinders to improve the combustion characteristics of the resulting fuel/syngas/air-mixture. With careful load balancing between the cylinders, this can yield lower fuel consumption and nitric oxide

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emissions at an overall stoichiometric fuel/air-feed to the engine, enabling use of a conventional three-way catalyst. This concept was first explored for gasoline fuel by Alger and co-authors [10,11] and later expanded to natural gas by Zhu et al. [12]. None of the studies surveyed here performed an exergetic analysis.

Exergetic analysis [13] is valuable for polygeneration processes, because different products like work, heat, and chemicals that are produced in different relative and total amounts are difficult to assess otherwise. Exergy, sometimes called available energy, is the part of the energy of a source that can be converted to any other form of energy while bringing the system into equilibrium with the environment on a reversible path. Unlike energy, exergy is a non-conserved property; it can be destroyed through irreversible entropy production. With this approach, not only product yields can be assessed, but also the amount of work and heat produced or consumed by the process. Alternatively, one could also use thermo-economic analysis [13], with the ambiguity that prices change with time.

In the present work, lean and rich operating conditions of an engine fueled with methane, CH_4, are compared in terms of work and heat output, exergetic efficiency, and product-gas composition. Methane was selected since it is the main component of natural gas and "biogas" and the main reactant used for syngas production in chemical industry. The experiments were performed at $0.64 < \phi < 1.74$ in SI operation. Additional HCCI measurements were carried out with n-heptane addition at $1.86 < \phi < 2.42$. The results were compared to those from a homogeneous, zero-dimensional engine model.

2. Experimental methods

The experiments were performed in a single-cylinder BASF-type engine usually used for octane-number testing of liquid fuels. The engine was modified to also run on gaseous fuels. The test bench consisted of the naturally aspirated spark-ignited two-valve engine and a three-phase dynamometer for constant engine speed.

The instrumentation of the engine is shown schematically in Fig. 1. A piezo transducer integrated into the spark plug measured the in-cylinder pressure as a function of the crank-angle given by an incremental optical rotary encoder on the engine crankshaft. The pressure was recorded by an indicating system every 0.1° crank angle (CA). The spark plug was mounted sideways in a prechamber. The off-center ignition in combination with the complex combustion-chamber geometry led to incomplete combustion even at stoichiometric conditions.

The product stream's major species were detected with a commercial exhaust-gas analyzer (ABB, Type Advance Optima 2020), with units measuring concentrations of carbon monoxide (CO, specified accuracy 0.3% absolute), carbon dioxide (CO_2, 0.3%), as well as methane (CH_4, 0.2%) (all by infrared absorption), hydrogen (H_2, 1%) (by thermal conductivity), and oxygen (O_2, 0.13%) (paramagnetically). The product stream was dried to a dew point of 3 °C to prevent interference due to cross-sensitivity of the analyzers to H_2O. Soot was measured as a filter smoke number (AVL smoke meter, Type 415S). The intake air flow was measured by an air flow meter (ABB, Type Sensyflow, accuracy 1% relative) combined with a compressor and a large plenum to control mean intake pressure and dampen pressure fluctuations, respectively. The engine exhaust was connected to a burner system to safely dispose of the flammable and toxic products.

Table 1
Engine properties and operation conditions.

Engine type	4-stroke 2-valve single-cylinder
Fuel, SI/HCCI	CH_4/CH_4 + 5 mol% n-C_7H_{16}
Displacement	332 cm^3
Bore/stroke	65/100 mm
Con. rod length	200 mm
Comp. ratio	10
Engine speed	600 min^{-1}
Intake temperature	50 °C (SI), 120 °C (HCCI)
Intake pressure	1 bar
Coolant temperature	100 °C
Spark timing	10°CA bTDC
Intake valve timing	25°CA aTDC – 45°CA aBDC
Exhaust valve timing	30°CA bBDC – TDC

The engine was operated on lean as well as rich CH_4/air mixtures in SI mode and on rich mixtures only in HCCI mode. Table 1 lists the key parameters of engine and operating conditions. For the gaseous methane fuel, the engine had continuous intake-manifold injection with the fuel flow controlled by a mass-flow controller (MFC) with a typical accuracy between 1% at rich conditions and 2% at lean conditions. Methane is not a very suitable fuel for HCCI operation due to its low reactivity (RON = 130) and single-stage ignition. Therefore, to enable compression ignition (CI) in this engine with its relatively low maximum compression ratio of 10, n-heptane (RON = 0) was added and the intake air was heated. The n-heptane was dispersed into the intake air by pulse-width modulated port-fuel injection (PFI) from a four-hole nozzle with 3 bar (abs.) fuel pressure. The nozzle had been characterized separately by adjusting the pulse width of injection and measuring the weight of the injected fuel per time. The n-heptane flow was obtained from the corresponding characteristic diagram with an accuracy of 0.1 mg/cycle or 1.4%.

Before taking data in SI operation, the engine was run on methane until a coolant temperature of 100 °C was reached, which was maintained for all experiments. Data recording was started when the measurements of the gas analysis were steady. At each operating condition, the product gas volume fractions, temperatures, and about 140 cycles of pressure data were recorded.

To transfer the engine from SI to HCCI, spark ignition was switched off and the intake temperature was increased to 120 °C. Because of the low reactivity of methane, no reaction took place under these conditions and thus the engine was motored. Upon adding n-heptane by PFI, auto-ignition started. Once stable HCCI operation was achieved, the equivalence ratio was varied by adjusting the fuel flow while keeping the ratio of CH_4/n-heptane constant at a molar ratio of 95/5. The relative accuracy of this ratio was 3.2%, and within the range of the metering uncertainty, the results were not sensitive to the concentration of the additive.

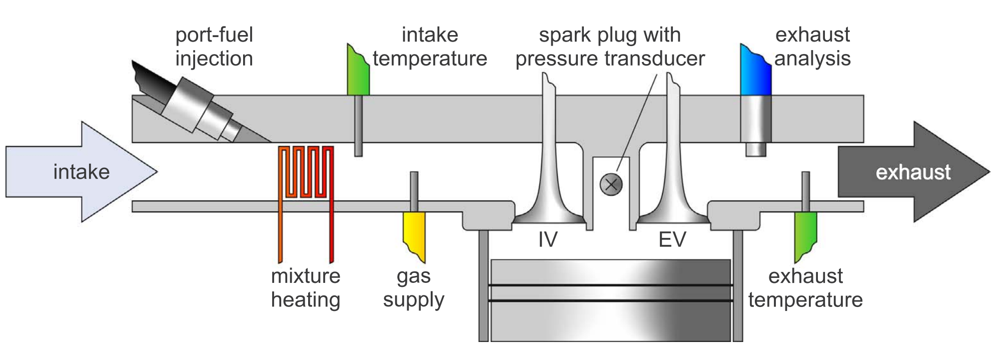

Fig. 1. Instrumentation and fuel supply of the single-cylinder engine.