THE INTERNAL COMBUSTION ENGINE AS A NATURAL GAS REFORMER: OPERATING CONDITIONS PROPOSED BY NUMERICAL OPTIMIZATION

H. Gossler and O. Deutschmann*
Karlsruhe Institute of Technology
Engesserstr. 18, 76131 Karlsruhe, Germany

Abstract

The production of hydrogen is studied numerically under uncatalyzed partial oxidation and homogeneous charge compression ignition (HCCI) conditions in an internal combustion engine fueled by natural gas. The HCCI process is modeled by a single-zone variable volume reactor using a global heat transfer model and elementary-step reaction mechanisms. Numerical optimization is applied to maximize the hydrogen yield at the end of the expansion stroke by varying the equivalence ratio, engine speed and initial pressure for a range of fixed initial temperatures. From these results, maximum hydrogen yield profiles and the associated operating parameter profiles as functions of initial temperature were obtained.

Keywords

Natural gas, Partial oxidation, Internal combustion engine, Hydrogen, Syngas, Optimization.

Introduction

Internal combustion engines (ICEs) can be viewed as highly dynamic high temperature/pressure reactors. Therefore, ICEs can possibly be an attractive alternative to conventional reactors for certain chemical synthesis applications. Depending on the operating parameters, reaction conditions are attainable that can hardly be achieved in conventional reactors. For example, ICEs posses the intrinsic feature to quench the reaction, which stems from the piston motion.

According to a study by Atakan (2011), the efficiency of gas turbines can be improved if they are operated as polygenerators. More precisely, the production of useful chemicals such as syngas simultaneously with mechanical energy shows potential to increase the energetic efficiency of the process viewed as a whole. Although gas turbines were the focus of Atakan's work, similar considerations hold for ICEs, which are addressed in this study. The use of ICEs to produce useful chemicals instead of CO_2 and H_2O is thus motivated by two different aspects: Firstly, the potential to increase overall process efficiency and secondly, the possibility to achieve conditions that are not feasible in conventional reactors arising from the piston motion. In addition, piston engines can be operated very flexibly and react promptly to changes in controls. This flexibility poses another advantage that can possibly also be exploited for a variety of chemical processes. The purpose of this work is to conduct a fundamental study employing numerical optimization to identify promising operating regions for the production of gaseous chemicals from natural gas in an ICE.

Numerical Approach

In a piston engine, the initial conditions can be varied to optimize the product composition at the end of the expansion stroke. In particular, the conversion, the

* To whom all correspondence should be addressed

selectivity or the yield of a certain chemical species can be maximized.

A newly developed code DETCHEM^{ENGINE} (Deutschmann et al., 2015) was coupled with the COBYLA (constrained optimization by linear approximations) optimization algorithm (Powell 1998). The combustion chamber is modelled as an idealized batch reactor with a variable volume profile. The temporal change of species concentrations, temperature and pressure is accounted for by using detailed kinetic mechanisms. Heat loss through the engine walls is taken into account by using a global heat transfer model. More details regarding the optimization procedure can be found in the publication by Gossler and Deutschmann (2015).

In this study, the hydrogen yield was chosen as an objective function to be maximized in the optimization. By varying the fuel-air equivalence ratio ϕ, engine speed N and initial pressure P_0 for a fixed initial temperature T_0 ranging from 473 K to 773 K, the H_2 yield at the end of the expansion stroke was maximized.

Optimization of Hydrogen Yield

The maximized hydrogen yield (Y) as a function of initial temperature T_0 is shown in Fig. 1 (top left) along with the associated fuel conversion (X). The corresponding optimization variables ϕ, N and P_0, required to obtain the objective function value Y, are depicted in the other diagrams. The optimal H_2 yield is 74.8 % at T_0 = 473 K and improves with rising temperature to 90.1 % at T_0 = 773 K. Both the hydrogen yield and the optimization variables (ϕ, N, P_0) increase linearly with increasing initial temperature T_0. The fuel conversion of the optimal configurations is high throughout the considered temperature range, increasing from 98.8 % to 99.2 %. The most significant parameter for high hydrogen yields seems to be the initial temperature and the equivalence ratio, while the the engine speed and initial pressure can be regarded as variables to fine tune the process, for example proper ignition timing.

Under the conditions proposed by the optimization, the engine does not produce significant amounts of power or may need to be externally motored. This does not pose a problem, since the engine could be operated in a mixed fuel-lean/fuel-rich fashion, i.e. some cylinders running conventionally could drive the other cylinders running under H_2-producing conditions. In principle, however, it is possible to operate the engine while simultaneously producing both power and H_2. Since the optimization took only the H_2-yield into account, any excess power produced by the engine was not considered. However, simultaneous power generation along with H_2 production can be added as a constraint in future optimization work.

Conclusions

The numerical results predict both high hydrogen yields and high fuel conversions throughout a large temperature range.

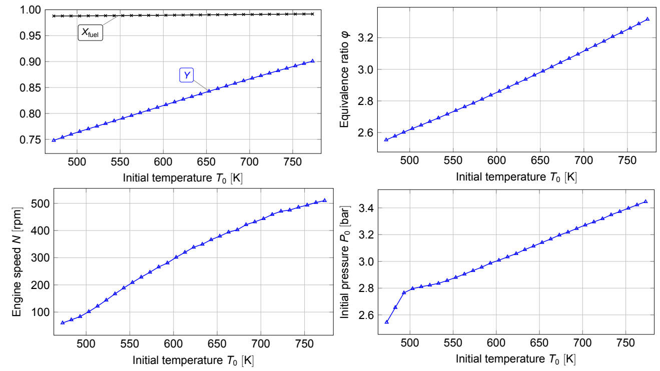

Figure 1. Results of the optimization for constant initial temperatures T_0 showing the maximized H_2 yield, fuel conversion (top left) and corresponding values of the optimization variables ϕ (top right), N (bottom left) and P_0 (bottom right).

The engine would need to be operated under very fuel-rich conditions, at relatively low RPMs and at elevated pressures. These pressures could be attained by a supercharger, for example.

In addition, a reaction pathway analysis has indicated that substantial amounts of H_2 are produced from precursors which are also valuable products, such as methanol, formaldehyde and ethylene. Therefore, there is potential that these products may also be obtained in reasonable yields if the engine design parameters and operating conditions are changed accordingly. This underlines our conception of the engine being a flexible chemical reactor and not a mere device for generating power.

Acknowledgments

Financial support of this work by the Deutsche Forschungsgemeinschaft within the framework of the DFG research unit FOR 1993 “Multi-functional conversion of chemical species and energy” is gratefully acknowledged.

References

Atakan, B. (2011). Gas turbines for polygeneration? A thermodynamic investigation of a fuel rich gas turbine cycle. *Int J Thermodyn, 14 (4),* 185–192.

Deutschmann, O., Tischer, S., Correa, C., Chatterjee, D., Kleditzsch, S., Janardhanan, V.M., Mladenov, N., Minh, H.D., Karadeniz, H., Hettel, M., Gossler, H. (2015). DETCHEM Software Package (Release v2.6).

Gossler, H., Deutschmann, O. (2015). Numerical optimization and reaction flow analysis of syngas production via partial oxidation of natural gas in piston engines. *Int J Hydrogen Energy, 40,* 11046–11058.

Powell, M.J.D. (1998). Direct search algorithms for optimization calculations. *Acta Numerica, 7*, 287–336.