Integrated Design of Renewable Fuel and Spark-Ignition Engine

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Abstract

Renewable fuels enable high efficiencies in spark-ignition engines. Their combustion properties allow to exploit advanced engine concepts for which conventional gasoline is not suitable, e.g., very high compression ratios and highly boosted conditions. Fuel design can identify such alternative fuels. So far, fuel design utilizes models of engine performance fitted to experiments using moderate engine conditions and conventional gasoline. This work proposes an integrated design approach utilizing an engine model fitted to and validated with measurement data of alternative fuels in an advanced single-cylinder research engine. Constraining volatility related properties, the optimal blend consists of methyl acetate and ethyl acetate and achieves a net indicated efficiency of 44% at high load engine operation. Without property constraints, the optimal blend consists of methyl acetate and methanol and achieves a net indicated efficiency of 45 %. In light of model uncertainties, the results require experimental validation.

**Keywords**: Renewable fuels, fuel design, integrated product and process design, engine model, engine efficiency.

* 1. Introduction

Computer-aided product design (CAPD) can identify alternative fuels that enable superior engine performance in specially built engines compared to that of conventional fuels in conventional engines. Typically, such alternative fuels are identified based on physico-chemical fuel properties and, in case of spark-ignition engines, the research octane number (RON) is used as a proxy for high engine efficiency (Dahmen and Marquardt, 2016, McCormick et al. 2017). CAPD studies for other products, however, suggest that the method can be improved by integrating a model for the product use, for example in solvent design for chemical processes and in working fluid design for energy processes (Muhieddine et al., 2022, Neumaier et al., 2023). In recent years, such approaches have also been applied to fuel design. Specifically, fuels for spark-ignition engines have been designed for maximum engine efficiency, using empirical correlations or a thermodynamic engine model (Gschwend et al., 2019, vom Lehn et al., 2021, Fleitmann, Ackermann et al., 2023). In all these cases, the models contained parameters fitted to engine data of conventional fuels or blends of alternative fuels with conventional fuels. Since models for conventional fuels cannot reliably predict the occurrence of engine knock for alternative fuels, it is uncertain to which extent these models can be used to predict the engine performance of newly designed fuels.

* 1. Method

We present a CAPD method to design fuels by maximizing the achievable indicated efficiency in a zero-dimensional thermodynamic engine model that was calibrated and validated with experimental data from alternative fuels in a spark-ignition single-cylinder research engine with a compression ratio of 16.4. Importantly, we include ignition delay models derived from kinetic simulations to accurately predict the onset of knock. We maximize the indicated efficiency by optimizing the compression ratio, considering knock and peak pressure limitations. The engine model and optimization are implemented in MATLAB R2020a. To design an optimal multi-component fuel, we then select possible alternative fuel constituents known from previous studies. We enumerate binary and ternary blends and use MATLAB’s local optimization solver fmincon to tailor the fuel composition for maximum indicated efficiency, utilizing the engine model with embedded optimization of the compression ratio. To design a fuel that is knock resistant under extreme conditions, we allow compression ratios of up to 20 and set the intake and exhaust pressure to 2 bar. Aiming for proper in-cylinder mixture formation, we constrain volatility-related fuel properties.

* 1. Results and Discussion
     1. Fuel Design with Volatility Constraints

The design runs for 12 CPU hours on an Intel® Core™ i5-8500 processor with 16 GB RAM. The optimal blends achieve an indicated efficiency of 44%, which constitutes a relative increase of 17% over the efficiency that conventional gasoline achieves in the simulation with an optimized compression ratio and at an intake pressure of 1 bar. The three top blends contain large shares of methyl acetate and ethyl acetate. As a pure component, methyl acetate violates the upper limit on the enthalpy of vaporization, whereas ethyl acetate violates the lower limit on the bubble point pressure. The mixture balances both properties and thus is feasible regarding the imposed volatility constraints.

* + 1. Fuel Design without Volatility Constraints

In a separate design run without volatility constraints, the optimal blend consists of 60 mol-% methyl acetate and 40 mol-% methanol and achieves a slightly higher predicted indicated efficiency of 45%. In the simulation, this blend outperforms its constituents as neat fuels by synergistically combining the charge cooling effect of methanol with the presumably higher knock resistance of methyl acetate. However, it should be noted that for this binary blend, the change in indicated efficiency as a function of the composition is in the order of magnitude of the fitting error, i.e., the deviation between the experimental data that has been used for model calibration and the model output. Experimental investigations will be necessary to confirm the higher knock resistance of methyl acetate and the synergistic behavior of the blend. Model uncertainties can be caused by the reduced-order modeling approach as well as fuel specific inaccuracies introduced by the choice of sub-models for fuel dependant processes. For example, the used combustion sub-model does not account for the influence of fuel chemistry on the combustion process that influences the pressure trajectory and thus the efficiency. Similarly, the sub-model for the evaporation process influences the temperature trajectory and thus the onset of knock.

* 1. Conclusions

In conclusion, this study identifies alternative fuel blends for advanced spark-ignition engines. Future work could improve the sub-models for fuel evaporation and combustion processes, as well as quantify the uncertainty. Furthermore, the approach could be extended to design fuels for operation under lean conditions and pre-chamber applications to further increase the indicated efficiency of the engine.

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