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FINAL REPORT

1308 | 2022 – Frankfurt am Main

## Kraftstoffzusammensetzung zur CO<sub>2</sub>-Reduktion

Wie können neue Generationen von Kraftstoffen und deren Zusammensetzung systematisch dazu beitragen, den Wirkungsgrad zu verbessern und die Emissionen für eine nachhaltige Mobilität zu reduzieren?

### *Fuel Composition for CO<sub>2</sub> Reduction*

*How can new generation of fuels and their composition contribute systematically to enhance thermal efficiency and reduce emissions for sustainable mobility?*

# Fuel Composition for CO<sub>2</sub> Reduction

Project no. 1348

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## How can new generation of fuels and their composition contribute systematically to enhance thermal efficiency and reduce emissions for sustainable mobility?

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### Final report

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#### Abstract:

Alternative fuels have the potential to improve the performance of spark-ignition engines in terms of increasing efficiency, i.e., reducing CO<sub>2</sub>, and decreasing engine-out emissions. In particular, engine operation with charge dilution using excess air is a promising way to achieve these goals simultaneously. However, the lean engine operation is limited by the combustion stability, which decreases with excess air dilution. Boosting the laminar burning velocity at the lean limit by alternative fuel usage stabilizes combustion and extends lean operation limits. To this end, we defined and investigated neat alternative fuels and their mixtures with a conventional gasoline pump fuel. A broad fuel property database was developed to identify high-potential fuel candidates in the fuel design process. Missing properties were estimated using machine learning approaches. Then, the highest-ranked fuels' combustions behavior were investigated by experimentally investigating laminar burning velocities and ignition delay times for 50%(v/v) mixtures with gasoline. Cyclopentanone and anisole were selected for detailed characterization due to their beneficial impact on increasing knock resistance and laminar burning velocities.

Both fuels were investigated as neat fuels, as mixtures with 50%(v/v) gasoline, and as mixtures with a maximum oxygen content of 5%(m/m), resulting in seven fuels in total, including the gasoline base fuel. First, the laminar burning velocity and the ignition delay time measurements of the neat fuels and the 50/50 mixtures were conducted for a broad range of conditions, functioning as validation targets for kinetic modeling. Kinetic models were developed for both neat fuels and their blends with gasoline. Second, thermodynamic investigations on a spark-ignition engine with compression ratios of both 10.8 and 13.5 were performed to evaluate the lean limits and the emission behavior using all seven fuels. Third, numerical 3D simulations were performed to assess both the mixture formation at the lean limit and the early flame kernel development. Fourth, numerical 0D simulations were used to evaluate the combustion process, using results from the engine experiments as input parameters. Fifth, a co-optimization of the fuel and the engine was simulated to quantify possible increases in the compression ratio considering the alternative fuels' improved knock resistance.

The investigations of the laminar burning velocities revealed higher overall values for cyclopentanone, especially under rich conditions, and higher values for anisole under lean conditions compared to conventional gasoline. Moreover, longer ignition delay times were measured for cyclopentanone/gasoline blends than for anisole/gasoline blends, yielding a higher knock resistance. The engine investigations showed that cyclopentanone and its gasoline mixtures achieved higher net indicated efficiencies and higher lean limits than their anisole counterparts. The numerical investigations revealed a more pronounced charge stratification with increasing anisole in the blend, yielding increased nitrogen oxide emissions. However, both fuels showed a high knock resistance. The co-optimization simulations showed that the compression ratio could be increased beyond 13.5 without knock restriction using both neat fuels. Although both fuels benefit combustion in spark-ignition engines, cyclopentanone has been proven to be more beneficial than anisole and can be considered a promising fuel for additional investigations in the future.

The objective of the research project was achieved.

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RTD performers: Chair of Thermodynamics of Mobile Energy Conversion Systems (tme), RWTH Aachen University  
Head: Univ.-Prof. Dr.-Ing. (USA) Stefan Pischinger

Institute for Combustion Technology (itv), RWTH Aachen University  
Head: Univ.-Prof. Dr.-Ing. Heinz Pitsch

Chair of High Pressure Gas Dynamics (HGD), RWTH Aachen University  
Head: Prof. Dr.-Ing. Karl Alexander Heufer

Institute of Automotive Engineering (IFS), University of Stuttgart  
Head: Prof. Dr.-Ing. Michael Bargende  
Prof. Dr.-Ing. André Casal Kulzer

Chair of Thermodynamics / Thermal Process Engineering (TDTVT), Brandenburg University of Technology Cottbus-Senftenberg  
Head: Prof. Dr.-Ing. Fabian Mauß

Research associate(s) / author(s): Patrick Burkardt, M.Sc. (tme)  
Florian vom Lehn, M.Sc. (itv)  
Raik Hesse, M.Sc. (itv)  
Hongchao Chu, M.Sc. (itv)  
Dipl.-Ing. Sascha Jacobs (HGD)  
Sebastian Crönert, M.Sc. (IFS)  
Tim Franken, M.Sc. (TDTVT)

Project coordination / user committee: Koji Kitano (Toyota Motor Corporation)  
Dr. Navid Shahangian (Toyota Motor Europe)

Scientific advisory committee chair: Dr.-Ing. Andreas Kufferath (Robert Bosch GmbH)

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