Potentials and Challenges of Tailor-Made Fuels from Biomass

S. Pischinger, M. Muether*
Institute for Combustion Engines (VKA)
RWTH Aachen University, Aachen, Germany

The Cluster of Excellence (CoE) ¨Tailor-Made Fuels from Biomass¨ (TMFB) takes an interdisciplinary research approach towards new synthetic fuels based on biomass feedstock. New target-designed synthesis pathways, employing novel catalytic systems, reaction solvents and tightly integrated production processes, which embed intensified process units for fuel production, are considered to create new tailor-made fuels most efficiently. The potential of the fuel as an optimisation parameter for future low-temperature combustion technologies for internal combustion engines will be fundamentally explored.

Introduction

World-wide increasing carbon dioxide (CO_2) emissions, a rising energy demand and limited availability of fossil energy resources constitute major challenges facing society today. Renewable raw materials are attaining increasing interest in this context.

In the European Union, the transport sector accounts for approximately 30 % of the total energy consumption and current forecasts even predict an increase in energy demand of 14 % for passenger transport and 74 % for freight transport between 2000 and 2030. Special emphasis is on transportation fuels, due to their specific requirements with respect to distribution, storage, preparation and combustion. Therefore, successful research activities on the fi eld of alternative fuels are strongly required for the transport sector.

The Cluster of Excellence (CoE) ¨Tailor-Made Fuels from Biomass¨ (TMFB) takes an interdisciplinary research approach towards new synthetic fuels based on biomass feedstock. New target-designed synthesis pathways, employing novel catalytic systems, reaction solvents and tightly integrated production processes, which embed intensified process units for fuel production, are considered to create new tailor-made fuels most efficiently. The potential of the fuel as an optimisation parameter for future low-temperature combustion technologies for internal combustion engines will be fundamentally explored.

The TMFB-Approach

The definition and production of these tailor-made biofuels with favourable characteristics represent a challenge for chemo- and biocatalysis, process and systems engineering, combustion research and engine technology. By striving for a new catalytic, selective and targeted transformation of the whole plant material (lignocellulose) into tailored fuel components, this CoE will provide the scientific basis to introduce the third generation of biofuels. These biofuels, in contrast to most of today's biofuels, will not be competing with the food chain.

The integrated approach, clustering expertise from natural and engineering sciences, will follow a model-based design procedure: a mixture of a few well-defined candidate fuel components with tailored properties will be derived from the requirements of the combustion process. The feasibility of this fuel will depend on the research success on attractive catalytic pathways and by the effort for their production. The viability of the desired blend of fuel components is therefore decided by technological, economic and ecological constraints, which critically depend on (bio-) chemical transformation, process engineering and combustion technology. The barriers between established research fields need to be overcome to achieve the CoE's objective and to find a systematically optimised solution, which cannot be provided by a single discipline alone.

The jointly founded ¨Fuel Design Center¨ documents the close collaboration of scientists from the faculty of Natural Sciences, Mathematics and Information Technology and the faculty of mechanical engineering at RWTH Aachen University, together with partners from the Fraunhofer Institute for Molecular Biology and Applied Ecology (Aachen) and the Max-Planck-Institute für Kohlenforschung (Mülheim an der Ruhr).

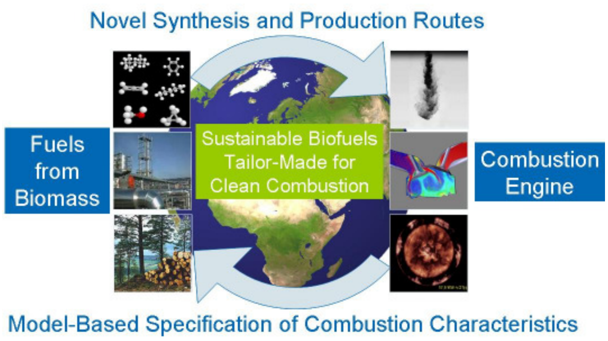

Fig. 1: The 3. Generation of Biofuels

* Corresponding author: muether@vka.rwth-aachen.de

Research Activities
To achieve the scientific vision of the CoE, the research groups from RWTH Aachen University and its partner institutions are focusing on three major ¨Integrated Research Fields (IRF)¨:

(i) ¨Molecular Transformation¨
(ii) ¨Reaction and Process Engineering for Biorenewables¨
(iii) ¨Fuel Injection and Combustion¨

These research fields are linked by two ¨Core Interactions Fields (CIF)¨:

(i) ¨Fuel Design¨ and
(ii) ¨Chemical and Physical Property Modelling¨

Additional activities are bundled in the¨Supplementary Cluster Activities (SCA)¨

IRF-1: MOLECULAR TRANSFORMATION
The integrated Research Field ¨Molecular Transformation¨ aims at the targeted conversion of biogenous substrates derived from the renewable feedstock streams cellulose, hemicellulose and lignin into the molecular constituents of a tailor-made fuel. A selected range of constitutive molecular transformations on the basis of catalysis as the key technology will be the core of IRF-1. Owing to the complexity of the required transformations, the complementary benefits of the three major catalysis disciplines, bio-, homo-, and heterogeneous catalysis need to be explored in an integrated approach ranging from the molecular to the mesoscopic scale.

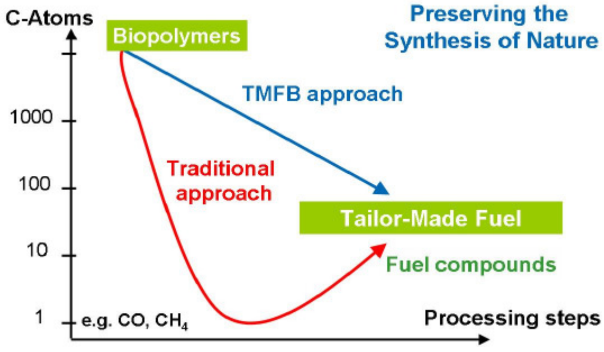

Fig. 2: Direct catalytic conversion of the plant material for energetically beneficial production processes

IRF-2: React ion and Process Engineering for Biorenewables
The Integrated ResearchField ¨Reaction and Process Engineering for Biorenewables¨ addresses key issues in process engineering related to the transition of biorenewable feedstock in fuel production. Research focuses on the foundations of integrated processes and intensified units; first, for the selective conversion of biomass to substrates and later, for their subsequent transformation into fuel components. Two novel and complementary biorefinery routes are investigated which target at the specific classes of biomass: whole green plants with high water content and wooden plants with low water content, respectively.

IRF-3: Fuel Injection and Combustion
The Integrated Research Field ¨Fuel Injection and Combustion¨ reconsiders the combustion process in combustion engines by using the fuel as a design parameter. The two traditional engine types, the spark ignition (SI) and the compression ignition (CI) engine, were designed to make use of the lighter or the heavier fraction of liquid hydrocarbons which can be distilled from crude oil. By tailoring the fuel obtained from biomass to specific engine needs, new engine combustion concepts will be developed which previously could not even be thought of. For CI engines, for example, auto-ignition of higher hydrocarbons, due to their low temperature chemistry, is viewed as beneficial but it is harmful for SI engines because the same chemistry is responsible for engine knocking. Tailor-made fuels having different temperature and pressure dependencies of auto-ignition chemistry may possibly avoid that contradiction. Since this feature and other properties differ from those of conventional fuels, tailor-made fuels will allow designing a new combustion process which shares common features of future SI and CI engines.

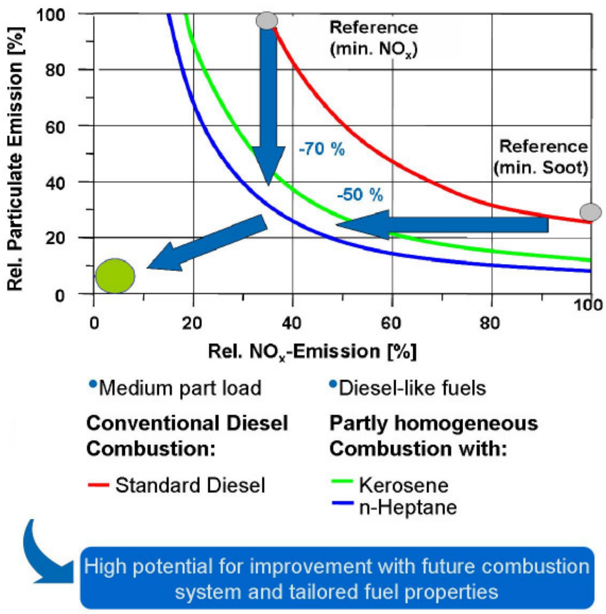

Fig. 3: Direct catalytic conversion of the plant material for energetically beneficial production processes

CIF-2: Physical and Chemical Property Modelling
Complex fluids consisting of intricate multifunctional molecules of biogenous origin and ionic liquids (IL) as solvents are of key importance for the research aims of the Cluster of Excellence. Today a lack of both, accurate description and fundamen-

tal understanding of the behaviour of such systems, is existing. Therefore, the goal of the Core Interaction Field ¨Physical and Chemical Property Modelling¨ is to build a fundamental understanding and to create predictive models with a sound physical basis which will contribute towards the development of tailor-made fuels. Quantum mechanics (QM) will be used to describe molecular properties while molecular simulations will reveal generic effects and analyse small-scale systems as a basis to develop and validate coarse-grained analytical engineering models. Beyond the scope of the proposed CoE, the results will be valuable for the development of biogenous feedstock based industries in general.

CIF-1: Fuel Design

In order to support the continuous pursuit of the ultimate goal of finding a tailormade fuel from biomass, the key activities focussing on the fuel definition are bundled in the cross-functional Core Interaction Field ¨Fuel Design¨. The Fuel Design process is a complex problem involving all disciplines of the CoE, ranging from reaction and process design, fuel production and fuel preparation in the engine to combustion and emission formation. Such an all encompassing approach has never been followed before. Only by using a systematic search procedure, assisted by suitable mathematical models and methods, the vast and unique opportunities in the design of novel fuels can be exploited. The methods and tools to be investigated not only allow identifying the promising compounds among known ones, but rather aim at the discovery of completely novel fuel components. In order to bridge the gaps still existing in models connecting molecular structure to reaction, process and combustion performance, appropriate data-driven and hybrid model descriptions are derived using experimental data and aggregated models from all IRFs and from CIF-2.

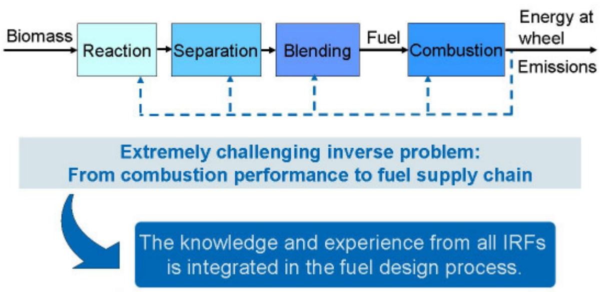

Fig. 4: Model-based description and optimisation of the overall process

SCA: Supplementary Cluster Activities

Supplementary Cluster Activities aim at the efficient networking of scientific processes within the CoE. Therefore, a conceptual framework has been developed to improve the cluster performance. In addition to this framework the enhancement of satisfaction of all employees within the network constitutes an important aspect as well as the initiation of learning processes within the cluster by the reflection of networking activities. For the future, a transfer of this model shall be enabled to complex, highly networked, scientific cluster approaches of a similar type.

Fuel Design Center Aachen

The Cluster of Excellence ¨Tailor-Made Fuels from Biomass¨ strives to concentrate the existing expertise to take advantage of methodological and scientific synergies. As a physical and visible focal point of the interdisciplinary collaboration, a ¨Fuel Design Center¨ will be established at RWTH Aachen University, which provides laboratory space of about 1000 m^2. Two new professorships and five junior professorships will be setup at RWTH Aachen University. In addition to a high profile international scientific advisory board with key researchers from renowned institutes such as Princeton, Yale and the MIT, a board of key industrial players ensures a direct feedback from the application side, among which are chemical industries such as Bayer, petrochemical industries such as BP and Shell, and automotive companies such as Daimler, Ford, Volvo and VW. Consequently, the research results will not only be introduced quickly into lectures and courses but also transferred into industrial application.

Acknowledgements

This work is funded by the Excellence Initiative by the German federal and state governments to promote science and research at German universities.