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L-IV | From CO$_2$ to Fuel Candidates: Evaluating the Homogeneous Catalysis Route

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The conversion of CO$_2$ into value-added products such as alcohols and acetals as high-value chemicals offers a promising synthetic route to reintegrate CO$_2$ into the value chain and contribute to the defossilization of the (petro)chemical industry. This requires a detailed understanding and adjustment of the catalysts involved for each transformation step. The target molecules are continuously evaluated for their properties in the application as a fuel additive in order to control the development at an early stage.

The successful development of a stepwise homogeneously catalyzed hydrogenation of CO$_2$ from furnace gases with subsequent build-up reaction to EtOH is the basis for further conversion to higher alcohols.[1] The process sequence includes methyl formate and methyl acetate as key intermediate platform chemicals.

HOMOGENEOUS CATALYTIC GUERBET-TYPE COUPLING OF ETHANOL TO BUTANOL

Methanol and ethanol can be produced from flue gases. The Guerbet coupling to higher alcohols, however, turns out to be a highly complex reaction network. Close inspection with Process Analytical Technologies, sound reaction engineering and a strong cooperation with catalyst researchers and potential users brought surprising insights into molecular intricacies and unsuspected side products so far. This led to a deeper understanding as the basis for all further work.
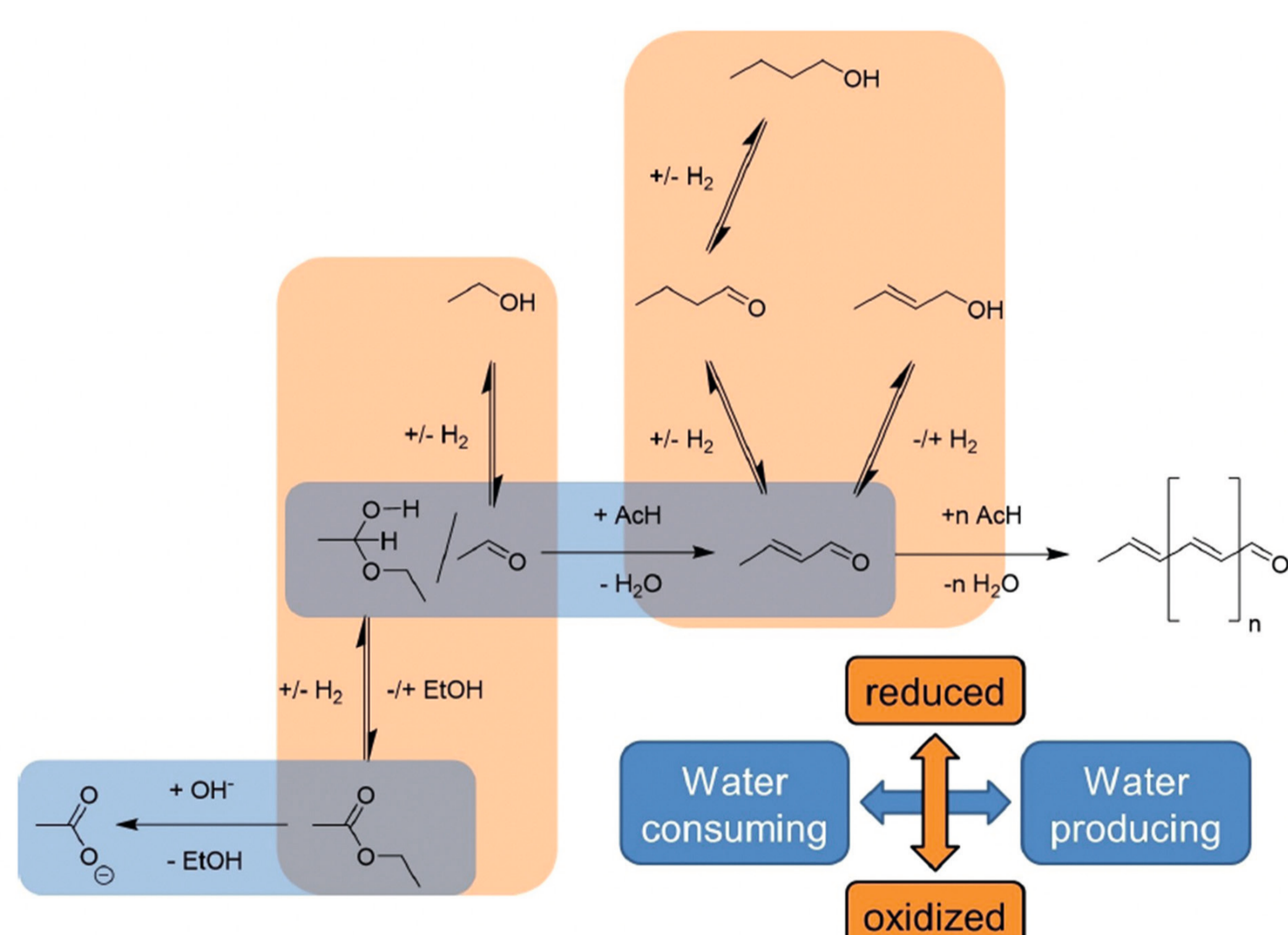

The Guerbet coupling network of ethanol to 1-butanol.

HYDROFORMYLATION WITH CO$_2$/H$_2$ AND ACETAL SYNTHESIS

In another approach, alcohols will be formed from C$_2$-C$_{4+}$ olefins, CO$_2$ and H$_2$. Therefore, CO$_2$ is used as a carbonylating agent for the hydroformylation of olefins. This is achieved by the reduction of carbon dioxide CO$_2$ to carbon monoxide CO in a reverse Water-Gas Shift reaction.

The formed CO can then be consumed in the hydroformylation, after subsequent hydrogenation alcohols of chain length C$_{n+1}$ are obtained. These alcohols can either find direct application as a fuel additive, or can be transformed into the respective acetals after conversion with CO$_2$ and H$_2$.
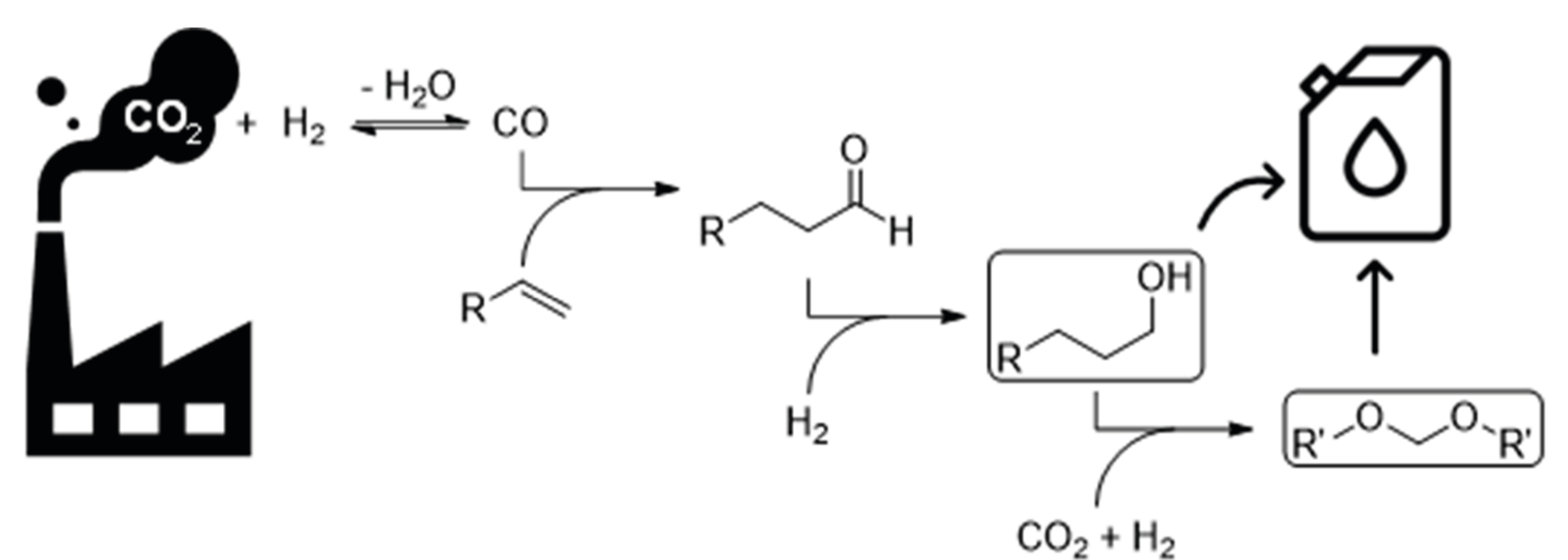
Reverse water-gas shift based access to alcohols and acetals.

EVALUATION AND ENGINE TESTING OF SYNALK-FUELS

From fundamental screening of ignition behavior with linear alcohols up to testing in a single-cylinder engine. C$_1$-C$_4$ alcohols show increased ignition delay times over a wide pressure and temperature range. Engine testing showed significant efficiency gains and emission reductions with these alcohols. A suitable mixture of alcohols was defined based on these results, consisting of ethanol, 1-propanol and 1-butanol.
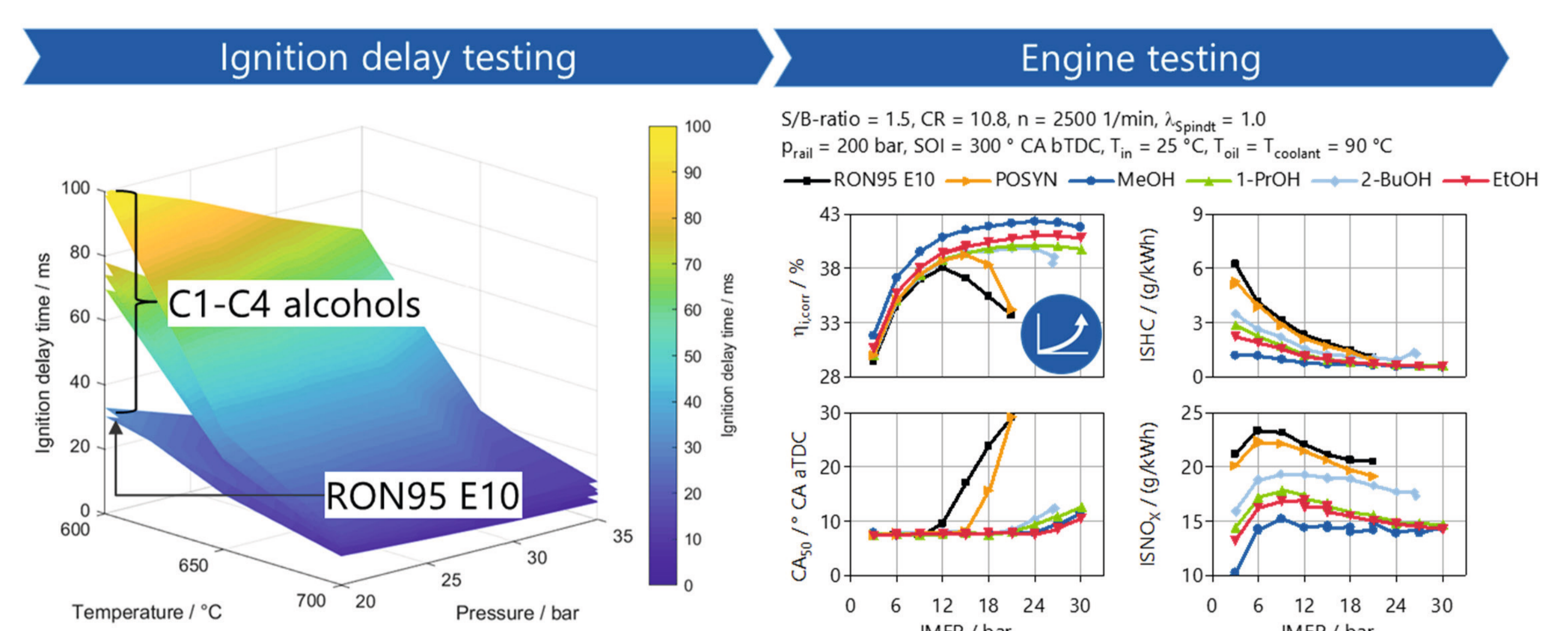
Ignition delay and engine testing of C$_1$-C$_4$ alcohols vs. gasoline.

References
[1] M. Schmitz, C. Erken, A. Ohligschläger, J. K. Schnoor, N. F. Westhues, J. Klankermayer, W. Leitner, M. A. Liauw, Chem. Ing. Tech. 2018, 90, 1476-1488.

A KEY BUILDING BLOCK FOR THE CLIMATE PROTECTION

CO$_2$ reduction by cooperation of process industrial sectors