

L-IV Downstream Process Development

Institute of Technical and Macromolecular Chemistry of the RWTH Aachen (ITMC), Chair of Translational Molecular Catalysis, Worringerweg 2, 52074 Aachen, Germany Carolin Schartmann*, Ole Osterthun, Jürgen Klankermayer, *schartmann@itmc.rwth-aachen.de

After having successfully demonstrated an efficient multi-step process for the conversion of furnace gas components carbon dioxide (CO_2) and molecular hydrogen (H_2) to higher alcohols (C_3-C_4 , see bottom figure) in the first project phase, the ITMC has now shifted focus to further processing the obtained product mixtures. Utilisation of the obtained products as possible fuel components is of particular interest.

SYNTHESIS OF ACETALS AS POTENTIAL FUEL DROP-INS

One possible approach to valorise the product mixtures obtained by the multi-step conversion of furnace gas (see bottom figure) is acetalisation. In that transformation, the obtained higher alcohols are again reacted with a gas mixture of CO₂ and H₂:

$$CO_2 + H_2 + 2 R-OH \rightarrow R-O-CH_2-O-R$$

Subsequently, the obtained acetals can be utilised as dropin fuels, which would generate lower particle emissions due to their comparatively high oxygen content. The focus is, therefore, set on optimising the reaction conditions as well as modifying the organometallic catalyst and its additives to further improve selectivity and yield of the reaction to then take the reaction from batch to a continuous process.

In a joint venture in collaboration with the Chair of Thermodynamics of Mobile Energy Conversion Systems (VKA) of the RWTH, the thusly produced drop-in fuels will be tested regarding their combustion properties and classified into diesel fuel or petrol fuel (additives).

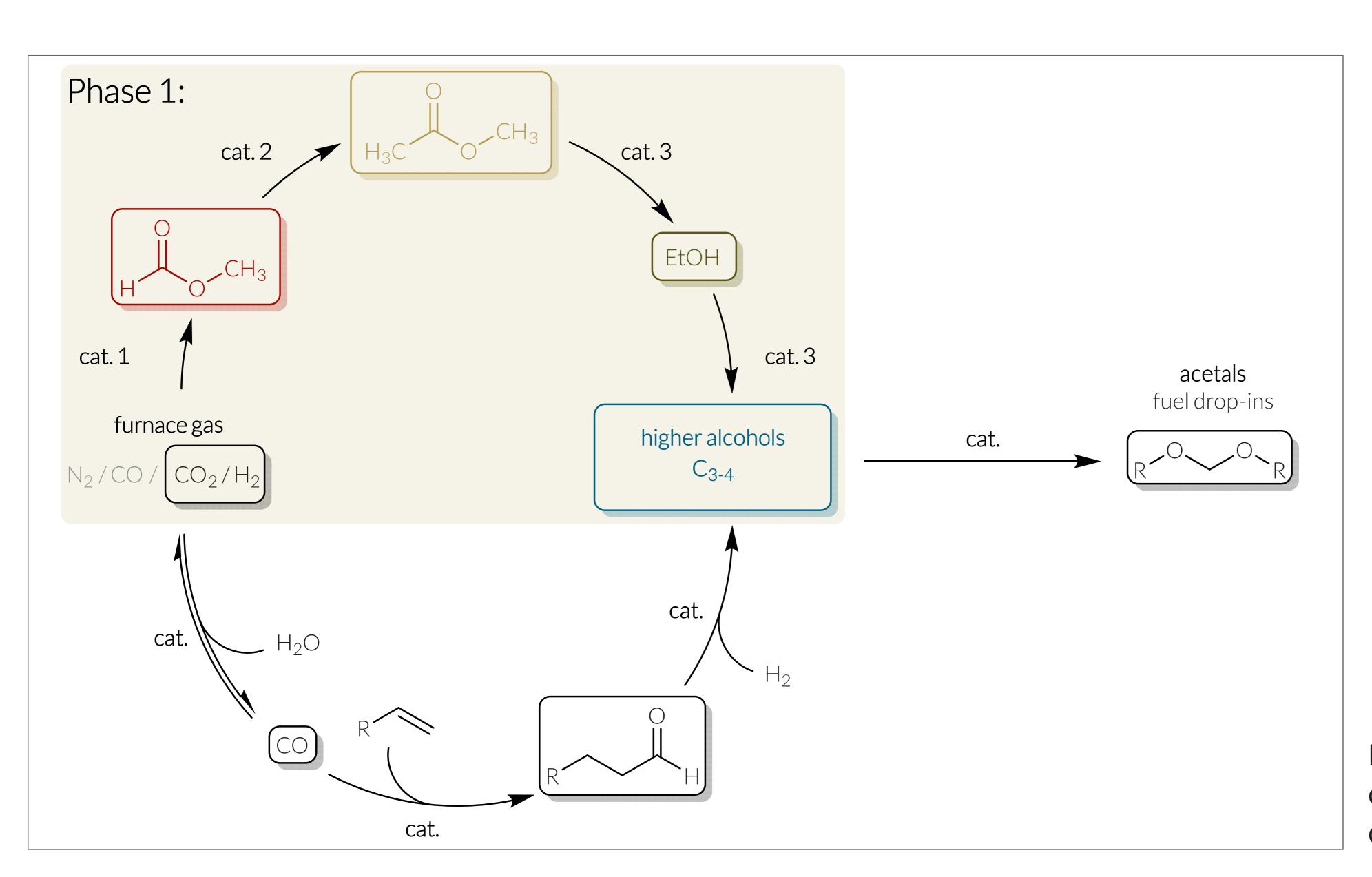
COMBINATION OF THE REVERSE WATER GAS-SHIFT-REACTION WITH A CARBONYLATION REACTION

Another way to further process furnace gases is the reverse Water Gas-Shift-Reaction (rWGS). The rWGS reaction is an equilibrium reaction in which carbon dioxide (CO₂) is reduced to carbon monoxide (CO):

$$CO_2 + H_2 \rightarrow CO + H_2O$$

The greenhouse gas CO₂ can, therefore, be utilised as a surrogate for the highly toxic carbonylating agent CO. The generated CO can then be reacted in a follow-up reaction, e.g. in a hydroformylation with olefins, generating aldehydes, which could subsequently be hydrated to form the corresponding alcohol.

In this second project phase, the reverse Water Gas-Shift-Reaction should be combined with a carbonylation reaction. One main objective is to run both transformations parallelly, as the constant withdrawal of CO would positively influence the reaction equilibrium of the reverse Water Gas-Shift-Reaction, increasing the yields of CO and consequently also the carbonylation products.



Multi-step process for the production of higher alcohols from furnace gas as demonstrated in the first project phase.

A KEY BUILDING BLOCK FOR THE CLIMATE PROTECTION

