



REDIFUEL

Deliverable report

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Executive Summary

The objective of the REDIFUEL project is to generate a sustainable and innovative synthetic biofuel which can compete with fossil based fuels. In the final REDIFUEL fuel mixture between 20 %-30 % of the fuel matrix will be made up by alcohols of various chain lengths.¹ The alcohols act as high value additives in the proposed synthetic fuel. It was proven that they show enhanced combustion behaviour and decrease the amount of pollutants.^{2,3}

Those alcohols are generated by converting C5-C10 olefins, coming from the Fischer-Tropsch process (the first step in the REDIFUEL project), into C6-C11 alcohols. The hydroformylation/hydrogenation reaction is very effective for this transformation.⁴ In the hydroformylation reaction carbon monoxide and hydrogen are added to an olefin double bond, generating aldehydes elongated by one carbon atom. In the second step the aldehydes are hydrogenated to alcohols. The reaction has nearly 100% atom efficiency and can be run under mild conditions. Both steps in the hydroformylation/hydrogenation reaction need to be catalysed. The most commonly used and very effective ones are homogeneous transition metal catalysts, e.g. catalysts based on rhodium or cobalt.⁵

The catalyst plays a key role and is the deciding factor for the overall yield and also the product distribution.⁶ Therefore an effective catalytic system is the starting point and influences the overall effectiveness of a future process to generate those alcohols (Figure 1).

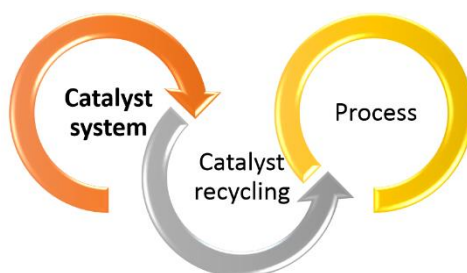


Figure 1: Steps in process development.

In this report, the development of two effective catalytic systems for this reaction are described and discussed. The first catalytic system is based on rhodium as the catalyst metal, with inexpensive and readily available tertiary amines as ligands. This catalytic system is able to catalyse both reactions, the hydroformylation and the hydrogenation, in a single step and therefore directly transforms olefins to alcohols. With this approach a yield of 60 % alcohols after 1.5 hours of reaction time can be achieved with 1-octene as model substrate. To the best of our knowledge, this new catalyst shows one of the highest activities for the tandem catalysed hydroformylation/hydrogenation reaction ever reported. In addition, the reaction is very selective, and the only by-products are olefin isomers.

The second catalytic system is also based on rhodium as the catalyst metal in combination with water-soluble phosphine ligands. This system catalyses the first hydroformylation reaction. The resulting aldehyde products are then hydrogenated over a solid nickel hydrogenation catalyst. Although in this case two catalysts for two separate reaction steps are needed, rhodium in combination with phosphines is very well known and highly active for the first crucial hydroformylation step.⁴ In our tests with the REDIFUEL mixture a yield between 40 % and 70 % of aldehyde products is generated in 1.5 hours with an extraordinary high catalytic activity. Again, the only mentionable by-products are olefin isomers. Furthermore, the water-soluble phosphine ligands make a liquid/liquid two phase catalyst recycling possible. Both mentioned systems are promising candidates for the production of alcohols. As the second catalytic system with sulfonated phosphine ligands allows for an easy and intrinsic catalyst recycling it will be the focus of future investigations. In case of a good recycling strategy can be developed also for the one step approach, the catalytic system can be adjusted.

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Project partners:

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- 3 - CSIC – AGENCIA ESTATAL CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS - ES
- 4 - VTT – Teknologian tutkimuskeskus VTT Oy - FI
- 5 - RWTH – RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN - DE
- 6 - OWI – OWI Oel-Waerme Institut GmbH - DE
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- 8 - NESTE – NESTE OYJ – FI
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