



## Press release

## Public Defence on 02 Dec 2022

# Biofuels: one way to carbon-neutral future

<b>Title of the doctoral thesis</b>	Hydrodeoxygenation of fatty acid esters for biofuel production over sulfur-free catalysts
<b>Content of the doctoral thesis</b>	<p>Liquid biofuel is playing an important role to reduce the carbon footprint for the transportation sectors. Catalytic hydrotreatment (also called hydrodeoxygenation) is an attractive technology to convert biological feedstock such as vegetable oils or animal fats into drop-in biofuels via the mechanism of oxygen removal. The main objective of this thesis was to gain new insights into the hydrodeoxygenation reaction mechanism over novel sulfur-free catalysts with the main focus on zirconia supported rhodium catalyst (<math>\text{Rh/ZrO}_2</math>). We are also aiming to develop a suitable kinetic model which can be used for design the hydrodeoxygenation process.</p> <p>Fatty acid esters were applied as the model compound of the bio-based feedstock. Deoxygenation of fatty acid esters over <math>\text{Rh/ZrO}_2</math> catalyst always led to the alkane products of one carbon number shorter than the reactants, which is attributed to the decarbonylation reaction mechanism. Both the active metal rhodium and the support <math>\text{ZrO}_2</math> could act as the active sites for the deoxygenation reaction. Thus, the selection of support is as crucial as the metal for catalyst development. The most-active zone is likely located at the perimeter of rhodium nanoparticles. It is therefore beneficial to create more perimeter sites when developing zirconia-supported metal catalysts for hydrodeoxygenation application. It was also found that acidic support <math>\text{H}\beta</math> was favorable for the deoxygenation purpose resulting in alkane products, whereas basic support <math>\text{MgO}</math> was not suitable for biofuel application as it was highly selective to the formation of alcohol. Two types of kinetic models, e.g., power-law and mechanistic models, were developed based on the proposed reaction mechanism. They were both able to describe the reaction data with satisfactory accuracy. The applied modelling methodology and mechanism hypotheses could also be applicable for the hydrodeoxygenation process of more complex feedstocks.</p>
<b>Field of the doctoral thesis</b>	Chemical Engineering
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<b>Public defence date and time</b>	02 December 2022 at 12 o'clock (in Finnish time)
<b>Remote defence</b>	<a href="https://aalto.zoom.us/j/68002531390">https://aalto.zoom.us/j/68002531390</a>
<b>Place of public defence</b>	Aalto University School of Chemical Engineering, Lecture hall Ke2 (Komppa-Sali), Kemistintie 1, (main door at Biologinkuja) Espoo
<b>Opponent(s)</b>	Professor Tapio Salmi, Åbo Akademi University, Finland
<b>Custos</b>	Professor Pekka Oinas, Aalto University School of Chemical Engineering
<b>Link to electronic thesis</b>	<a href="https://aaltodoc.aalto.fi/handle/123456789/51">https://aaltodoc.aalto.fi/handle/123456789/51</a>
<b>Keywords</b>	hydrodeoxygenation, HDO, biofuel, fatty acid ester, kinetic modelling, reaction mechanism, rhodium, zirconium dioxide, noble metal catalyst, cobalt catalyst