

Newsletter



C123 – Methane oxidative conversion and hydroformylation to propylene

No. 3, December2021

C123 conference contributions

The C123 project was profiled at the 2021 AIChE annual meeting in Boston. Two different lectures were given in two different sessions of the AIChE meeting.

The first lecture had the topic 'Shaped Catalysts for Oxidative Coupling of Methane' at the session 'Hydrocarbon Conversion: C1 Aromatization and Coupling' given by Jordan Guillemot from CNRS on Tuesday, Nov 9.

In this lecture promising results obtained on supported catalysts under relevant conditions for Oxidative Coupling of Methane (OCM) with high CO₂ content in the feed were presented. The catalyst characterization combined with kinetic modeling for the identifications of key catalyst parameters that drive activity and selectivity were discussed. The results included contributions from partner Axel'One.



Lecture 1 of C123 at AIChE 2021

The second lecture had the topic 'C123: From Methane to Value-Added C3 Chemicals Via Ethylene' at the session 'Value-Added Chemicals from Natural Gas I' given by Jeroen Poissonnier from Ghent University on Wednesday, Nov 10, with contributions from partners Johnson Matthey, SINTEF, Linde and CNRS.

In this lecture a breakthrough technology to upgrade natural gas to propanal was presented. The process consists of the Oxidative Conversion of Methane (OCoM), rather than OCM, where ethylene and synthesis gas are formed, and the heterogeneously catalyzed hydroformylation of ethylene to propanal. C123 is closing the gap between the operating conditions of both process steps as much as possible using a model supported multiscale approach and will ultimately develop a unified catalyst and process at TRL 5.



Lecture 2 of C123 at AIChE 2021

In addition to these lectures, the C123 project submitted two abstracts for the books of abstracts of two conferences in September 2021. Unfortunately, COVID-19 restrictions prohibited the completion of these conference presentations.

The first abstract is published in the book of abstracts (p. 459) of the XII International Conference on Chemistry for Young Scientists "Mendeleev 2021" held on September 6-10 2021 in St Petersburg, Russia. The topic was 'New trends in oxidative conversion of methane. Effect of catalyst'. The authors of this abstract were S. N. Osmanova, G. N. Azimova, E. H. Ismailov, D. B. Taghiyev, and S. M. Zulfugarova from partner ANAS and J. W. Thybaut from Ghent University.

The second abstract is published in the book of abstracts (p.149-150) of the IV Russian Congress on Catalysis "ROSCATALIZ" held on September 20-25 2021 in Kazan, Russia. The topic was 'Oxidative

conversion of methane. The choice of catalyst and perspective directions of the reaction' by E. H. Ismailov, D. B. Taghiyev, S. M. Zulfugarova, S. N. Osmanova , and G. N. Azimova from ANAS and J. W. Thybaut from Ghent University.

C123 publications

The first two C123 publications, by Amieiro et al. and Dubois et al., have been published back-to-back in *Johnson Matthey Technology Review*. The first manuscript, highlighting the technical challenges addressed within C123 and entitled "A Disruptive Innovation for Upgrading Methane to C3 Commodity Chemicals", can be accessed at <u>https://doi.org/10.1595/205651321X16051060155762</u>. The second manuscript, describing the market and viability potential of the C123 project and entitled "C123 – Methane oxidative conversion and hydroformylation to propylene", can be accessed at https://doi.org/10.1595/205651321X16051080751506.

Home / Johnson Matthey Technology Review, Volume 65, Number 2



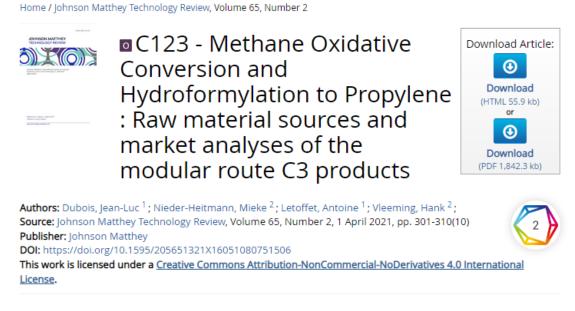
A Disruptive Innovation for Upgrading Methane to C3 Commodity Chemicals : Technical challenges faced by the C123 European consortium



Authors: Fonseca, Alvaro Amieiro ¹; Heyn, Richard H. ²; Frøseth, Morten ²; Thybaut, Joris W. ³ ; Poissonnier, Jeroen ³; Meiswinkel, Andreas ⁴; Zander, Hans-Jörg ⁴; Canivet, Jérôme ⁵; Source: Johnson Matthey Technology Review, Volume 65, Number 2, 1 April 2021, pp. 311-329(19) Publisher: Johnson Matthey

DOI: https://doi.org/10.1595/205651321X16051060155762

This work is licensed under a Creative Commons Attribution-NonCommercial-NoDerivatives 4.0 International License.



A third C123 publication has been published in the ACS journal *Industrial & Engineering Chemistry Research*. The manuscript 'Kinetics Assessment of the Homogeneously Catalyzed Hydroformylation of Ethylene on an Rh Catalyst' by S. Siradze, J. Poissonnier, M. Frøseth, R. Stensrød, R. H. Heyn and J. W. Thybaut (from UGent and SINTEF) can be assessed at https://pubs.acs.org/doi/10.1021/acs.iecr.1c02572.

RETURN TO ISSUE <th<< th=""><th>Rh Catalyst</th><th></th></th<<>	Rh Catalyst	
DPF (2 MB) Supporting Info (1) * SUBJECTS: Hydroformylation, Hydrocarbons, Ligands, Equilibrium, Catalysts		Industrial & Engineering Chemistry Research
Abstract The homogeneously catalyzed hydroformylation of ethylene to propanal using an Rh(H)(PPh ₉) ₃ (CO) catalyst has been assessed experimentally in a gas-liquid batch reactor and via microkinetic modeling, based on Wilkinson's dissociative mechanism. A higher reaction rate was observed with increasing temperature, up to 10° °C. Even higher temperatures resulted in catalyst deactivation, which was also attributed to lower total pressures and PPh ₉ /rhodium molar ratios. The model and its parameters were statistically significant and could be used to simulate the trends observed in the experimental data. Activation energies for the insertion of ethylene and the oxidative addition of H ₂ of 42 and 48 kJ mol ⁻¹ , respectively, were obtained. Ethylene insertion and oxidative addition of H ₂ were identified as the most kinetically relevant steps in the reaction mechanism.		(A, 60 A, CASIM (A, 60

All publications are available via Open Access. Enjoy reading!

Start of a project video

A project video is under production. The making of the script was started at beginning of October 2021. The video is expected be ready by early 2022.

Webinar: New and innovative methods for the conversion of alkanes to olefins

In this webinar, the three Horizon 2020 sister projects **C123** – Methane oxidative conversion and hydroformylation to propylene, **ZEOCAT-3D** – Development of a bifunctional hierarchically structured zeolite-based nano-catalyst using 3D-technology for direct conversion of methane into hydrocarbons via methane dehydroaromatization and **BIZEOLCAT** – Bifunctional Zeolite based Catalysts and Innovative process for Sustainable Hydrocarbon Transformation presented their research on the common topic of conversion of alkanes to olefins and aromatics.

Different speakers from the three sister projects gave various lectures. The overview of the projects was presented by Joris Thybaut (UGent for C123), Maria Tripinan (IDENER for ZEOCAT-3D) and Ana Villacampa (Fundació Eurecat for BIZEOLCAT).

More information about the projects can be found on

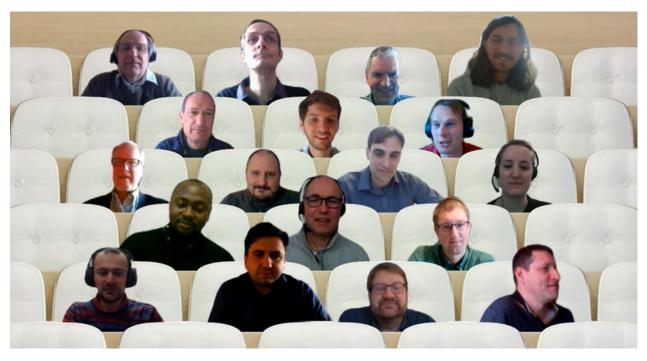
C123: https://www.sintef.no/projectweb/c123/ ZEOCAT-3D: https://www.zeocat-3d.eu/ BIZEOLCAT: https://www.bizeolcat.eu/

C123 27M and 33M progress meetings on 3-4 March 2021 and 9-10 September 2021, online

The H2020-funded C123 project had its fifth project meeting with 37 participants from the 11 consortium partners over a total of 4 online sessions on 3 and 4 March 2021.

The sixth project meeting took place on 9 and 10 September 2021 and had a total of 4 online sessions.

The entire consortium had scientific discussions on the technical work packages. The work package meetings showed promising status updates the partners made throughout every WP. With respect to the Oxidative Conversion of Methane (OCoM) the catalytic tests showed great results. Catalyst synthesis and kinetic modeling of the hydroformylation (HF) have taken a major step forward during the last period. The design of the OCoM reactor and C123 process is getting into its final shape and, while challenging, a more sustainable C123 process concept compared to the conventional C3 production routes has been established. A meeting of the consortium's General Assembly concluded the proceedings.



C123 participants in the virtual meeting room during the 27M progress meeting

Editorial from the C123 Executive Board

The increases in energy costs, specifically those for natural gas in Europe, has been featured in the news cycle this fall and early winter. The reasons are, of course, complex, but they can be related to a number of coincidental factors, including a large increase in demand from countries that are willing to switch from coal-fired power plants to a cleaner energy source, low national natural gas storage volumes at the beginning of the winter season and geopolitical aspects, such as the increase tension in Ukraine and the delayed start of the Nordstream 2 gas pipeline.

Not all the regions of the world are affected the same way. In the USA, the delayed restart of shale gas production, after the low prices during the Covid pandemic, has had an impact. Also, the possibility to export liquefied natural gas from places where it was not possible before has increased local prices. The disruption of LNG transport resulting from COVID-induced logistics gridlocks is another economic impact.

The lack of natural gas has forced some countries to restart coal-fired power plants. This shows that, despite a large demand for natural gas, countries will switch to cheaper energy (coal) from economic considerations, even if they had previously made strong commitments to limit emissions of Greenhouse gases. There is therefore a natural price regulation for natural gas, in that it cannot be too expensive otherwise energy production switches to coal and that it must be cheaper (on an energy content basis) than crude oil since natural gas is more difficult to transport and to store.

This picture, though, only holds for large production and consumption of natural gas. For the remote sites, there is still production where gas is often flared – when not vented – and for these sites there are still no clear solutions today. Thus, consumption on site, which is the goal of the C123 project, still makes sense if the resulting product is easy to transport and store. There is a big reservoir of this type of natural gas in line with the small plants that we have considered in the project.

For biogas, the high gas prices will in the short term push the biogas to the fuel market, where there are mandates and credits. Thus, it will likely not be available for conversion to chemicals. Once prices get back to previous levels, and there are no more fuel mandates but a level playing field, then the biogas will be used for chemical applications. Indeed, the push toward sustainable material exploitation will continue despite any current price for natural gas.

The current increases of gas prices are mainly limited in regions like Europe. Globally there is still a large excess of natural gas which is not yet utilized but still flared, especially at remote locations. The goals of the C123 project are still highly relevant, even in economic situations where the natural gas price is high.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 814557.