

Supervisor	Period	Funding
Joris Thybaut	2019-2023	H2020-C123

Hydroformylation of ethylene: assessment of the reaction kinetics and development of an integrated process with OCoM

Aim

Construction of Single-Event MicroKinetic (SEMK) models for ethylene hydroformylation over homogeneous and heterogeneous catalysts. Development of a generic software (μ KE) for kinetic model construction and reactor simulation. Exploitation of this knowledge using the developed software in the development of an integrated process comprising an Oxidative Conversion of Methane (OCoM) and a hydroformylation step.

Justification

OCoM refers to a novel combination of reactions aiming at transforming methane to an appropriate product spectrum for further conversion into C₃ products, such as propanal, propanol and/or propylene. Instead of focusing on C₂ optimization (ethane/ethylene) as in the Oxidative Coupling of Methane (OCM), OCoM aims at an effluent with an optimized ratio of C₂H₄, CO and H₂ which is subsequently sent to a hydroformylation reactor. Apart from the desired chemical transformation into C₃ products, hydroformylation also ensures an easy product separation and, hence, recycle of the unreacted feed. In this way cheap and unexploited carbon resources can be directly valorised in the production of valuable propylene. Within the framework of the Horizon 2020 project 'C123', a collaboration between eleven industrial and academic partners, the development of a comprehensive process is considered. This ranges from catalyst design to mapping the chemical knowledge in powerful mathematical models and ultimately to the integration in an industrially viable process.

Program

Development of a software for the construction of two SEMK models for ethylene hydroformylation. The bulk of the necessary experimental data for the SEMK model construction will be acquired and provided by project partners. Complementary data can be measured in-house. The existing microkinetic engine (μ KE) software will be further developed to account for the reactor modelling needs in this project. This will range from accounting for non-isothermicity and diffusion limitations to ensuring the compatibility between the μ KE and process simulation tools such as ASPEN and Pro/II.

The developed tools will then be used to develop an integrated process for an OCoM and an ethylene hydroformylation step in close collaboration with the (industrial) partners in the C123 project.