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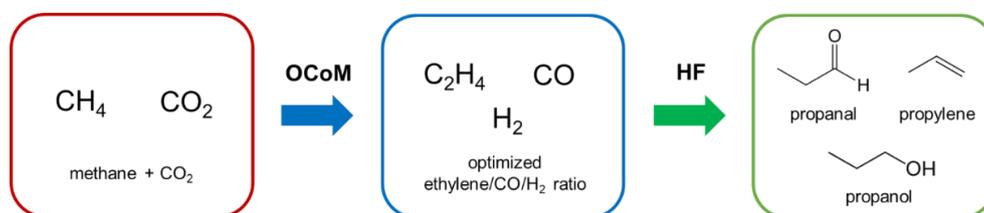
Reactor and process modelling of ethylene hydroformylation over a heterogenized catalyst

Aim

Developing a code for the simulation of an industrial reactor for the heterogeneously catalyzed hydroformylation of ethylene, enabling the modelling of the C123 process integrating the hydroformylation of ethylene with OCoM (Oxidative Coupling of Methane) to produce propanal starting from the greenhouse gases methane and CO₂ in a sustainable manner.

Justification

The hydroformylation of ethylene is a reaction which is used to convert a mixture of ethylene and syngas (H₂ and CO) to propanal. This reaction can be combined with OCoM which produces ethylene, H₂ and CO starting from methane and CO₂. By tuning the reaction conditions of the OCoM process, it is possible to obtain a ratio of components which serves as the ideal feed for the hydroformylation of ethylene. This will then lead to a process which produces valuable C3-products based on cheap and unexploited carbon resources. This process is currently being investigated within the H2020 C123 project, a collaboration between 11 industrial and academic partners from 7 different European countries.



A kinetic model has been developed for hydroformylation of ethylene over a heterogenized Rh catalyst at the LCT. As a part of the master thesis, a code will be developed in Fortran to simulate an industrial reactor starting from the existing code. Such a model will need to include the effects of mass and heat transfer on the reaction in order to simulate the reactor composition. The model will afterwards be implemented in the simulation tool ASPEN to assess the hydroformylation of ethylene as a part of an industrial process and determine which reaction conditions lead to the optimal conversion to propanal.

Program

1. Literature survey of the heterogeneously catalyzed hydroformylation of ethylene and its possible industrial applications
2. Development and testing of a Fortran code for the simulation of an industrial ethylene hydroformylation reactor using a heterogenized Rh catalyst
3. Simulation of the industrial process of ethylene hydroformylation in ASPEN