

<b>Coaches</b> ir. Sébastien Siradze	<b>Supervisors</b> prof. dr. ir. Joris Thybaut, dr. ir. Jeroen Poissonnier	<b>Funding</b> C123
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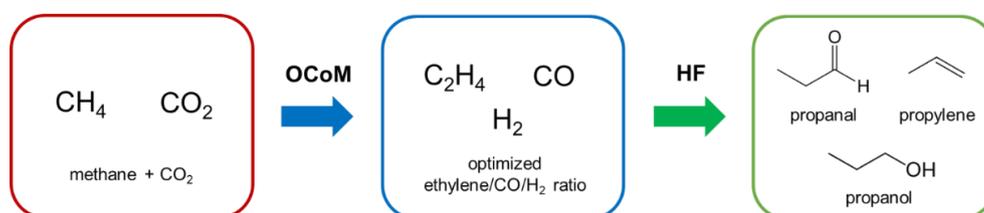
## Reactor and process modelling of ethylene hydroformylation

### Aim

Developing a code for the simulation of an industrial reactor for the 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 methane.

### Justification

The hydroformylation of ethylene is a reaction which is used to convert a mixture of ethylene and syngas ( $H_2$  and  $CO$ ) to propanal. This reaction can be combined with OCoM which produces ethylene,  $H_2$  and  $CO$  starting from methane and  $CO_2$ . 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 the hydroformylation of ethylene 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 for the kinetics. 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 hydroformylation of ethylene and its industrial applications
2. Development and testing of a Fortran code for the simulation of an industrial ethylene hydroformylation reactor
3. Simulation of the industrial process of ethylene hydroformylation in ASPEN