

Supervisor Joris Thybaut	Period 2019-2023	Funding H2020-C123
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Oxidative Conversion of Methane: unravelling the kinetics and optimizing the process for alternative propylene production

Aim

Understanding and quantifying of the Oxidative Conversion of Methane (OCoM) by the development of a detailed kinetic model combined with experimental investigation. Exploitation of this knowledge in the development of an industrial reactor and process model to provide guidelines for the optimal configuration and operating conditions.

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 optimized ratio of C₂H₄, CO and H₂ by combining OCM with a variety of reactions such as ethane dehydrogenation, methane (dry) reforming, catalytic partial oxidation, the (reverse) water gas shift reaction and CO₂ induced OCM. 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

Experimental data of the reactions integrated in OCoM will first be acquired in a broad range of operating conditions on a benchmark catalyst, supplied by a project partner. The operating conditions will be determined aiming at the acquisition of so-called intrinsic kinetics, i.e. in absence of heat and mass transfer limitations. These data, in combination with critically evaluated literature data, will be employed in the development of a detailed kinetic model.

Subsequently, the potential of performing various reactions in a single OCoM reactor will be examined in terms of different reactor technologies, configurations and operating conditions by development of integrated reactor models to ultimately optimize the CO/C₂H₄ yield such that it can be directly fed to an ethylene hydroformylation reactor. This optimization will be performed in the framework of the development of a C123 process in close collaboration with the (industrial) partners of the consortium.