LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Coach	**Supervisor(s)**	**Funding**
Laurien Vandewalle	Prof. dr. ir. Kevin M. Van Geem	FWO Flanders

CFD based design of a gas-solid vortex reactor for oxidative coupling of methane

Aim

The objective of this work is to optimize the design and operating conditions of the gas-solid vortex reactor (GSVR) in order to obtain high product yields during oxidative coupling of methane (OCM). Multiphase computational fluid dynamic (CFD) simulations will be performed in the open-source CFD package OpenFOAM.

Justification

The low natural gas price and the large amounts of shale and natural gas have created a renewed interest in methane as a source of liquid energy carriers or as a raw material for the chemical industry. In this work one of the most promising processes for valorizing methane to longer hydrocarbons, the oxidative coupling of methane (OCM), will be studied. Two key challenges have to be addressed before OCM can be considered as an alternative gas-to-chemical technology, namely the low yields of ethylene and what to do with the substantial heat release of the reaction. In order to prevent the unwanted propagation of the gas-phase reactions and efficiently address the large amount of heat released, reactors with short gas-phase residence time and efficient heat transfer are preferred for OCM. Hence the gas-solid vortex reactor (GSVR), developed at the Laboratory for Chemical Technology, emerges as an excellent reactor choice for demonstrating the OCM process.

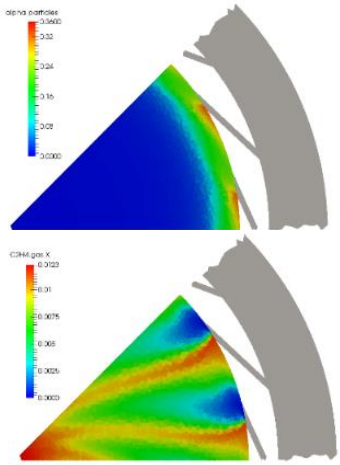

Figure 1. Catalyst volume fraction (top), and ethylene mole fraction (bottom) in a 16 slot GSVR.

In combination with modeling, valuable experimental studies can be carried out for different operating conditions. Nevertheless, these time intensive experimental studies can be drastically reduced by focusing on high level computational fluid dynamics (CFD) simulations. These simulations will allow to optimize the reactor geometry and operating conditions specifically for OCM.

In this project, both reactive and non-reactive CFD simulations of the GSVR are performed using the open-source CFD package OpenFOAM. The developed reactive CFD model takes into account a detailed OCM microkinetic model consisting of both homogeneous and heterogeneous reactions. The simulations are validated against the results obtained on the experimental setups available at the LCT.

Program

- Literature study on the state-of-the-art for oxidative coupling of methane: catalysts and reactor technologies.
- Getting acquainted with the OpenFOAM software package by performing some preliminary non-reactive CFD simulations, including validation with cold-flow experimental data.
- Reactive simulation of the GSVR for OCM and validation with experimental data.
- Optimization of operating conditions and design of the GSVR reactor specifically for the oxidative coupling of methane. Different microkinetic models will be tested for different catalysts. Benchmarking of the GSVR reactor technology through comparison with classical reactor techniques.

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