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Coach	**Supervisor(s)**	**Funding**
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Putting CO2 to use: CFD-DEM modeling of super-dry reforming reactors using detailed kinetic models

Aim

Particle-resolved CFD simulations of packed bed reactor configurations for super-dry reforming of methane, under a wide variety of operating conditions and bed properties

Justification

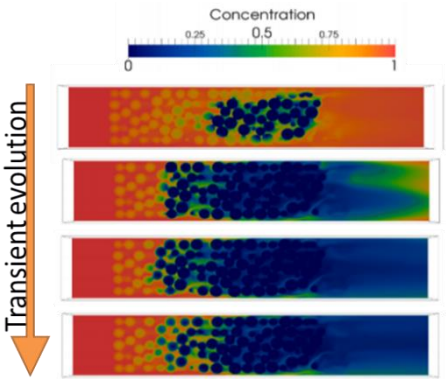

Figure 1: Transient evolution of concentration profile in a packed bed reactor using resolved CFD-DEM.

Process intensification of existing technologies and the development of novel Carbon Capture & Utilization (CCU) technologies will be of tremendous importance for the chemical industry to become CO2 neutral in the next decades. Today, dry reforming of methane, which converts two important greenhouse gases (CH4 and CO2) into CO and H2, is considered one of the most efficient technologies to realize a maximum global warming impact reduction. As an alternative to conventional dry reforming technologies, reforming based on chemical looping is considered a game changer. The super-dry reforming (SDR) technology, recently developed at the Laboratory for Chemical Technology (LCT), combines dry reforming with chemical looping to convert even more CO2 compared to regular dry reforming. Along with an appropriate design of chemical looping materials, the choice of the reactor configuration is vital for the practical realization of chemical looping processes such as SDR. Two types of reactor configurations are currently being considered for SDR: a multi-packed bed reactor or a circulating fluidized bed reactor configuration.

Instead of experimentally studying various reactor designs and sets of operating conditions, in-silico reactor design by multi-scale modeling using detailed chemical kinetics is much more efficient. Fundamental multiscale modeling will be the key to obtain a better understanding of the super-dry reforming system, to optimize existing reactor configurations and develop novel reactor concepts. Computational fluid dynamics (CFD) is hereby needed to predict flow fields and transport phenomena, while the use of microkinetic models for both gas and surface chemistry allows an accurate description of each elementary step at the microscale. A particle-resolved CFD-DEM approach allows to accurately design and hence also compare packed bed reactor configurations and circulating fluidized bed reactors, and is therefore the ultimate modeling strategy to optimize SDR. In this thesis, highly-detailed dynamic multi-region and CFD-DEM packed bed reactor simulations will be performed of the various sub-processes happening during SDR (dry reforming, CO2 sorption, redox chemistry). Using this particle-resolved model, effects of material use, hybrid structuring, composition, loading, porosity etc. on the functionality and effectiveness can be investigated.

Program

- Literature survey on reactor modeling for chemical looping processes
- Cold flow simulations of packed bed reactors and comparison with MRI experimental data from literature
- Reactive flow simulations of the various sub-processes during SDR
- Use the results from the above simulations to derive heat and mass transfer correlations to be used in simpler simulation frameworks
- Comparison with engineering 1D reactor models

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