

Bachelor-Project(s) - Chemical Engineering (Verfahrenstechnik)
Transport Limitations of Non-Catalytic Heterogeneous Reaction

Chemical Looping Combustion (CLC), as well as Chemical Looping Reforming (CLR) are two extremely interesting processes to reduce CO₂ emissions. In these processes porous particles play a central role, since they host the active substance (e.g., iron oxide). The reduction and oxidation of the particles is affected by reaction kinetics, the morphology of the active substance residing in the pores, transport within the pores of the particles, as well as flow characteristics of the process.

In our previous “NanoSim” Project (<http://www.sintef.no/projectweb/nanosim>) we have developed the simulation tool “*ParScale*” that enables a detailed prediction of the reduction and oxidation process of porous particles. ParScale uses a radially-discretized representation of a particle, and solves heat and species balances that occur in the solid, gas, and liquid phase of a particle. Most important, ParScale can be linked to particle and fluid flow simulations, enabling the direct simulation of small (lab-scale) reactors involving up to O(10⁵) particles.

The Bachelor project(s) (one student, or a team of 2 students) should (i) benchmark the predictions of ParScale against known analytical solutions for simple chemical reactions (literature study required), (ii) check the validity of approximate (analytical solutions) for more complex reactions, as well as (iii) probe the computational speed of ParScale on XEON workstations at our institute. Finally, the bachelor students should document their results in a thesis, as well as in the form of tutorials for users of ParScale. The student should bring (i) solid background in transport phenomena, (ii) ambition to perform numerical (simulation) work, and (iii) some experience with Matlab.



(<https://github.com/CFDEMproject/ParScale-PUBLIC>).

We offer

- high industrial and scientific relevance (e.g., for energy conversion processes)
- computer(s) with installed, and tested simulation software ParScale. Basic tutorials, screencasts, and personal training on the simulators (including the Linux operating system) can be provided. Based on the interest of the student(s), an introduction to C/C++ programming can be provided, but this is not critical for the success of the projects
- desk and office space for writing the bachelor thesis

Contact

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The bachelor thesis projects can be started as soon as possible.