

Development of reactor models using tabulated chemistry for the direct reduction process

Master thesis at Zittau

Mission

In the pursuit of more sustainable steelmaking, stakeholders are engaging in a transformative exploration of hydrogen-based direct reduction as an alternative to conventional blast furnaces. Potential for optimization of these new facilities is large, ranging from reactor design and operation, to fuel flexibility and heat integration of entire plants. The institute of low-carbon industrial processes has developed a particle resolved numerical tool to accurately model the direct reduction in fixed bed reactors. The goal of this master thesis is to initiate the development of simplified reactor models, in order to address optimization challenges at industrial scales.

Work steps

- Developing Python-based 0D/1D models of fixed beds for the direct reduction process of iron ore using H₂/CO as reducing gas
- Generating a table of apparent reaction rates, using the existing particle-resolved CFD fixed bed model
- Coupling the developed 0D/1D models with the tabulated values of reaction rates
- Validating the models against the CFD results

Skills required

- Currently studying physics, chemistry, mechanical engineering, aerospace engineering or a comparable field
- Interest in theory, modelling and simulation of physical processes
- Knowledge of fluid dynamics and CFD simulations
- Programming experience in C++, Python or other scientific programming languages is preferable

Start: 06.2024

Place: Zittau

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