OTTO VON GUERICKE UNIVERSITÄT MAGDEBURG | VST | FAKULTÄT FÜR VERFAHRENS- UND SYSTEMTECHNIK

Masterarbeit Nr.: LSS-Mxx
Aufgabenstellung für die Masterarbeit von: xxx (Matr.-Nr. xxx)

TITLE: **Improved kinetic description of polypropylene gasification under supercritical conditions**

SHORT DESCRIPTION:
Plastic recycling is becoming extremely important to mitigate the increasing problems coming with pollution, energy prices, and climate change. One of the most promising solutions to recycle mixed plastic wastes involves gasification under supercritical conditions. Due to the very high temperature and pressure used in the process, experimental studies are extremely complex, so that accurate numerical simulations are essential for better process understanding and optimization. The highest accuracy is achieved by Direct Numerical Simulation (DNS, [1]). To describe particle conversion, a suitable kinetic mechanism is of course needed. Only very few relevant studies can be found in the literature [2]. The objective of the present thesis is to optimize the kinetic scheme used in [1] based on [2] in order to increase noticeably the quality and accuracy of the simulation results.

Major steps:
- Get acquainted with the subject by reading the available literature on the topic, starting with [1] and [2]
- Get fully acquainted with the kinetic mechanism employed up to now
- Test modifications of this mechanism in order to improve quality and accuracy of the simulations using genetic optimization (GA)
- Document and analyze the obtained results

Pre-requisites:
- Good knowledge of chemistry
- First practical experience with multi-step kinetics
- Interest for chemical processes and recycling

Supervision:
- Prof. Gábor Janiga (ISUT/LSS)
- Dr. Cheng Chi (ISUT/LSS)
- M.Sc. Wei Guan (ISUT/LSS)

Beginning: **as soon as possible**
Due: xxx

[1] C. Chi, W. Guan, Z. Ou, K. Sundmacher, and D. Thévenin, "Direct numerical simulations of polypropylene gasification in supercritical water," *Physics of Fluids,* in press (2023).
[2] B. Bai, W. Wang, and H. Jin, “Experimental study on gasification performance of polypropylene (PP) plastics in supercritical water,” *Energy* 191, 116527 (2020).