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Simulation of pyrolysis process of waste plastics

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Recycling of waste represents one of the major goals to close the carbon cycle and to achieve circular economy concepts. The thermal conversion of plastic waste via pyrolysis to base chemicals for the production of new plastics represents one of the key technologies.
The talk provides an overview of fundamental research carried out at the Institute for Technical Chemistry (ITC) at KIT, with the objective to develop and optimize high-temperature process techniques for plastics pyrolysis suited for industrial-scale applications. Particular focus of the work is to study the plastics pyrolysis process by means of high-fidelity numerical simulations, which can be regarded as a "digital twins" of the real systems. In this way, the simulations provide detailed information for the temporal evolution and spatial distributions of the flow and chemical scalar fields, such as pressure, velocity, and temperature or species concentrations, which often cannot be assessed experimentally. Moreover, the modeling concept enables detailed analyses of the mutual interactions between underlying chemical-physical processes, such as heat transfer and chemical reactions, which dominate the pyrolysis process of plastics.
A couple of ongoing studies will be presented, ranging systematically from basic setups using a single plastic particle to a fully captured laboratory-scale fluidized bed reactor, which covers millions of sand and plastic particles. The results reveal strong correlations between characteristics behaviors of the pyrolysis process with the applied operating parameters. These correlations can be used to develop a more efficient reactor design for the pyrolysis of plastic waste. The opportunities and challenges for applications of the modeling concept concerning a compromise between simulation accuracy and computational cost, as well as the predictability of the underlying chemo-physical effects, e.g. pyrolysis reactions and melting behavior, will be highlighted at the end.

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