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ADVANCED NUMERICAL TOOLS FOR CHEMICAL PROCESS INTENSIFICATION: INNOVATIONS IN 3D PRINTING, MEMBRANE REACTORS, AND BUBBLE DYNAMICS

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Abstract. Chemical process intensification (CPI) is concerned with making innovations for chemical processes to make them smaller and faster, and more sustainable and efficient. Typically, CPI aims for utilizing and enforcing a synergy of the different chemical-physical processes in a reactor and involves a deep understanding of the reactor behavior and being able to control the different aspects of the reactor system. We therefore work on the development of digital twins for various reactor system types, along with experimental validation and verification. In this talk, I will give an overview of the numerical and experimental technologies and innovations that were developed in our group, aiming to stimulate other researchers to identify process intensification opportunities in their research. One area of interest is 3D printing of catalysts. Catalysts speed up chemical reactions, and with 3D printing, we can create custom-designed catalysts that enhance heat transfer while keeping the pressure drop within limits, leading to more efficient reactors. We have developed a number of logpile structure designs, that outperform conventional reactors relating to the pressure drop and heat transfer. Another intensification technology concerns fluidized bed membrane reactors. These reactors use a membrane to separate and control the reaction environment, and by properly extracting the product, it drives equilibrium reactions to the product side, resulting in better performance and higher yields. Our digital twin models help to gain insight in the placement of the membranes in the reactor under reactive conditions. Finally, we dive into the realm of two-phase gas-liquid flows, from bubble column reactors to modern electrolyzers. Understanding how bubbles form, grow, release, and rise can significantly improve the efficiency and design of e.g. electrodes and reactor structures. We have set out to develop digital twins using various approaches; by traditional numerical modelling (e.g. Euler-Lagrange CFD type models), as well as by developing deep-learning based techniques e.g. novel graph neural network architectures. The latter helps us to accelerate the simulation of complex physical systems, with a focus on bubble front-tracking in multiphase flow. Besides, machine learning techniques can also assist us to perform validation experiments. We demonstrate a machine-learning based technique for bubble detection and optical bubble characterization. We will explore how we can reconstruct the 3D shapes of bubbles, providing deeper insights into their behavior and improving their role in model validation.

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