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Digitalization in Catalysis and Reaction Engineering: Automatizing Work Flows

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Extended abstract

Digitalization and surrounding efforts fostered by the advent of Industry 4.0 have been a development topic in the fields of chemistry and chemical engineering for several years – so timing may be right to look back and to question what the impact of efforts made, and to judge the impact of workflows and technologies developed. First and foremost, the first two key principle of Industry 4.0, namely *Interconnectivity* and *Information Transparency* play the crucial role in the context of Digitalization as only a seamless flow of data based on standardized formats remains key to enabling *Decentralized Decisions* and *Technical Assistance*. Digitization and digital tools play a key role in the acceleration data transfer and development efforts, the automation and autonomation of technical equipment employed, and the digital transformation of “classical” chemical reaction engineering processes towards an ideal originally projected by the high-tech agenda of Industry 4.0.

In this presentation we will start our journey with fully integrated environments on a laboratory level where data are not only made available in data warehouses but can be used to drive feedback loops to autonomously drive experimental devices. The concrete example shows how chemometrics, based on complex chemical analytics can be used to trigger autonomous decision making in order to harvest the maximum value of experimental resources [1]. We will continue with illustrative cases where we tap into the power of simulation software, that facilitates the understanding of physicochemical processes and assists in the optimization of design and operation points of chemical and electrochemical reactors. The development of the required kinetic models is an iterative process, which can be sped up by automized work flows [2]. Furthermore, efficient research data management systems can ensure the (re)usability and traceability of experimental data for the development of novel catalysts and mechanisms [3]. To allow for in-depth insights into the underlying strategy of coupling of simulation and experiment, examples from the fields of reaction engineering including heterogeneous catalysis, electrochemistry and the production of alternative energy carriers are chosen.

A variety of tools have been developed and are under construction in the NFDI consortia such as NFDI4Cat [4]. Now, strong efforts are taken to combine the individual tools. Exemplarily, the Figure illustrates the communication between software tools that manage infor-

mation on catalyst synthesis, characterization, and performance as well as drivers for numerical simulation of catalytic reactors using these catalytic materials. Recently developed optimization tools to speed up model development and scale-up will soon extend this picture [5, 6].

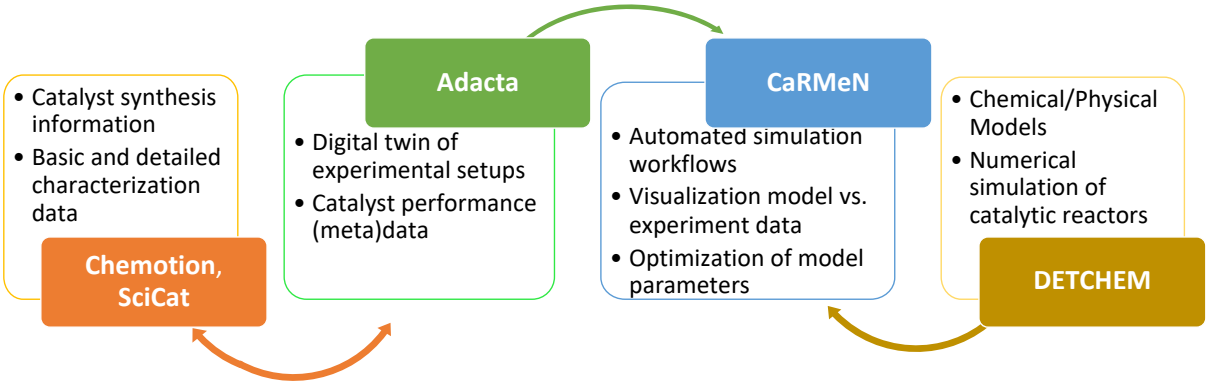

Figure 1: Functions and communication interfaces between software tools recently developed for digitalization in catalysis and reaction engineering.

The presentation is concluded by an overview of the work in the consortium NFDI4Cat, where digital tools, workflows and service offerings are developed in a community driven effort for catalysis related sciences including chemical engineering and process design.

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