Efficient multiphase chemical processes – from advanced modelling, simulation and measurement to novel reactor concepts and technologies

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Introduction
The chemical and process industry is one of the major industrial consumers of primary energy resources worldwide. Hence, this industry is especially concerned with rising energy prices and demands for reduction of greenhouse gas emissions [1]. In recent years, many advances in energy efficiency have been made especially in the production of bulk chemicals. Efficient heat recovery, efficient plant and production structures as well as improved synthesis routes and catalysts are examples for that. A further increase of efficiency is hardly achievable by simple improvements and game-changing technologies will most possibly only punctually come up. Gradual improvement of processes and equipment still has the highest potential to achieve a broader impact, particularly if a methodological base for optimal process designs is developed that can be applied to many of the different processes and process classes in chemical production [2].

Discussion
With the Helmholtz Energy Alliance "Energy Efficient Chemical Multiphase Processes" a broader network of groups and scientist is dealing with a variety of potential measures for improved chemical processes [3]. Thereby multiphase reactions, such as oxidation, hydrogenation, or hydroformylation, are in the central focus of the research work. As key factors of improved processes, efficient heat recovery of strongly exothermic reactions at elevated pressures and temperatures as well as improved selectivity of complex reactions is targeted. The first topic is demonstrated for the hydrogenation of nitrobenzene to aniline at an elevated temperature level, for which efficient micro-structured reactors as well as novel structured reactor concepts together with new catalyst developments are being considered. As an exemplary reaction with selectivity enhancement potential, the partial oxidation of isobutane to TBHP is under investigation. A further strong fundamental focus is on a multi-scale modelling of chemical reactions and processes from the micro-scale including reaction and kinetics to the device scale with various modelling approaches, such as computational fluid dynamics and compartment modelling. New methodological developments in experimental and measurement techniques target an improved understanding of the multiphase flow, local mass transfer and reaction and comprise tomographic and fluorescence imaging techniques, time-resolved Raman spectroscopy and distributed temperature measurement. Eventually new manufacturing technologies for designed reactor structures, such as additive manufacturing as well as new open-pore foams as catalyst supports and internals for intensified phase contacting are being applied and developed. The technical work is further accompanied by comprehensive analyses of the environmental and economic impacts of the new concepts.

Conclusions and Outlook
The contribution will give an overview over general needs for further progress in chemical process efficiency and discuss the necessity to fully understand and model the full complexity of chemical processes from the reaction via the apparatus to the whole process chain. Recent advances within of the author groups in this field are being discussed in more detail.

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