Shifting frontiers in applied catalysis

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Abstract

A typical challenge in the field of catalyst development and application is to cope with the reaction enthalpy associated to a chemical reaction.

Strongly **exothermic** gas phase reactions, such as selective oxidation, are typically operated in so-called multitubular reactors. Those reactors consist of up to 30,000 tubes loaded with a solid catalyst bed. The heat that is released during the reaction is taken up by a cooling medium, such as molten salt or steam. Due to heat transfer limitations, a radial and axial temperature gradient in the catalyst bed is formed leading to hotspots that can be up to 100°C higher than the temperature of the cooling medium. In those situations, minor deviations in the plant conditions can lead to a dangerous reactor runaway. It is therefore a pre-requisite for safe plant operation that the catalyst packing in all tubes of a multitubular reactor is close to identical. This allows for comparable gas flow and heat transfer through the individual tubes. A case study illustrates the requirements as regards the uniformity of the catalyst packing in the tubes and the relevant parameters to achieve this.

In case of an **endothermic** reaction, the productivity of a chemical plant can be significantly increased by effectively supplying to and distributing the required heat over the catalytic bed. The presentation elaborates on two fundamentally different approaches how this challenge has been addressed in the fields of Steam Methane Reforming and the Dehydrogenation of Propane.

As an example for a classical approach to cope with this challenge, a case study in **Steam Methane Reforming** (SMR) is shown. In SMR, heat is supplied from outside of the reactor. A better and more effective distribution of heat in the catalyst bed can be achieved by optimization of the catalyst shape, which influences the heat and mass transfer properties of the catalytic bed and the catalyst particle itself. Classical design criteria have been applied and they have led to a new shape with improved heat and mass transfer properties.

Such shape design and optimization can be done in a much faster and more focused way: with modern modelling tools for the simulation of fluid dynamic properties of a catalyst packing and subsequent experimental verification using 3d printing technology for fast prototyping of new shapes.

In the case of endothermic **Dehydrogenation of Propane** to Propylene according to the Houdry® process, an entirely different approach was chosen to more evenly supply and distribute the required heat to the catalytic bed. Rather than exclusively supplying the heat from outside of the reactor tubes, so called **HGM ("Heat Generating Material")** is introduced into the reactor. It supplies heat in-operando via an exothermic phase transfer of an inorganic material during the oxidation and reduction cycle. Various tests in a bench-scale test reactor have been conducted to find the optimal configuration of HGM and catalyst bed and its influence on the temperature profile and resulting catalytic performance.