FROM LABORATORY TO INDUSTRIAL OPERATION: MODEL-BASED DIGITAL DESIGN AND OPTIMIZATION OF FIXED BED CATALYTIC REACTORS

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Abstract

Careful design of catalytic reactors can reduce both the cost and risk associated with new designs, as well as reduce ownership costs significantly through better performance during operation. The Advanced Process Modeling (APM) approach allows performing detailed design of multitubular reactors taking into account multi-scale effects – from catalyst pore to industrial reactor scale – by combining high fidelity models with model-targeted experimentation, followed by implementation of the detailed model online for monitoring, forecasting and optimization.

This paper introduces the APM approach to model-based digital design and optimization of fixed-bed catalytic reactors and demonstrate them on industrial cases.

Keywords

Fixed-bed reactors, Model-based design and optimization, gPROMS-CFD Multitubular interface.

Introduction

Optimization of the design and operation of fixed-bed catalytic reactors requires highly detailed models that can represent the complexity at all levels from the microscale reaction and diffusion phenomena occurring in the catalyst to the macroscale operation within the full industrial reactor geometry. Despite such methods being known for decades, their applications across the R&D-to-operation lifecycle are still not being seen widely. One of the reasons for not applying state-of-the-art methods is often the required skills and time it takes to develop those. However, there are now ready-to-use tools on the market, as well as established methodologies that can accommodate the required model-based activities over the whole R&D-to-operation lifecycle.

Advanced Process Modelling approach

This paper introduces the Advanced Process Modelling (APM) approach to model-based design and optimization of fixed-bed catalytic reactors and subsequent operational optimization in the following steps: (1) capturing all physics relevant to the problem of interest using a modular model library that allows construction of reactor models of various configurations by users without mathematical modeling background; (2) evaluation of model parameters, such as (i) heat transfer and flow resistance properties of the catalyst bed, and (ii) parameters of reaction kinetics, as well as determining the required pilot plant experiments targeting evaluation of these properties; (3) performing optimization-based reactor design, where the objective function considers all key Operational and Capital expenditure contributions and the key decision variables and constraints include the reactor geometry and operation parameters (while considering the reactor in conjunction with other unit operation units such as separation columns if necessary); (4) making final adjustments to the reactor design based on a hybrid model that includes a CFD representation of the complex reactor shell-side geometry; and (5) implementation of the detailed model online within a digital applications framework for operational monitoring, forecasting and optimization.

The presentation emphasizes the significant advantage in using the same Advanced Models of catalytic bed for the model validation (i.e. evaluation of bed properties and reaction kinetics) and for the optimization activities and any online or offline decision support tool for operations.

The steps of the APM approach are illustrated using industrial cases that include design of a reactor for production of Dimethyl Sulfide, simultaneous optimization of reactor and separation section for propylene oxide production, high-performance terephthaldehyde reactor design, and online implementation of an acetylene hydrogenation reactor model.

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