A Comparison of Homogeneous and Heterogeneous Dynamic Models for Industrial Catalytic Reactors in the Face of Catalyst Deactivation

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Abstract

Simulations of a fixed-bed industrial methanol reactor have been studied in the presence of long term catalyst deactivation. The performance of the reactor was investigated using two different dynamic models: (a) a homogeneous model, and (b) a heterogeneous model. Both the models were found to predict the identical results at industrial operating conditions. The models have been verified against daily observed process data of a methanol plant for four years of operation and good agreement was found. By analyzing the results of the homogeneous model, it was shown that there is a non-uniform catalyst deactivation along the reactor. Simple model, of the type presented here, represents a useful beginning in the optimization and control of reactor for methanol synthesis, since it is capable of describing many of the qualitative trends observed with such reactors.

Keywords: Heterogeneous; Homogeneous; Methanol; Low-Pressure; Synthesis

1. Introduction

The computer simulation and mathematical modeling of the physical and chemical processes involved in catalysis has a wide range of uses. Firstly mathematical modeling can be used to study the phenomena involved in a catalytic process and obtain further understanding of the system without the need for costly, time-consuming experimentation. Secondly, it can be used to obtain values of physical parameters that are very difficult or impossible to obtain by experiment, because they are present in highly convoluted data. Thirdly, modeling can be used in the interpretation of the experiments.

Dynamic simulation of processes has a wide range of applications including; investigation of start-up and shut-down, identification, safety, control, dynamic optimization, investigation of dynamic behavior of the system and operability studies. Furthermore, dynamic model should be preferred to steady-state models, since the former provides a realistic description of the transient states of reactor, and the numerical solution strategy of dynamic model is more robust than the solution of steady-state model. Thus, it allows for safe and trustworthy studies of the control and optimization of reactor [1, 2].

So far quasi-steady-state models of multiphase methanol reactors have been extensively developed in several reviews [3, 4], while there is no information available in the literature regarding the use of a dynamic model for industrial methanol synthesis in the face of long term catalyst deactivation.