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Modeling of the Methanol Synthesis Catalyst Deactivation in a Spherical Bed Reactor: An Environmental Challenge

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Abstract

Catalyst deactivation and its environmental consequences are believed to be an important issue seriously needed to be dealt with. In this study, a mathematical model of a spherical bed along with the catalyst deactivation in a long-term operation period for the methanol synthesis was investigated. The inside space of the two spheres reactor configuration was filled with the catalyst. The materials in the outer surface of the inner hemisphere were understudied. The equations solved at two dynamic and static levels via the finite difference method. It was revealed that, the resulting pressure drop as well as operation costs might have been lowered while the production capacity enhanced in comparison with the conventional reactors and overall leading to better environment protections. Furthermore, the analysis of the catalyst deactivation behavior indicated that a series of parameters including the reactor temperature and size, as well as the entering carbon monoxide and feed rates played an important role in the catalyst deactivation.

Keywords: Spherical reactor, Catalyst deactivation, Methanol synthesis, Modeling

1. Introduction

Methanol is one of the three most important products produced thru the chemical industries world from which too many materials derived [1, 2]. Due to shortage of energy resources foreseeable in future, the direct use of the methanol as a clean fuel in such places as in fuel cells and hydrogen production is an issue under

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serious considerations. Hence its environmental aspects are undertaken. In the methanol synthesis from the synthesis gas, the catalyst plays an important role for which the activity reduction during the process might cause the methanol production lowering. This leads to production of competing undesirable species in the reaction scheme as well as wasted energy both for this and other needed downstream separations hence; creating environmental concerns. Generally, a good industrial catalyst provides high activity and selectivity toward production of desired species. In addition, one important factor in selecting an industrial catalyst is that its activity and selectivity not only remain high but also, stays near the optimum level for a long period of time. Due to the presence of such environmental toxins as CO and CO_2 in the reactor feed as well as high operating temperatures catalysts become deactivated. On the other hand, it is an unavoidable complex phenomenon taking place hence; should be carefully investigated [3, 4]. Moreover, the use of spherical bed reactors in order to improve the methanol synthesis is widely understudied. This might therefore be a good alternative to regular conventional tubular reactors (TR). In spherical reactors known as the RF-SPBR, the space between the two concentric spheres is filled by catalyst. In short, the design is such that the feed inlet enters the vessel across the external wall and radially proceeds inward through the bed. Then it flows outward via a pipe collector. Advantages of this type reactor in comparison with the usual conventional TR types are a small pressure drop, low manufacturing costs as a result of a small wall thickness, and a high production capacity [5] hence, better environmental and economic outcomes. Ultimately, good deals of researches were performed on the synthesis of methanol in spherical bed reactors [5-10].

The present proposed model focuses on discussing the influences of the various reaction and reactor parameters on the catalyst deactivation and performance of the reactor for a spherical geometry. The main purpose of this study is to scrutinize the influence of various factors involved in deactivation of the $CuO/ZnO/Al_2O_3$ catalyst in spherical beds. Homogeneous and one-dimensional aspects have been considered throughout this study. The basic structure of this model is composed of heat and mass balance conservation equations coupled through thermodynamic and chemical kinetic relationships as well as auxiliary correlations for predicting physical properties.

2. Spherical Reactor Modeling

The Methanol synthesis from syngas (CO, CO_2 and H_2) in presence of the catalyst is widely used in industry. The schematic diagram of the spherical reactor is shown in Figure 1.

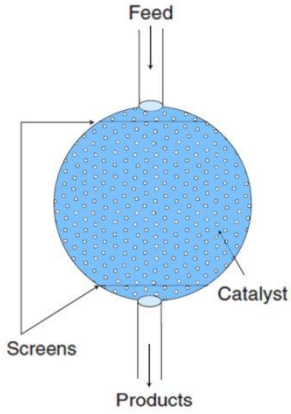

Fig. 1. Schematic diagram of a methanol synthesis in a spherical bed reactor