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Analysis of Hydrodynamic Parameters Effect on the Hydropurification Reactor Operation through Numerical Simulation

Abbas Azarpour[a,]*, Mohamed Ibrahim Abdul Mutalib[a], Shuhaimi Mahadzir[a], Anita Ramli[b]

[a]*Chemical Engineering Department, Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak, Malaysia*
[b]*Fundamental & Applied Sciences Department, Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak, Malaysia*

Abstract

In the class of three-phase catalytic reactors, trickle-bed reactors (TBRs) are the most extensively used in industry. They are utilized in petrochemicals, petroleum, chemicals, waste treatment, electrochemical and biochemical processing, and many other applications. One of the most significant applications of TBRs is their utilization in the process of purification. Since the purified product has to meet the required specifications of a high quality chemical, the TBRs operation control is very critical. Considerable fluctuation of the operating parameters values adversely affects the reactor efficient performance. In this paper, the effect of hydrodynamic parameters on the hydropurification TBR operation is investigated considering the product quality. A first principle heterogeneous model incorporating the hydrodynamic parameters and catalyst deactivation has been developed to analyze the reactor performance under the fluctuation of the hydrodynamic parameters. The devised model along with its mathematical solution has been coded into MATLAB R2016a environment. The results reveal that the deviation of hydrodynamic parameters of liquid holdup and gas holdup considerably influence the efficiency of the purified terephthalic acid reactor operation in term of product quality. Moreover, the impact of liquid holdup on the reactor operation is more than gas holdup in term of product quality. These research findings might be applied into an actual operating system mentioning that the deviation from trickling flow regime is to be avoided in the reactor.

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Keywords: Hydrodynamic; Reactor; Modeling; Deactivation; Hydropurification; Catalyst

* Corresponding author. Tel.: +605 368 7638; fax: +605 365 6176.
E-mail address: abbas.azarpour@utp.edu.my; abbas.azarpour@gmail.com

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1. Introduction

Trickle-bed reactor (TBR) is a multiphase reactor in which gas and liquid phases pass cocurrently downward through a fixed bed of solid catalyst particles. TBRs are widely employed in hydrotreating processes in petrochemical industries, petroleum refineries, and in many chemical industries. When the gas and liquid are fed cocurrently upward through the catalyst bed, the system is called a flooded bed reactor or upflow reactor. The upflow arrangement is utilized rarely in industrial application where TBRs dominate. Due to the unmoving catalyst bed, almost plug flow is established in TBRs, and in this case they are preferred to other three-phase catalytic reactors where the catalyst is either fluidized or slurried. From industrial and economic viewpoints, TBRs' low energy dissipation rate and high catalyst loading per unit volume of the liquid make them superior to the slurry reactors. Though, the disadvantages of TBRs are their low efficiency for the reactions with rapidly deactivating catalysts, such as in heavy oil hydrotreating processes, and the possibility of improper liquid distribution, which might result in hot spots and reactor runaway. The economic impact of how properly TBRs run is significant since; for instance, in the petroleum industry alone TBRs yearly processing capacity for different hydrotreating processes such as hydrodesulfurization, hydrocracking, hydrorefining, hydrodemetallization, hydrodenitrogenation, and etc. is estimated around 1.6 billion metric tons [1]. Thus, any improvement in TBRs performance will lead to the significant savings.

Nomenclature

a	deactivation parameter	*Subscripts*	
C	concentration (kmol m^{-3})	B	bed
H	Henry's constant (barg kmol m^{-3})	c	catalyst
k_d	deactivation model constant (d^{-1})	d	deactivation
$k_{i,ls}$	liquid-solid mass transfer coefficient ($m\ s^{-1}$)	g	gas phase
m	sintering order	i	index of component
r	rate of reaction (kmol kg$_c^{-1}$ s^{-1})	k	index of reaction
r_d	rate of deactivation (d^{-1})	l	liquid phase
R	universal gas constant (J mol^{-1} K^{-1})	P	particle
t	time (s)	s	solid
T	Temperature (K)	*Superscripts*	
u	superficial velocity (m s^{-1})	S	surface of catalyst
z	axial coordinate (m)		
Greek letters			
ε_B	bed void fraction		
ε_g	gas phase holdup		
ε_l	liquid phase holdup		
ε_P	particle porosity		
η	catalyst effectiveness factor		
ξ	specific surface area of the phase interface (m^2 m^{-3})		
ρ_B	bulk density (kg m^{-3})		

One of the utilizations of TBRs is in the hydropurification process. Purified terephthalic acid (PTA) is the chemical which is used to produce polyethylene terephthalate (PET). In the process of PTA production, crude terephthalic acid (CTA) is produced via the oxidation of para-xylene (PX). CTA powder containing around 2000-3000 *ppm* of 4-carboxybenzaldehyde (4-CBA) is not suitable to be utilized in a polymerization process to produce polyester. Therefore, CTA is purified in a TBR consisting of palladium supported on carbon (0.5wt. % Pd/C) catalyst through the hydrogenation reaction of 4-CBA which converts to para-toluic acid (PT) [2].

The most important parameters that can influence the operation of a TBR are hydrodynamic variables such as gas holdup, liquid holdup, pressure drop, and flow regime transition. To incorporate the mentioned parameters effects