Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

Development of a rigorous two-dimensional mathematical model for a novel thermally coupled reactor for simultaneous production of xylenes, hydrogen, and toluene

*Nazanin Hamedi, Mahshid Nategh, Fariba Keshtkari, Mohammad Reza Rahimpour**

Department of Chemical Engineering, School of Chemical and Petroleum Engineering, Shiraz University, Shiraz 71345, Iran

ARTICLE INFO

Article history:
Received 29 March 2017
Received in revised form 2 September 2017
Accepted 7 September 2017
Available online 20 September 2017

Keywords:
Thermal coupling
Heavy aromatics to xylenes
MCH dehydrogenation
Hydrogen production
Two-dimensional model
Coupling of mass

ABSTRACT

In this study, a novel reactor configuration has been proposed, in which the exothermic process of heavy aromatics upgrading to xylenes and endothermic process of dehydrogenation of methylcyclohexane to toluene and hydrogen are thermally coupled. Because of the existence of different components in the feedstock of the exothermic side, an elaborate kinetic model is applied to provide a reliable reactor model. A two-dimensional, comprehensive mathematical model is developed to predict the reactor performance, which is solved by means of finite difference method. The results indicate that by employing the coupled configuration, the xylenes and hydrogen production rates are improved, acceptably. Additionally, the effect of coupling of mass (recycling toluene from the endothermic side to the exothermic side) is investigated, which results in higher yield of xylenes in the first part of the reactor; while it lowers the xylenes yield in the second part.

1. Introduction

1.1. Heavy reformates conversion to xylenes

Aromatic components, including BTX (benzene, toluene, and xylenes), are highly demanded in the petrochemical industry as intermediate materials to produce end-products with applications in domestic, agricultural, and pharmaceutical sectors. Having a high octane number, such aromatics are used as suitable compounds to produce gasoline (Tsai et al., 1999). Catalytic reforming and naphtha pyrolysis are regarded as two important processes used to produce BTX. While, benzene and xylenes are used more frequently, the mentioned processes are more likely to produce toluene. Accordingly, some processes are used to convert toluene into xylenes and benzene (Tsai et al., 1999; Waziri et al., 2010). On the other hand, in most of the refineries a stream of heavy reformates (9-carbon aromatics or higher) is separated from gasoline to provide a more environmentally benign fuel with less aromatic contents (Ali et al., 2011). The heavy reformates and toluene can

Abbreviations: A_{10}, aromatic with 10 carbons; A_9, aromatic with 9 carbons; A_8, aromatic with 8 carbons; *B*, benzene; *BTX*, benzene, toluene, xylenes; *CCR*, continuous catalytic reforming; *CR*, conventional reactor; *EB*, ethylbenzene; *MCH*, methylcyclohexane; *MEB*, methylethylbenzene; *MX*, meta xylene; N_6, naphthene with 6 carbons; N_7, naphthene with 7 carbons; *OX*, ortho xylene; P_1, paraffin with 1 carbon; P_2, paraffin with 2 carbons; P_3, paraffin with 3 carbons; P_4, paraffin with 4 carbons; P_5, paraffin with 5 carbons; *PB*, propylbenzene; *PET*, poly ethylene teraphthalate; *PTA*, purified terephthalic acid; *PX*, para xylene; *TMB*, trimethylbenzene; *TOL*, toluene; *TCR*, thermally coupled reactor; *TR*, tubular reactor; *Xs*, xylenes.

* *Corresponding author*. Fax: +98 711 6287294.
E-mail address: rahimpor@shirazu.ac.ir (M.R. Rahimpour).

http://dx.doi.org/10.1016/j.cherd.2017.09.009

Nomenclature

a	Catalyst activity
A	Cross sectional area of exothermic side (m^2)
A_i	Inner lateral area (m^2)
A_o	Outer lateral area (m^2)
C_T	Total concentration of exothermic side ($kmol\,m^{-3}$)
C_i	Coefficients of the correlations for heat capacity and viscosity estimation
C_j	Concentration of component j in exothermic side ($kmol\,m^{-3}$)
C_j^{endo}	Concentration of component j in endothermic side ($kmol\,m^{-3}$)
C_{j0}	Inlet concentration of component j in exothermic side ($kmol\,m^{-3}$)
C_p	Specific heat capacity of exothermic side ($kJ\,kmol^{-1}\,K^{-1}$)
D_{jm}	Effective diffusivity of component j in the gas mixture ($m^2\,s^{-1}$)
D_o	Outer diameter (m)
D_i	Inner diameter (m)
d_p	Particle diameter (m)
E_i	Activation energy for ith reaction ($kJ\,kmol^{-1}$)
F_j	Molar flow rate of jth component ($mol\,s^{-1}$)
F (m,n)	Value of function F in the position m, n
h_{endo}	Heat transfer coefficient of endothermic side ($W\,m^{-2}\,K^{-1}$)
h_i	Heat transfer coefficient of the inner tube ($W\,m^{-2}\,K^{-1}$)
h_o	Heat transfer coefficient of the outer tube ($W\,m^{-2}\,K^{-1}$)
h_r	Step size in r direction (m)
h_{trans}	Heat transfer coefficient of exothermic side (transalkylation side) ($W\,m^{-2}\,K^{-1}$)
h_z	Step size in z direction (m)
K	Thermal conductivity ($W\,m^{-1}\,s^{-1}$)
K_{0i}	Frequency factor for Reactions (1)–(20) and (32) ($mol\,Pa^{-2}\,s^{-1}\,kgcat^{-1}$) (i = 1–20 and i = 32)
K_{0i}	Frequency factor for Reactions (21) and (22) ($mol\,Pa^{-4}\,s^{-1}\,kgcat^{-1}$) (i = 21 and 22)
K_{0i}	Frequency factor for Reactions (23)–(31) and (33)–(39) ($mol\,Pa^{-1}\,s^{-1}\,kgcat^{-1}$) (i = 23–31 and i = 33–39)
K_{ei}	Chemical equilibrium constant of the reaction i
k_{eff}	Thermal conductivity of the gas-phase ($W\,m^{-1}\,K^{-1}$)
K_{eq}	Chemical equilibrium constant for MCH dehydrogenation reaction (atm^3)
K_i	Rate constant for Reactions (1)–(20) and (32) ($mol\,Pa^{-2}\,s^{-1}\,kgcat^{-1}$) (i = 1–20 and i = 32)
K_i	Rate constant for Reactions (21) and (22) ($mol\,Pa^{-4}\,s^{-1}\,kgcat^{-1}$) (i = 21 and 22)
K_i	Rate constant for Reactions (23)–(31) and (33)–(39) ($mol\,Pa^{-1}\,s^{-1}\,kgcat^{-1}$) (i = 23–31 and i = 33–39)
k_w	Thermal conductivity of reactor wall ($W\,m^{-1}\,K^{-1}$)
L	Length of the reactor (m)
LOR	Length/radius ratio of the reactor
m	Numerator for nodes in r direction in exothermic side
mm	Numerator for nodes in r direction in endothermic side
mt	Numerator for total number of nodes in r direction
n	Numerator for nodes in z direction
N_m	Number of nodes in r direction in exothermic side
N_{mm}	Number of nodes in r direction in endothermic side
N_{mt}	Total number of nodes in r direction
N_n	Number of nodes in z direction
p	Exothermic side inner perimeter
P_j	Partial pressure of jth component (Pa)
P	Total pressure (Pa)
q	Number of reactions in exothermic side
Q	Volumetric flow rate ($m^3\,s^{-1}$)
r	Radius of the reactor (m)
R	Gas constant ($kJ\,kmol^{-1}\,K^{-1}$)
R	Exothermic side radius (m)
R	Recycle ratio
R^{endo}	Endothermic side radius (m)
r_i	Rate of reaction for ith reaction ($mol\,kgcat^{-1}\,s^{-1}$)
r^{endo}	Rate of reaction for MCH dehydrogenation ($mol\,kgcat^{-1}\,s^{-1}$)
s	Number of components in exothermic side
t	Time (s)
T	Temperature of gas phase (K)
$\overline{T}$	Average temperature (K)
T_0	Inlet temperature (K)
T_{ref}	Reference temperature
u	Overall heat transfer coefficient ($W\,m^{-2}\,K^{-1}$)
U_z	Axial velocity ($m\,s^{-1}$)
X_{A9}	A_9 conversion
Y	Yield

Greek letter

ε	Void fraction of catalyst bed
μ	Viscosity of gas phase ($kg\,m^{-1}\,s^{-1}$)
ν_{ij}	Stoichiometric coefficient of component j in reaction i
ρ	Gas density ($kg\,m^{-3}$)
ρ_B	Reactor bulk density ($kg\,m^{-3}$)
ΔC_p	Specific heat capacity change of the reactions ($kJ\,kmol^{-1}\,K^{-1}$)
δ	Thickness of the reactor wall (m)
ΔH_0	Heat of reaction in standard condition ($kJ\,kmol^{-1}$)
ΔH_i	Heat of ith reaction ($kJ\,kmol^{-1}$)
ΔG_0	Standard Gibbs free energy change of the reactions ($kJ\,kmol^{-1}$)
ΔG_i	Gibbs free energy change of the reactions ($kJ\,kmol^{-1}$)
Δr	Control volume radius (m)
Δz	Control volume length (m)
φ_s	Sphericity

Superscripts and subscripts

i	Numerator for reaction
j	Numerator for component
endo	Endothermic side