



Multi-zone parallel-series plug flow reactor model with catalyst deactivation effect for continuous catalytic reforming process



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HIGHLIGHTS

- The multi-zone parallel-series PFR modeling approach is proposed.
- An axial catalyst deactivation model is designed and integrated into PFR model.
- The prediction performance is validated by the commercial plant datasets.
- The effect of zone number on prediction and computational cost is studied.
- Both concentration and temperature distributions are thoroughly investigated.

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ABSTRACT

Accurate and reliable modeling of continuous catalytic regenerative (CCR) reforming process plays a significant role not only in product and temperature distributions prediction, but also in real-time optimization and control. In this study, a new multi-zone parallel-series plug flow reactor (PFR) model is proposed for the CCR reformer with four-stage stacked radial flow moving bed reactors (RFMBRs). A 27-lumped kinetic model is used to describe the aromatics aimed CCR reforming process. An empirical catalyst deactivation model is designed to describe the axial catalyst activity distribution information and integrated into the multi-zone parallel-series PFR model. The effectiveness of the proposed model is validated by the industrial plant datasets from a commercial reforming process. The zone number of 4 is reasonably determined by balancing the trade-off between the prediction accuracy and computational cost. Moreover, the detailed distributions of component mass fraction, temperature and catalyst activity are thoroughly investigated by means of the simulation results of the 4-zone parallel-series PFR model. The prediction results illustrate that the proposed model could provide accurate predictions of product and temperature distributions, which indicates that the proposed modeling approach could be greatly helpful for assisting in real-time optimization and control of CCR reforming process.

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1. Introduction

Catalytic naphtha reforming process, as one of the most important processes in refining industries, is widely used for producing high-octane gasoline and aromatics (Rahimpour et al., 2011a,b,c). The valuable byproduct hydrogen of catalytic naphtha reforming process also provides a rich source for hydrogen-consuming processes in most refineries (Rahimpour et al., 2011a,b,c). According to the mode of catalyst regeneration, the existing catalytic naphtha reforming processes can be generally divided into three distinct types: cyclic regenerative (CR), semi-regenerative (SR) and continuous catalyst regenerative (CCR) (D'Ippolito et al., 2008;

Rahimpour et al., 2013). Although the most commonly used processes are also the SR type, more than 95% of the new catalytic naphtha processes are designed with CCR type due to its advantages of higher catalyst activity and lower operational pressure (Mahdavian et al., 2010; Wei et al., 2016). In addition, originally designed SR type has been starting to be revamped to CCR type. In last decades, the mathematical model based optimization approaches has been developed not only to assist in optimal design of reactor configuration, but also to optimize the operation conditions for improving the reformate yields, the hydrogen yields and the octane number (Rahimpour et al., 2011a,b,c; Karimi et al., 2013). However, how to develop a simple, accurate and reliable model for performing real-time optimization of commercial CCR reforming process is still a challenging task, as it usually requires

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Nomenclature

a_{acid}	catalyst deactivation factor of acid site, dimensionless
a_{metal}	catalyst deactivation factor of metal site, dimensionless
A_j	activation energy of the j th reaction, s^{-1}
b_{acid}	catalyst deactivation factor of acid site, dimensionless
b_{metal}	catalyst deactivation factor of metal site, dimensionless
$c_{p,i}$	specific heat capacity of the i th component, $J\ mol^{-1}\ K^{-1}$
E_j	frequency factor of the j th reaction, $J\ mol^{-1}$
h	axial location of reactor, dimensionless
$h_{n-1,m}$	top location of the n th zone of the m th RFMBR, dimensionless
$h_{n,m}$	bottom location of the n th zone of the m th RFMBR, dimensionless
k_j	kinetic constant of the j th reaction, s^{-1}
K_{RP}	reaction equilibrium constant of $R \leftrightarrow P$, dimensionless
N	total number of zones in a RFMBR, dimensionless
P	operation pressure, MPa
P_0	standard atmospheric pressure, MPa
Q_{nm}	volume flow rate of the n th zone of the m th RFMBR, $m^3\ s^{-1}$
r_{ij}	reaction rate of i th lumped components for the j th reaction, $mol\ s^{-2}$
r_j	reaction rate of the j th reaction, $mol\ s^{-2}$
R	universal constant of gases, $J\ mol^{-1}\ K^{-1}$
T	reaction temperature, K
$T_{in}^{(m)}$	inlet temperature of the m th RFMBR, K
$T_{in}^{(nm)}$	inlet temperature of the n th zone of the m th RFMBR, K
$T_{out}^{(m)}$	outlet temperature of the m th RFMBR, K
$T_{out}^{(nm)}$	outlet temperature of the n th zone of the m th RFMBR, K
$T_{out,actual}^{(m)}$	actual outlet temperature of the m th RFMBR, K
$T_{out,cal}^{(m)}$	calculated outlet temperature of the m th RFMBR, K
w_i	weight of the i th lumped components, dimensionless
w_m	weight of the outlet temperature of the m th RFMBR, dimensionless
y_i	molar flow rate of the i th component, $mol\ s^{-1}$
$y_{i,in}^{(m)}$	inlet molar flow rate of the i th lumped component in the m th RFMBR, $mol\ s^{-1}$
$y_{i,in}^{(nm)}$	inlet molar flow rate of the i th lumped component in the n th zone of the m th RFMBR, $mol\ s^{-1}$
$y_{i,out}^{(m)}$	outlet molar flow rate of the i th lumped component in the m th RFMBR, $mol\ s^{-1}$
$y_{i,out}^{(nm)}$	outlet molar flow rate of i th lumped component in the n th zone of the m th RFMBR, $mol\ s^{-1}$
$y_{i,out,actual}^{(4)}$	actual molar flow rate of the i th lumped component in the outlet of the 4th RFMBR, $mol\ s^{-1}$
$y_{i,out,cal}^{(4)}$	calculated molar flow rate of the i th lumped component in the outlet of the 4th RFMBR, $mol\ s^{-1}$
y_P	molar flow rate of product, $mol\ s^{-1}$
y_R	molar flow rate of reactant, $mol\ s^{-1}$
z_m	radial length of the catalyst layer in the m th RFMBR, dimensionless

Greek letters

α_j	pressure factor of the j th reactions, dimensionless
φ_{acid}	catalyst activity in acid site, dimensionless
$\varphi_{acid}^{(nm)}$	catalyst activity in acid site of the n th zone of the m th RFMBR, dimensionless
φ_{metal}	catalyst activity in metal site, dimensionless
$\varphi_{metal}^{(nm)}$	catalyst activity in metal site of the n th zone of the m th RFMBR, dimensionless
φ_j	catalyst activity of the j th reaction, dimensionless
ΔrH_j	enthalpy of the j th reaction, $J\ mol^{-1}$

Subscript

<i>acid</i>	acid site
<i>actual</i>	actual industrial data
<i>cal</i>	calculation result
<i>i</i>	number of lump components, dimensionless
<i>in</i>	inlet of reactors
<i>j</i>	number of reactions, dimensionless
<i>m</i>	number of reactors, dimensionless
<i>metal</i>	metal site
<i>n</i>	number of zones, dimensionless
<i>out</i>	outlet of reactors
<i>P</i>	product
<i>R</i>	reactant

Abbreviations

5N	alkyl-cyclohexane
6N	alkyl-cyclopentane
A	aromatic
CCR	continuous catalytic regenerative
CFD	computational fluid dynamics
CR	cyclic regenerative
EB	ethylbenzene
HA	heavy aromatic
HP	heavy paraffin
LA	light aromatic
LP	light paraffin
MADS	mesh adaptive direct search
MEB	methylethylbenzene
N	naphthene
ODE	ordinary differential equation
P	paraffin
PB	propylbenzene
PFR	plug flow reactor
R1	the first-stage reactor
R2	the second-stage reactor
R3	the third-stage reactor
R4	the fourth-stage reactor
RFMBR	radial flow moving bed reactor
SR	semi-regenerative
TMB	trimethylbenzene
WNSSE	weighted normalized sum square error
XY	xylene

to balance the trade-off between model accuracy and computational cost especially from an industrial perspective.

Note that accurate and reliable modeling of a CCR reforming process usually calls for a thorough understanding of complex reaction network, catalyst deactivation behavior as well as practical reactor configuration. As the main feedstock of CCR reforming process, naphtha consisting of more than 300 components is a very complex mixture of hydrocarbons, and different reactions occur between these components, including dehydrogenation, dehydro-

cyclization, isomerization, hydrodealkylations, hydrocracking and coking (Boyás and Froment, 2008; Stijepovic et al., 2009; Rodríguez and Ancheyta, 2011). Hence, it is often practically impossible and unnecessary to establish a kinetic model with the inclusion of all components and their corresponding reactions (Marin and Froment, 1982). To tackle such complex reaction network problems, lumped kinetic modeling approach has been introduced, in which components with similar chemical properties and kinetic behaviors are lumped into a pseudocomponent (Zhou et al.,

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