Mathematical modeling, simulation, and analysis for predicting improvement opportunities in the continuous catalytic regeneration reforming process

Badiea S. Babaqi [a,b,d], Mohd S. Takriff [a,b,*], Siti K. Kamarudin [a,c], Nur Tantiyani A. Othman [a]

[a] Department of Chemical and Process Engineering, Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia
[b] Research Centre for Sustainable Process Technology, Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia
[c] Fuel Cell Institute, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia
[d] Department of Chemical Engineering, Faculty of Engineering and Petroleum, Hadhramout University, Mukalla, Hadhramout, Yemen

ARTICLE INFO

ABSTRACT

A mathematical model and simulation of the continuous catalytic regeneration reforming process (CCRRP) were developed to identify the key opportunities for predicting the output parameters and improving the process performance. This proposed model was used to monitor the profiles of reformate yield, temperatures and pressures of reactors, octane number, hydrogen yield, and light gases. It includes a description of reforming reactions by using the lumping technique to reduce the complexity of the reactions that occur during the CCRRP. The new network model of various reactions containing 36 lumps and 55 reactions was investigated. The primary reactions included dehydrogenation, dehydrocyclization, isomerization, hydrocracking, and hydrodealkylation of the reforming process. The simulation results of the model have been validated by comparison with plant data. Average absolute deviation (AAD%) of reformate yield, temperatures and pressures of reactors, octane number, hydrogen yield, and light gases reached 2.5%, 1.03%, 2.6%, 1.3%, 0.43%, and 0.93% respectively. The evaluation of the output parameters was within the acceptable limit and a fair agreement.

1. Introduction

Modeling and development of processes for improving design efficiency represent the main challenges in realizing strategic economic benefits. Simulation and analysis of industrial processes are often carried out to study the behavior of the products, and the operating conditions and energy consumption. The process simulation is described by mathematical equations of the process parameters such as feed composition, pressure, temperature, and geometrical configurations, which form an integrated approach to the system. In any oil refinery sector, simulation is used to monitor the process

Nomenclature

P_{nP_x}	partial pressure of component nP_x, kPa
P_{iP_x}	partial pressure of component iP_x, kPa
P_{N_x}	partial pressure of component N_x (AKCH or AKCP), kPa
P_{A_x}	partial pressure of component A_x, kPa
P_{H_2}	partial pressure of component H_2, kPa
P_t	total pressure of components, kPa
$P_{A_{x+n}}$	partial pressure of component, $n = 1$, kPa
$\overline{P_x}$, $\overline{iP_x}$	light gases respect to breaking probability
r_j	rate of reaction
K_j	constant of rate, kmol/kg cat h kPa
K_c	equilibrium constant
K_j	rate constant of reaction
k_o	frequency factor or pre-exponential factor
E	activation energy, kJ/kmol
R	gas constant (8.314 kJ/kmol K)
T	temperature, K
T_o	temperature standard usually 298 K
ΔH^R	heat of reaction, kJ/kmol
ΔH°_f	enthalpy of formation for the reactants or the products at T
ΔH°_f	enthalpy of formation of component at T
ΔH°_{f0}	standard enthalpy of formation at standard temperature (298 K)
T_0	temperature at standard (298 K)
T	temperature at the reaction, K
F_{xm}	mole flow rate of component (x) in reactor (m) by kmol/h
r_{jm}	rate of reaction (j) of component (x) in reactor (m) by kmol/kg h
w_m	weight of the catalyst in reactor (m) by kg
T_{xm}	temperature of component (x) in reactor (m) by K
Cp_{xm}	specific heat capacity of component (x) by mol kJ/kmol K
P_m	pressure of fluid by (kPa) in reactor (m)
w_m	weight of the packed bed of catalyst by m in reactor (m)
G_{u_m}	mass flux through the system by kg/m^2 s in reactor (m)
D_{p_m}	particle diameter in the bed by m in reactor (m)
A_s	area external curved surface of catalyst (m^2)

Greek letters

$\varnothing_m$	void fraction, dimensionless in reactor (m)
μ_m	viscosity of fluid by kg/m s in reactor (m)
ρ_{f_m}	density of fluid by kg/m^3 in reactor (m)
ρ_c	density of catalyst by kg/m^3
ΔH^R_{jm}	heat of reaction by kJ/kmol

Subscript

x	number of components 6, 7, 8, 9, 10
j	number of reactions 1, 2, 3, …, n
$\frac{1}{m}$	fraction respect to sum of breaking probability
s_p	stoichiometric coefficient of the product from the balanced reaction
s_r	stoichiometric coefficient of the reactants from the balanced reaction

Abbreviations

nP_x	component of paraffinic hydrocarbons (P)
iP_x	component of paraffinic hydrocarbons branshed (IP)
N_x	component of naphthenes, alkylcyclohexane (AKCH) or alkylcyclopentane (AKCP)
A_x	component of aromatic, alkyl benzene (A)
RON	research octane number

performance and as a tool for guiding and controlling the operations to achieve optimum production.

Catalytic reforming is one of the most important processes in oil refineries that produce high-octane-number gasoline. Catalytic reforming processes are commonly classified into three types based on the regeneration systems of the catalyst: (i) semi-regenerative catalytic reforming process (SRCRP), (ii) cyclic regenerative catalytic reforming process (CRCRP), and (iii) continuous catalytic regeneration reforming process (CCRRP). These processes vary according to the need to shut down the reactor for catalyst regeneration. The mechanism for the regeneration steps could be classified into fixed-bed catalyst system; fixed-bed catalyst combined a swing reactor and a move-bed catalyst with special regenerator of SRCRP, CRCRP or CCRRP type respectively (Babaqi et al., 2016).

Several reactions occur in the catalytic reforming process that increase the gasoline octane number: (i) dehydrogenation of naphthenes, (ii) dehydrocyclization of paraffins, (iii) isomerization of normal paraffins, (iv) hydrocracking of paraffins and conversion into lower-molecular-weight paraffins, and (v) hydrodealkylation of aromatics. Dehydrogenation, dehydrocyclization, and isomerization are the desired reactions because they control the octane number and hydrogen purity. In contrast, hydrocracking is undesirable because it cracks paraffins into smaller paraffins that produce light gases (lower octane, LPG). Additionally, hydrocracking consumes hydrogen that decreases the reformate yield (George and Abdullah, 2004; Sadighi and Mohaddecy, 2013; Zahedi et al., 2008).

The catalytic reforming process plays a significant role in the transformation of low-octane naphtha into higher-octane-number reformate for gasoline blending and aromatic-rich reformate for petrochemical production. It also produces high-purity hydrogen gas as a by-product. Because of the significance of the desirable gasoline for increasing the quantity and quality, process improvement is necessary. Most previous research focused on the catalytic reforming process with different types of units via the simulation and modeling of reactors for improving the process design. For example, in 1997, Vathi and Chaudhuri carried out the modeling and simulating of a commercial catalytic reforming process. This study focused on the concentration and temperature profiles of each reactor to evaluate the process performance (Vathi and Chaudhuri, 1997). In 2005, Yongyou et al. simulated a commercial catalytic reforming process and focused on dynamic simulation. The dynamic simulation provides information on the control system analysis and process design with dynamic process optimization. They used a numerical technique for dealing with partial differential equations, and linked the reaction model with catalyst deactivation, the furnace model, and the separator model (Yongyou et al., 2005). Weifeng et al. (2006) simulated and optimized a whole industrial catalytic reforming process and focused on the process profit. They