ARTICLE IN PRESS

Applied Mathematical Modelling xxx (2014) xxx–xxx

Contents lists available at ScienceDirect

Applied Mathematical Modelling

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

Dynamic modeling and simulation of a naphtha catalytic reforming reactor

Ignacio Elizalde [a,b,*], Jorge Ancheyta [b]

[a] Centro Mexicano para la Producción más Limpia, Instituto Politécnico Nacional, Ticomán, México, D.F. 07340, Mexico
[b] Escuela Superior de Ingeniería Química e Industrias Extractivas, Instituto Politécnico Nacional, Zacatenco, México D.F. 07738, Mexico

ARTICLE INFO

Article history:
Received 26 March 2013
Received in revised form 27 May 2014
Accepted 11 July 2014
Available online xxxx

Keywords:
Dynamic modeling
Start-up
Perturbation
Reforming reactions

ABSTRACT

Modeling of reforming reactor was conducted by expressing the heat and mass balances under non-steady state conditions. Kinetic and thermodynamic parameters were taken from the literature. Simulation in steady-state and transient state was carried out by using Matlab software. It was determined that some compounds exhibit net increase in concentration such as low molecular weight paraffins, while other compounds undergo net disappearance. Depending on the compound the time to attain the pseudo-steady-state is different. Perturbation of feed temperature was also modeled. The time to achieve the quasi steady-state was obtained and when compared it with the start-up condition time they were almost similar under the conditions used in this study.

1. Introduction

Naphtha is a complex mixture of different families of hydrocarbons such as paraffins (alkanes), naphthenes (cycloalkanes) and aromatics containing 5–12 carbon atoms whose normal boiling point ranges between 30 and 200 °C. Catalytic reforming is a process that allows for upgrading low octane to high octane naphtha by means of a series of gas phase transformations of linear to branched and to cycloalkanes, and reaction of naphthenes to yield aromatics. The octane number is defined as the volume percent of iso-octane in blending with n-heptane that equals the performance of the naphtha being tested. As the concentration of aromatics and branched paraffins (reformate) increases as result of the reforming reactions so does the octane number and hence better performance of internal combustion engines is obtained.

A number of reactions occur during the catalytic reforming namely hydrocracking of paraffins, cyclization of straight alkanes, dehydrogenation/hydrogenation of naphthenes and aromatics, hydrodealkylation of substituted aromatics among the most important reactions [1]. As result of dehydrogenation reactions, hydrogen byproduct is obtained which is needed for hydrotreating and hydrocracking operations [2].

Modeling of naphtha catalytic reforming has been studied by employing different approaches. For instance Ancheyta et al. [2,3] have considered a number of reactions and complex network to properly simulate the reforming process, whereas Sotelo and Froment [4] have used a fundamental kinetic approach based on the single event concept that consists of modeling the huge number of reactions occurring in naphtha catalytic reforming in a reduced number of elementary steps while retaining details of each reaction such as pathway and intermediaries. While the fundamental approaches are not fully applied other approaches such as lumping kinetic procedure, that consist of grouping hydrocarbons of the same family with

* Corresponding author at: Centro Mexicano para la Producción más Limpia, Instituto Politécnico Nacional, Ticomán, México, D.F. 07340, Mexico. Tel.: +52 (55) 5729 6000x52602; fax: +52 (55) 5729 6000x52600.
E-mail address: ielizaldem@gmail.com (I. Elizalde).

http://dx.doi.org/10.1016/j.apm.2014.07.013
0307-904X/

Please cite this article in press as: I. Elizalde, J. Ancheyta, Dynamic modeling and simulation of a naphtha catalytic reforming reactor, Appl. Math. Modell. (2014), http://dx.doi.org/10.1016/j.apm.2014.07.013

Nomenclature

A_i	aromatic compound
A_r	cross-section reactor
C_A	molar concentration
C_{PG}	gas heat capacity at constant pressure
C_{PS}	solid heat capacity
E_a	activation energy
k	reaction rate constant
L	reactor length
MW_G	molecular weight of gas
N_i	naphthenic compound
P	pressure
P_i	paraffinic compound
P_0	reference pressure
R	universal gas constant
$\overline{r_A}$	mean reaction rate in the catalyst element weight
r_i	reaction rate
T	absolute temperature
T_∞	temperature length function at steady-state condition
t	time
u_G	linear gas velocity
w	catalyst weight
Y_i	molar concentration of i compound/total molar concentration
$Y_{i\infty}$	molar concentration of i compound at steady-state/total molar concentration at steady-state
z	axial position within the reactor

Subscripts

g	gas phase
i	ith-component
r	reactor
s	solid phase
0	inlet reactor condition or initial condition

Greek symbols

Δ	finite element
ε_G	gas holdup
ε_S	solid fraction
$\in_B$	bed porosity
ρ_B	bulk density
ω	acentric factor

the same number of carbons as one pseudo-component, are more versatile from an industrial point of view because the parameters to formulate the kinetics and reactor model can be obtained directly from experimental conditions and the kinetic model could work with acceptable accuracy. When modeling with the lumping approach it is better to use a greater number of pseudo-components due to closer agreement between experimental and simulations can be obtained although the identification of the huge number of feed components imposes severe restrictions for using such an approach.

Different catalytic processes are available for catalytic reforming such as: semi-regenerative, cyclic regeneration and continuous regeneration [2]. In semi-regenerative process the system consists of three or four in series reactors packed with catalyst particles [3]. Industrial reformers operate adiabatically, and because of the nature of reactions involved, the heat of endothermic reactions predominates over the heat of exothermic ones.

While kinetics of catalytic reforming reactions has been subject of continuous research, reactor modeling has received lesser attention. Important stages of reforming process such as start-up, shut-down, effect of transients due to changes in feed composition, and temperature increase due to catalyst deactivation are needed to be understood in order to improve the process and reactor design. According to Mederos et al. [5] capturing these features including the steady-state condition can be done by using a dynamic reactor model that also provides a more robust numerical solution.

In the present contribution the dynamic responses of start-of-run and perturbation by changing feed temperature of an adiabatic catalytic reactor where naphtha reforming is carried out was investigated by means of modeling. Kinetic

Please cite this article in press as: I. Elizalde, J. Ancheyta, Dynamic modeling and simulation of a naphtha catalytic reforming reactor, Appl. Math. Modell. (2014), http://dx.doi.org/10.1016/j.apm.2014.07.013