Advanced Powder Technology 29 (2018) 2568–2581

Contents lists available at ScienceDirect

Advanced Powder Technology

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

Original Research Paper

Numerical investigation of influence of treatment of the coke component on hydrodynamic and catalytic cracking reactions in an industrial riser

D.C. Pelissari [a], H.C. Alvares-Castro [b], J.L.G. Vergel [a], M. Mori [a,*]

[a] University of Campinas, School of Chemical Engineering, 500 Albert Einstein, Campinas, SP, Brazil
[b] Technological Units of Santander (UTS)/AC Ingenieria Virtual, Bucaramanga, Colombia

ARTICLE INFO

Article history:
Received 9 December 2017
Received in revised form 25 April 2018
Accepted 19 July 2018
Available online 31 July 2018

Keywords:
Riser
Fluid catalytic cracking
Numerical simulation
CFD

ABSTRACT

A three dimensional gas-solid reactive flow model based on the Eulerian-Eulerian approach was used to simulate the hydrodynamic, heat transfer and catalytic cracking reaction within in a conventional Fluid Catalytic cracking (FCC) riser. A 12-lump kinetic model was used to represent the catalytic cracking reaction network. It was proposed a catalyst deactivation model as a function of the weight percentage of coke amount on the catalyst to replace the deactivation model dependent of the residence time. It was compared the effects of novel treatment for coke component (coke produced in the solid phase) with common treatment (coke produced in the gas phase) on the fluid dynamic and catalytic cracking. The results showed that the treatment for coke component affects radial distribution of coke mass flow. It also showed that the treatment for coke plays an important role in simulation with catalyst deactivation as a function of coke amount on catalyst.

1. Introduction

The worldwide increase in demand for petroleum products, combined with the increase in the supply of low-grade crude oil, has forced the refineries to use chemical process to refine the atmospheric residue and vacuum gas oil of distillation [1,2]. In this context, the fluid catalytic cracking (FCC) process has been highlighted, and it is estimated that 45% of the world's gasoline comes from this process [3–5]. According to Fahim et al. [6], in the FCC unit, the heavy oil fractions of low commercial value are converted into products with higher added value, mainly gasoline and diesel, through the contact between the feedstock and catalyst in a fluidized bed regime. In addition, it stands out for its flexibility, adjusting the profile of the products to the market demand, through the control of the operational variables.

Among the several equipment in the FCC unit, it is in the reactor, called a riser, that the initial contact between the gasoil and the catalyst occurs, and consequently the catalytic reactions. The riser is described as a cylinder with a high height/diameter ratio, which aims to promote the contact between the feedstock and the catalyst for a specific time. The phenomena that occur within the riser are extremely complex, due to the heterogeneous reactions, mass, momentum and energy transfer between the phases, catalyst deactivation by coke deposition and volumetric expansion. Furthermore, the riser operates at high temperature and pressure, which makes the experimental study in an industrial riser unachievable [7].

In this context, to overcome the lack of knowledge about this important process, researchers have used computational fluid dynamics (CFD) as a tool to predict and analyze the phenomena that occur in this kind of flow. As a result, a wide range of studies using CFD and different kinetics model have been conducted to improve FCC riser performance from analysis of different geometries and operating conditions. Theologos et al. [8] studied the influence of the number of nozzles on the fluid dynamics and the gasoline yield. They used an Eulerian-Eulerian approach applied in a 3D gas-solid flow and a 10-lump kinetic model. The simulations results showed that increasing the number of nozzles from four to twelve increased the gasoline yield by 4%, since it provide a more uniform catalyst distribution. Lopes et al. [9] simulated the FCC riser using a 3-D three-phase model and 4-lump kinetic model. In their work, it was studied the influence of the geometry of the riser outlet on the flow and products yield. It was observed that small changes in the riser outlet configuration have a significant effect on the process. An increase in gasoline yield was observed with increasing reactive mixture residence time. However, in their kinetic model the gasoline does not crack, in this

* Corresponding author.
E-mail address: mori@feq.unicamp.br (M. Mori).

https://doi.org/10.1016/j.apt.2018.07.012
0921-8831/

Nomenclature

C_i	molar concentration of component I [kmol m^{-3}]
C_D	drag coefficient [–]
C_μ	constant 0.09
$C_{\in,1}$	constant 1.44
$C_{\in,2}$	constant 1.92
d	particle diameter [m]
g	gravitational acceleration [m^2 s^{-1}]
G	elasticity modulus [Pa]
G_0	constant of elasticity modulus function [Pa]
H	static enthalpy [J mol^{-1}]
k	turbulent kinetic energy [m^2 s^{-2}]
m_{coke}	reaction rate of coke in the solid phase [kg m^{-3} s^{-1}]
Nu	Nusselt number [–]
p	static pressure [Pa]
p^k	shear production of turbulence [Pa s^{-1}]
Pr	Prandtl number [–]
R_i	reaction rate of component i [kg m^{-3} s^{-1}]
Re	Reynolds number [–]
t	time [s]
T	static temperature [K]
$\boldsymbol{u}$	velocity vector [m s^{-1}]
Y_{coke}	mass fraction of coke [–]
Y_i	mass fraction of component i [–]

Greek symbols

β	interphase momentum transfer [kg m^{-3} s^{-1}]
ε	volume fraction [–]
$\in$	turbulence dissipation rate [m^2 s^{-3}]
γ	interphase heat transfer coefficient [W m^{-2} K^{-1}]
λ	thermal conductivity [W m^{-1} K^{-1}]
μ	viscosity [Pa s]
ρ	density [kg m^{-3}]
σ_k	constant 1.00
$\sigma_\in$	constant 3.00

Subscripts

g	gas phase
lam	laminar
r	reaction
s	solid phase
turb	turbulent

way, longer residence times increase the gasoline yield. Behjat et al. [10] conducted a 3D reactive three-phase-flow numerical experiment, including feedstock coalescence and vaporization, to evaluate the influence of the number of nozzles on the riser fluid dynamics and heat transfer. The results showed that the increase in the number of nozzles improved the catalyst distribution, a result that corroborates those of Theologos et al. [8]. Chang et al. [3] simulated an industrial riser using a 12-lumps kinetic model and considering the vaporization phenomenon. The results of the simulation showed that the decrease in the nozzle angle increases the feedstock conversion and coke yield, while the decreasing the yield of diesel and gasoline. Li et al. [11] analyzed the effects of nozzle jet velocity, nozzle position and nozzle angle. The nozzle jet velocity played a significant role on the gas-solid flow. Regarding the nozzle position, it was not observed significant effects on the fluid dynamic profile or on the riser efficiency. It was observed that nozzle angle had significant effect on the radial temperature distribution and gasoline yield. The catalyst-to-oil ratio was studied by Nayak et al. [12], Chang et al. [3] and Alvarez-Castro et al. [4]. It was observed an increase in the conversion with the increase of catalyst-to-oil rate. Regarding the gasoline, the three works diverged. Nayak et al. [17] reported an increase in gasoline yield with the increase of catalyst-to-oil rate, whereas Chang et al. [3] and Alvarez-Castro et al. [4] reported no significant effect and decrease in gasoline yield, respectively. Alvarez-Castro et al. [4] also evaluated the influence of catalyst inlet temperature. The authors observed that increasing the temperature decreases the gasoline and diesel yield, while increases the conversion and the yield of coke, LPG and dry gases.

As previously seen, several studies are conducted to obtain better yield and understand better the phenomena that occur in the FCC process due to its importance. However, such research is only possible with the development of both fluid dynamic and kinetics models, capable of predicting the phenomena that occur within the riser. The modeling of the reactions that occur in the riser is not a trivial task, due to the high number of components present and, consequently, to the high number of reactions that occur in this process. In this context, several approaches have been developed to represent the kinetics of catalytic cracking reactions. Among the different approaches found in the literature, the most used one was developed by Weekman and Nace [13] and called "lumps," in which petroleum components that have similar properties and behaviors (molecular weight, boiling point, number of carbons) are grouped into pseudo-components (lumps). In the Weekman and Nace [13] model all reactions are represented by the kinetics of three chemical species (gasoil, gasoline and other products).

As the composition of gasoil can vary depending on the petroleum, models such as those by Weekman and Nace [13], in which the feedstock is represented by a single lump, make it necessary to estimate the kinetic constants for each type of feedstock. Considering this, Jacob et al. [14] proposed a 10-lump model in which gasoil is divided according to its chemical characteristics into 4 lumps (aromatic, aromatics with substituents, naphthenic, and paraffinic), in which the dependence of the kinetic parameters, according to the feedstock composition, is considered.

Due to the different demands of petroleum products and the different types of petroleum, different catalytic cracking processes were proposed. Yang et al. [7] reported some of them in their work, such as the maximizing iso-paraffin in cracked naphtha (MIP) process and flexible dual-riser fluid catalytic cracking (FDFCC). Thus, from the models by Weekman and Nace [13] and Jacob et al. [14] other models have been proposed to fulfill the deficiencies of previous models or to meet the needs of their project. As a result, kinetic models of different lumps have been proposed (3-lumps [13], 5-lumps [14], 6-lumps [15], 10-lumps [16,17], 14-lumps [18]). In addition to the different numbers of lumps, the kinetics models also differ, considering different mechanisms, such as gasoline cracking, catalyst deactivation type, deactivation by basic nitrogen poisoning and absorption of aromatic, and asphaltenic resins.

Deactivation of the catalyst is another important factor that must be considered in the kinetic modeling of reactions. The deposition of coke on the catalyst surface lowers the activity thereof. The literature shows two main models to represent the catalyst deactivation: as a function of residence time and as a function of coke concentration. Cerqueira et al. [19] used the 12-lump model to evaluate different functions to describe the catalyst deactivation, and they observed that an exponential function with only one variable parameter generates satisfactory results. Depending