DOI: 10.1590/0104-6632.20160333s20150124

Brazilian Journal
of Chemical
Engineering

ISSN 0104-6632
Printed in Brazil
www.abeq.org.br/bjche

Vol. 33, No. 03, pp. 559 - 566, July - September, 2016
dx.doi.org/10.1590/0104-6632.20160333s20150124

STUDY OF FEEDSTOCK INJECTION TO IMPROVE CATALYST HOMOGENIZATION IN THE RISER OF A FCC

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(Submitted: February 26, 2015 ; Revised: July 12, 2015 ; Accepted: July 27, 2015)

Abstract- A three dimensional gas-solid reactive flow model based on the Eulerian-Eulerian approach was used to study the effects of different nozzle designs with internal parts inside the FCC riser. The simulations were solved using Computational Fluid Dynamics (CFD) with CFX version 14.0 as tool. The results showed that the nozzle designs have a significant influence on the gas-solid behavior, resulting in an important role in the hydrodynamics and thermal behavior of the riser. Furthermore, the simulations show it is possible to improve the catalyst-gas distribution with an appropriate nozzle design.
Keywords: Nozzles; Riser; Fluid Dynamic; FCC.

INTRODUCTION

Fluidized bed reactors (FBR) have been the basis for gas-solid reactions in various types of industries because of their better mass and heat transfer when compared to other systems with the same purpose. Many applications of FBR highlight their use in the refining industry like the fluidized catalytic cracking process (FCC), which consists of the production of petroleum light fractions with high economic value (gasoline, diesel) from the heavy fractions of less commercial interest.

According to Fahim *et al*. (2010), the FCC unit's basic structure consists of a riser (reactor), where gas oil, catalyst and steam are fed, and a regenerator where the coke deposited on the catalyst surface during the reactions is burned-off to regenerate the catalyst. The riser is a long vertical tube with high height/diameter ratio, in order to promote pneumatic transport and the optimal conditions for the desired reactions to take place.

At the bottom of the riser, the regenerated catalyst is introduced and fluidized steam is also injected at the bottom below the catalyst entrance. About 5 m above this region is located the injection zone, where the feedstock (gas oil) is fed and the initial contact between the feedstock and the hot catalyst occurs, resulting in high gradients of temperature and concentration. According to Fan *et al*. (2002), Gao *et al*. (1999) and Theologos *et al*. (1997), the initial contact is one of the most important aspects of the process, which affects the fluid dynamics and kinetics of the

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This is an extended version of the work presented at the 20th Brazilian Congress of Chemical Engineering, COBEQ-2014, Florianópolis, Brazil.

catalytic reaction. The feedstock is injected into the riser through nozzles, which aim to atomize the charge into small droplets and promote a perfect contact between the catalyst and the feedstock, thus minimizing regions of high catalyst concentration in order to avoid undesired reactions.

McCarthy *et al*. (1997), Chen (2006) and Wolschlag *et al*. (2010) show studies of the technological advances in the FCC process, which emphasize the important role that nozzles have on the riser performance. According to Chen (2006) and McCarthy *et al*. (1997), the injectors reduce thermal cracking, since they promote a rapid feedstock vaporization and efficient mixing between the catalyst and gas oil droplets. However, according to Theologos *et al*. (1997), Theologos and Markatos (1993), Mauleon and Coorcelle (1985) and Behjat *et al*. (2010) the flow in the riser is very complex and is characterized by high turbulence and non-uniformity in the phase distribution, particularly in the injection zone. Therefore, studies related to the injection zone, especially experimental research, are not common.

Due to this complex behavior in the riser, experimental research linked with the FCC riser are normally tested experimentally in a cold-riser model. In this respect, the works of Fan *et al*. (2002) and Fan *et al*. (2010) focused on the lift region and injection zone, and Gupta and Berruti (2000) and Harris *et al*. (2003) investigated the effects of riser outlet geometry. Despite using cold-riser models, these experiments generated important data about the boundary and initial conditions, which were essential for numerical models.

Numerical simulations using CFD have become an important tool in understanding the phenomena occurring in the riser. Theologos *et al*. (1997) simulated a FCC riser using a one-dimensional model with 10-lump kinetic model to describe the reactions of catalytic cracking, studying the influence of the number of nozzles on the reactor performance. The simulation results showed that the desired reaction yield was improved by increasing the number of nozzles, since it provided a better catalyst homogenization.

Lopes *et al*. (2011) showed in their work the importance of using three-dimensional models to predict the phenomena that occur in the riser. Then Lopes *et al*. (2012) and Barbosa *et al*. (2012) used three-dimensional models to study the influence of different riser outlet and inlet geometries, respectively. It was observed that small changes in the riser geometry influence the hydrodynamics and the product profile.

Li *et al*. (2013) used a 14-lump model to simulate the FCC riser, with variation in the feedstock injection velocity, the injection angle and the injector positions. The results showed that the injection velocity and angle played an important role in the process, while the nozzle positions do not have significant influence.

Due to the high profitability of the FCC process, many studies have been granted patents covering different settings for the riser in order to improve contact between the catalyst and gas oil. Among those works, many of them are related to zone injection, with either new nozzle design, injection angle, flow direction or arrangement (Chen *et al*., 1998; Haruch, 2000; Chen, 2011; Delesdernier *et al*., 2011; Wilson *et al*., 2013). However, patents are not detailed scientific works, and they are usually derived from trial and error experiments, which do not generate data for further work.

In this study, four different nozzle designs were evaluated using a three-dimensional gas-solid reactive flow model, a catalytic cracking kinetic model of 12-lumps and detailed feedstock injectors with changes in the design in order to improve the homogenization of the injection zone.

MATHEMATICAL MODEL

The simulations were conducted in the Solver CFX 14 tool. A 3D model was used to describe the flow transport phenomena with an Eulerian-Eulerian approach, where both phases are considered to be continuous and interpenetrating. In this approach the conservation equations for mass, momentum and energy, (Equations (1) to (6)) in Table 1, were solved simultaneously. All the meanings and description of the variables, subscripts and superscripts in Table 1 are presented in the Nomenclature section.

The gas-particle interactions present in the momentum equation (see Equations (12), (13) and (14)) are represented by β , the interphase momentum transfer, and G, the elasticity modulus, and they were approximated by Gidaspow (1994). The heat transfer coefficient was calculated with the Nusselt number, which was approximated by Ranz-Marshall, (see Equation (16)). The *k-epsilon* model was used to estimate the turbulence (see Equations (7), (8), (9), (10) and (11)). The 12-lump catalytic cracking kinetic model taken from Wu *et al*. (2008) and Chang *et al*. (2012) was used, in order to consider the effects on the riser fluid dynamics.

Table 1: Governing Equations and Complementary Correlations.

Governing equations	
Continuity equations of gas and solid phases	
$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g\right)+\nabla\cdot\left(\varepsilon_g\rho_g\boldsymbol{u}_g\right)=0$	(1)
$\frac{\partial}{\partial t}\left(\varepsilon_s\rho_s\right)+\nabla\cdot\left(\varepsilon_s\rho_s\boldsymbol{u}_s\right)=0$	(2)
Momentum equations of gas and solid phases	
$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g\boldsymbol{u}_g\right)+\nabla\cdot\left(\varepsilon_g\rho_g\boldsymbol{u}_g\boldsymbol{u}_g\right)=\nabla\cdot\left[\varepsilon_g\mu_g\left(\nabla\boldsymbol{u}_g+\left(\nabla\boldsymbol{u}_g\right)^T\right)\right]-\varepsilon_g\nabla p+\varepsilon_g\rho_g\boldsymbol{g}+\beta\left(\boldsymbol{u}_s-\boldsymbol{u}_g\right)$	(3)
$\frac{\partial}{\partial t}\left(\varepsilon_s\rho_s\boldsymbol{u}_s\right)+\nabla\cdot\left(\varepsilon_s\rho_s\boldsymbol{u}_s\boldsymbol{u}_s\right)=\nabla\cdot\left[\varepsilon_s\mu_s\left(\nabla\boldsymbol{u}_s+\left(\nabla\boldsymbol{u}_s\right)^T\right)\right]-\varepsilon_s G\nabla\varepsilon_s+\varepsilon_s\rho_s\boldsymbol{g}+\beta\left(\boldsymbol{u}_g-\boldsymbol{u}_s\right)$	(4)
Energy equation of gas and solid phases	
$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g H_g\right)+\nabla\cdot\left(\varepsilon_g\rho_g\boldsymbol{u}_g H_g\right)=\nabla\cdot\left[\varepsilon_g\lambda_g\nabla T_g\right]+h_{gs}\left(T_s-T_g\right)+\varepsilon_g\rho_g\sum_r\Delta H_r\frac{\partial C_r}{\partial t}$	(5)
$\frac{\partial}{\partial t}\left(\varepsilon_s\rho_s H_s\right)+\nabla\cdot\left(\varepsilon_s\rho_s\boldsymbol{u}_s H_s\right)=\nabla\cdot\left[\varepsilon_s\lambda_s\nabla T_s\right]+h_{gs}A_{g/s}\left(T_g-T_s\right)$	(6)
Additional models and correlations	
Turbulence Equation ($k-epsilon$ model)	
$\mu_g=\mu_{lam,g}+\mu_{turb,g}$	(7)
$\mu_{turb,g}=\rho_g C_\mu\frac{k^2}{\epsilon}$	(8)
$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g k\right)+\nabla\cdot\left(\varepsilon_g\rho_g\boldsymbol{u}_g k\right)=\nabla.\left[\varepsilon_g\left(\mu_{lam,g}+\frac{\mu_{turb,g}}{\sigma_k}\right)\nabla k\right]+\varepsilon_g P^k-\varepsilon_g\rho_g\epsilon$	(9)
$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g\epsilon\right)+\nabla\cdot\left(\varepsilon_g\rho_g\boldsymbol{u}_g\epsilon\right)=\nabla.\left[\varepsilon_g\left(\mu_{lam,g}+\frac{\mu_{turb,g}}{\sigma_\epsilon}\right)\nabla\epsilon\right]+\frac{\varepsilon_g\epsilon}{k}\left(C_{\epsilon,1}P^k-C_{\epsilon,2}\epsilon\rho_g\right)$	(10)
$P^k=\mu_{turb,g}\nabla\boldsymbol{u}_g.\left(\nabla\boldsymbol{u}_g+\left(\nabla\boldsymbol{u}_g\right)^T\right)$	(11)
Drag Force (Gidaspow, 1994)	
$\beta=\begin{cases}150\frac{\varepsilon_s^2\mu_g}{\varepsilon_g d_s^2}+\frac{7}{4}\frac{\left\lvert\boldsymbol{u}_s-\boldsymbol{u}_g\right\rvert\varepsilon_s\rho_g}{d_s} & \varepsilon_s>0.2\\ \frac{3}{4}C_D\frac{\left\lvert\boldsymbol{u}_s-\boldsymbol{u}_g\right\rvert\varepsilon_s\varepsilon_g\rho_g\varepsilon_g^{-2.65}}{d_s} & \varepsilon_s<0.2\end{cases}$	(12)
$C_D=\begin{cases}0.44 & Re_s>1000\\ \frac{24}{Re_s}\left[1+0.15\left(Re_s\right)^{0.687}\right] & Re_s<1000\end{cases}$	(13)

Continuation Table 1

Continuation Table 1

Governing equations	
Solid Pressure (Gidaspow, 1994)	
$G = G_0 exp\left[c\left(\varepsilon_s - \varepsilon_{s,max}\right)\right]$	(14)
Heat transfer coefficient between phases	
$h_{gs} = \dfrac{\lambda_g Nu}{d_p}$	(15)
Ranz-Marshall Correlation	
$Nu = 2.0 + 0.6Re^{0.5}Pr^{0.33}$	(16)

SIMULATION

In this work a riser geometry adapted from Alvarez-Castro *et al*. (2014) was used. The general riser geometry, nozzle designs and dimensions are shown in Figure 1 and Table 2. In Figure 1A, it can be seen that the riser is composed of a fluidized steam entrance, catalyst entrance and feedstock inlet, each one independent. The feedstock inlet is composed of eight feedstock nozzles equally distributed around the riser with an angle of 45º. In order to study the effect of different nozzles on the gas and catalyst mixture, four cases were proposed, as shown in Figure 1B, C, D and E, where Figure 1B shows a design without internal parts in the riser.

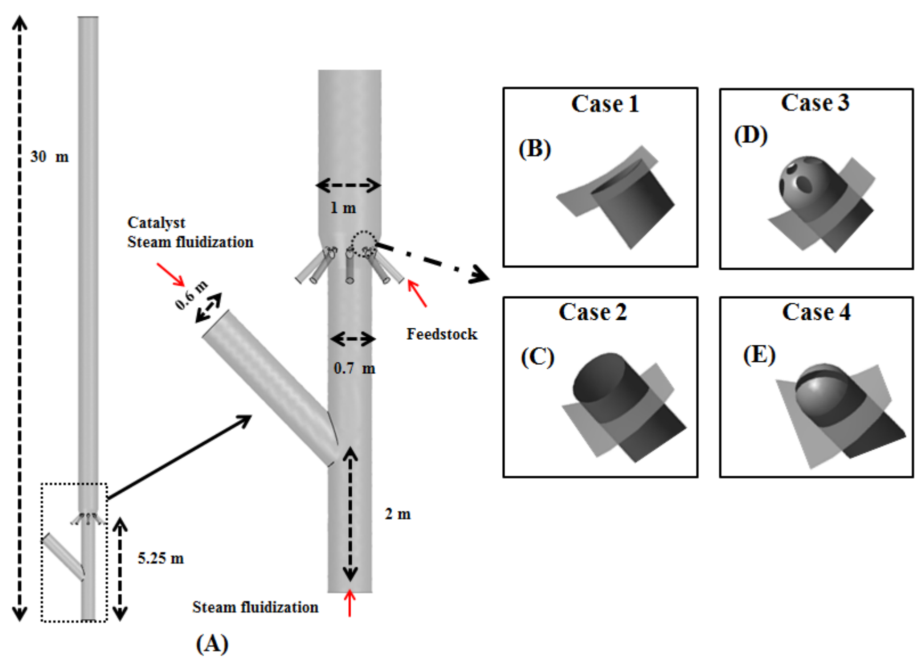

Figure 1: Riser geometry and nozzle designs: (A) General Riser geometry; (B) Case 1(without internal parts in the riser) (C) Case 2; (D) case 3 and (E) Case 4.

Table 2: Dimensions of the simulated riser.

Length (m)		30
Bottom diameter (m)		0.7
Upper diameter (m)		1.0
Number of nozzles		8.0
Nozzles diameter (m)		0.12
Nozzles angle		45°
Catalyst entrance diameter (m)		0.6
Catalyst entrance angle		45°
Nozzle outlet area (m^2)	Case 1	0,0128
	Case 2	0,01131
	Case 3	0,0044
	Case 4	0,0037

The computational meshes employed in the simulations were adapted from Alvarez-Castro *et al*. (2012) and ranged from about 675,000 to 1,300,000 elements according to the nozzle design complexity. The mesh is in agreement with previous Alvarez-Castro *et al*. (2012) mesh tests shown in Table 3. The operating conditions used were taken from Chang *et al*. (2012), shown in Table 4 and the component properties are the same used by Alvarez-Castro *et al*. (2015), which were taken from Lopes *et al*. (2011). The no slip condition on the wall was assumed for the gas phase and the free slip condition for the solid phase.

Table 3: Mesh Test (Alvarez-Castro, 2012).

Elements Number	334,000	534,000	765,000	980,000	1,457,000
Gasoline mass fraction	0.43	0.46	0.45	0.45	0.45
Pressure (Pa)	6,052	6,068	6,042	6,052	6,014

Table 4: Main operating conditions (Chang *et al*., 2012).

Reaction temperature (K)	793.15
Pressure drop (kPa)	163
Reaction time (s)	3.22
Flux of fresh feedstock (t/h)	124.46
Inlet temperature of fresh feedstock (K)	543.15
Catalyst temperature at the riser inlet (K)	913.15
Ratio of catalyst to oil	8.1

The commercial software ANSYS CFX 14 was used to solve the numerical discretization (space and time) of mass, momentum, energy and species conservation equations through the finite volume method. Transient expressions were estimated via the second order backward Euler. The high resolution interpolation scheme was used, with RMS of 10^{-4} as convergence criterion. The simulation time was fifteen seconds, enough time for variables to present a cyclic behavior according to Lopes *et al*. (2011) and Alvarez-Castro *et al*. (2015).

RESULTS AND DISCUSSION

Figure 2 shows a riser top view, highlighting the gas oil flow direction through the nozzles in streamline view. Figures 2A and B show a nozzle design similarity and the only difference is the fact that Case 2 has internal parts in the riser. It also can be seen that the two cases have similar flow behavior, but the gas oil flow in Case 2 reaches a more central region, implying that the use of injectors with internal parts strongly affects the flow in the riser. Those results are better seen in Figure 3, which shows the gas phase volume fraction in cross-sectional planes. In Case 2 a more concentrated central region is observed when compared to Case 1.

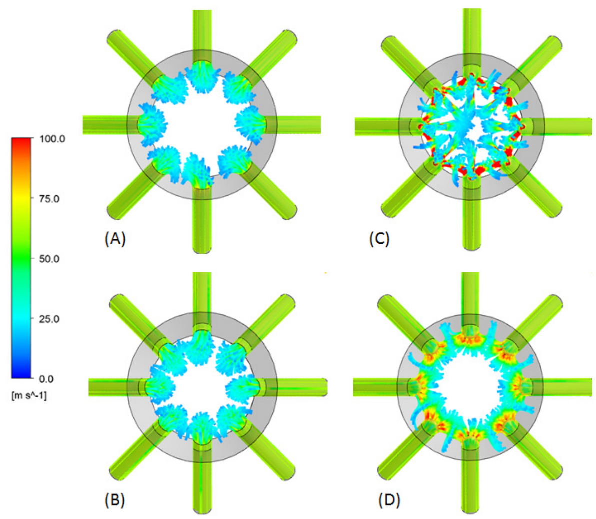

Figure 2: Stream line gas phase velocity: (A) Case 1; (B) Case 2; (C) Case 3 and (D) Case 4.

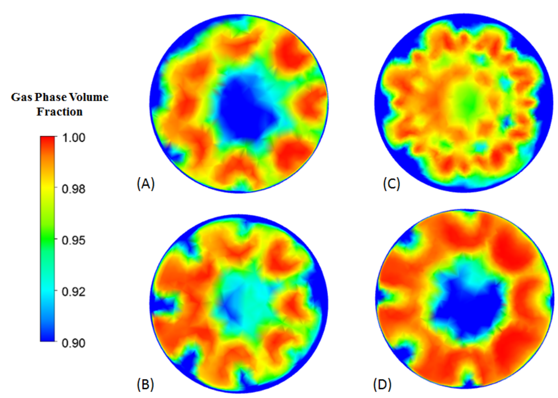

Figure 3: Gas phase volume fraction in cross-sectional planes 0.1 m after the feedstock injection: (A) Case 1; (B) Case 2; (C) Case 3 and (D) Case 4.

It can be observed in Figures 2B, C and D that the different nozzle designs play an important role in the injection zone flow profile. It can be noted that the nozzle designs in Figures 2C and D provide gas oil outflows with higher speed than the nozzle design in Figure 2B. In Case 3 a better gas phase distribution can be seen (Figure 3C). The gas flow covers the greater part of the riser. However, in Case 4 (Figure 3D), a similarity can be observed in the fluid dynamic profile with Cases 1 and 2, although Case 4 generates higher output speed when compared to them.

The different flow effects on the riser fluid dynamic are shown in Figure 4, which shows the solid fraction in the axial plane. It can be seen in Cases 1, 2 and 4 that the catalyst is shifted toward the riser center in the injection zone due to the injected gas oil, which is in agreement with previous work reported by Li *et al*. (2013) and Alvarez-Castro *et al*. (2015). In Case 3 a better homogeneous catalyst distribution is observed, without catalyst accumulation in the riser center as compared to other cases, resulting in better flow distribution shown in Figure 2C.

Figure 5 shows the temperature profile for the different nozzles in an axial plane. The temperature profile is similar to the profile of the catalyst volume fraction, in which high temperature can be noted in regions with high catalyst concentrations, that is in the central region and regions close to the wall. It can be noted that Case 3 has a better homogeneous temperature distribution, without regions with large temperature differences as in Case 1.

Figure 6 shows the catalyst volume fraction and temperature profiles, at a height of 6 m, as a function of radius for Cases 1, 2, 3 and 4. All these cases present an accumulation of catalyst and high temperature near the wall and in the central region. In addition, it can be noted that Case 3 also shows high temperature and catalyst concentrations near the wall, but it presents a more homogeneous temperature profile and catalyst distribution when compared to Cases 1, 2 and 4. Besides it favors a lower temperature gradient between the central region and the wall, showing better catalyst distribution inside the riser.

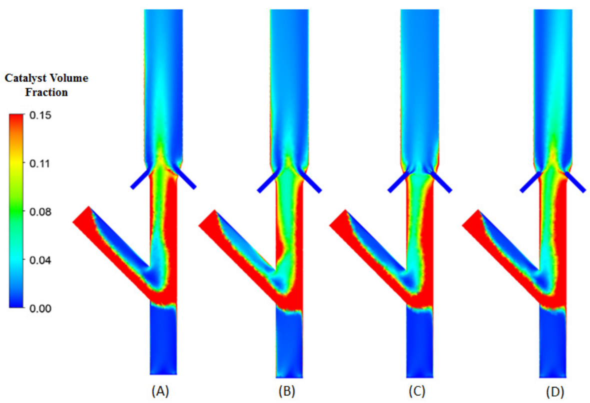

Figure 4: Catalyst volume fraction: (A) Case 1; (B) Case 2; (C) Case 3 and (D) Case 4.

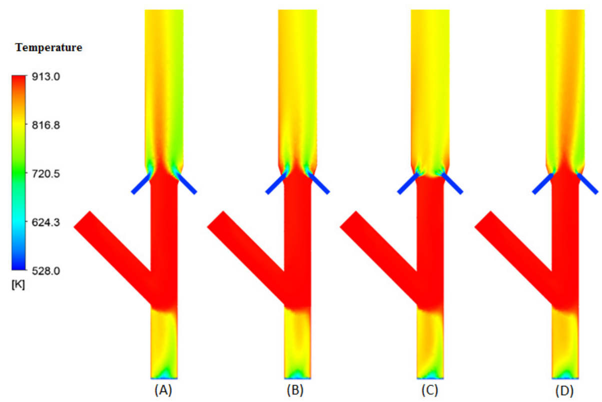

Figure 5: Temperature: (A) Case 1; (B) Case 2; (C) Case 3 and (D) Case 4.

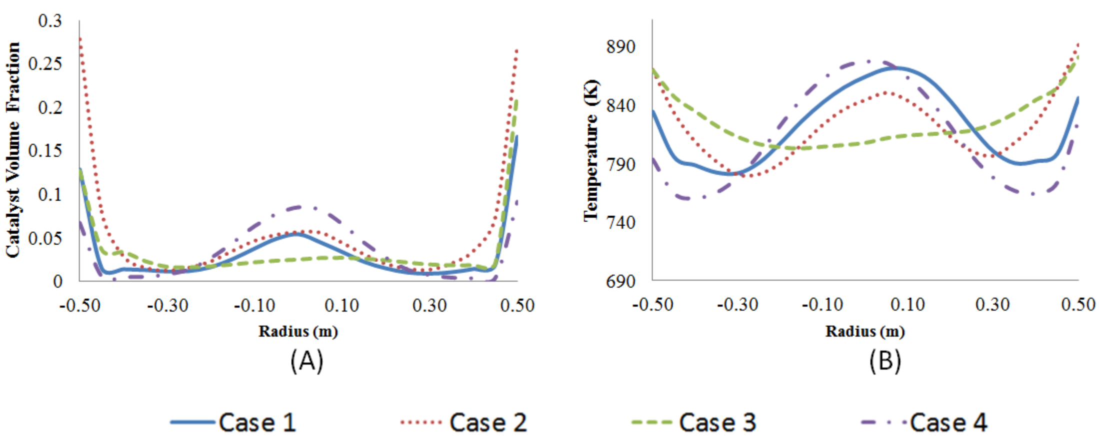

Figure 6: (A) Catalyst Volume Fraction; (B) Temperature radial distribution, at 6 m of height.

CONCLUSIONS

The FCC riser's injection zone fluid dynamic profile was determined using a three dimensional, multiphase and reactive model, through numerical simulations. The effects of using nozzles with internal parts in the riser and different designs were evaluated. The results for the flow direction, the catalyst distribution and the temperature showed that the nozzles with internal parts in the riser and nozzle designs have a significant influence on the gas-solid interaction, resulting in an important role on the riser fluid dynamics and thermal behavior. The simulation results indicated that a high gas oil output speed through the nozzles did not guarantee a better mixture between the phases. It is necessary to consider the jet directions. According to the results, it can be concluded that it is possible to improve the catalyst distribution inside the riser through changes in the nozzle design, thus emphasizing their importance in improving the catalytic cracking process.

ACKNOWLEDGEMENTS

The authors thank CAPES and Petrobras for the financial support of this research.

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}]
Nu	Nusselt number [-]
p	Static pressure [Pa]
p^k	Shear production of turbulence [Pa s^{-1}]
Pr	Prandtl number [-]
Re	Reynolds number [-]
T	Static temperature [K]
$\boldsymbol{u}$	Velocity vector [m s^{-1}]

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

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