

Three Dimensional Model of Computational Fluid Dynamic to Predict Products Yield and Residence Time in Riser of FCC

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The fluid catalytic cracking (FCC) process is at the heart of a modern refinery oriented toward maximum commercial (gasoline and diesel) production. In order to describe the large number of components present in heavy distillates and the kinetic models that are able to predict the profiles of heavy and light chemical fractions in industrial risers, the 12 lump approaches has been used. Gas acceleration inside the reactor due to molar expansion and catalyst deactivation were considered by simulating unsteady state cases over a time long enough to show that the variables had a cyclic behavior. The tracer particle was instantaneously injected following the tracer technique, to get an estimation of the residence time. The governing equations were solved numerically by finite volume method with a commercial CFD code, CFX version 14.0. Appropriate functions were implemented in the model by considering the heterogeneous kinetics, catalyst deactivation and function tracer. The simulation results were validated against the experimental results. This work was carried out in order to evaluate the predictions of product yields and to estimate the residence time distribution in industrial reactors.

1. Introduction

The fluid catalytic cracking (FCC) process involves the fluidization of solid particles (the catalyst) in gas; the process can be described by employing the conservation of mass and energy. The solution of the governing equations is an inherently difficult task due to the absence of comprehensive understanding of the nature of the contact between phases. The configuration of each FCC unit can be dissimilar but their common aim is to upgrade low-cost hydrocarbons into more valuable products (Barbosa et al., 2013). The FCC and ancillary units, such as the alkylation unit, are responsible for about 45 % of the gasoline produced worldwide. Gasoil conversion and product yields are evaluated through a three dimensional model simulating the FCC riser, where gasoil is fed through nozzles and enter in contact with the catalyst and the accelerant steam in the injection area. The performance of the injection area to guarantee rapid vaporization of the gasoil and a good contact of the gasoil droplets with the catalyst is crucial to improve the FCC riser productivity; the feedstock nozzles are positioned at about 5–12 m above the bottom of the reactor. Depending on the kind of FCC design, the number of feedstock injections can vary from 1 to 15. Almost all of the riser reactions take place between 1 and 3 s (Sadeghbeigi, 2012a). The Eulerian-Eulerian approach has been used in this work due it lower computational demand when compared to other approaches. In the Eulerian-Eulerian methodology the solid phase is treated as a continuum for all hydrodynamic purposes; the FCC reactions are then studied through the lumping approach which is shown to be very powerful when a large number of components is involved. The real reactive system is mimicked by using a finite number of lumps with each lump constituted by many components having comparable characteristics and in a definite array of molecular weight (Ancheyta-Juárez et al., 1997). In order to represent the catalytic cracking reaction behavior, a 12 lump model was employed. The 12 lump model presents the advantage of a better description of both products and feedstock, being one of the most complete models reported in literature by Wu et al., (2009). The 12 lump model is considered in combination with the fluid dynamic model of the industrial riser of the FCC unit; the complete

model (including hydrodynamics and catalytic reactions) is thus solved. In addition, a computational fluid dynamic (CFD) approach is undertaken to calculate the residence time of the solid and gas phases.

2. Mathematical Model

Table 1 summarizes the governing equations for the dynamic fluid adapted from Alvarez-Castro et al., (2015) and catalytic cracking kinetic models were taken and adapted from Chang et al., (2012). In order to study the kinetics, the catalyst phase deactivation and the residence time, Equations 8 to 18 were coupled in the CFX setup.

Table 1: Governing equations for transient two fluid models

Governing equation	Equation	N°
Continuity equations	$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g) = 0$	(1)
	$\frac{\partial}{\partial t}(\varepsilon_s \rho_s) + \nabla \cdot (\varepsilon_s \rho_s \mathbf{u}_s) = 0$	(2)
Momentum equations	$\frac{\partial}{\partial t}(\varepsilon_g \rho_g \mathbf{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g \mathbf{u}_g) = \nabla \cdot [\varepsilon_g \mu_g (\nabla \mathbf{u}_g + (\nabla \mathbf{u}_g)^T)] + \varepsilon_g \rho_g \mathbf{g} - \varepsilon_g \nabla p + M$	(3)
	$\frac{\partial}{\partial t}(\varepsilon_s \rho_s \mathbf{u}_s) + \nabla \cdot (\varepsilon_s \rho_s \mathbf{u}_s \mathbf{u}_s) = \nabla \cdot [\varepsilon_s \mu_s (\nabla \mathbf{u}_s + (\nabla \mathbf{u}_s)^T)] + \varepsilon_s \rho_s \mathbf{g} - \varepsilon_s \nabla p - M$	(4)
Turbulence: The k-epsilon mixture model		
Heat transfer model	$\frac{\partial}{\partial t}(\varepsilon_g \rho_g H_g) + \nabla \cdot (\varepsilon_g \rho_g u_g H_g) = \nabla \cdot (\varepsilon_g \lambda_g \nabla T_g) + \gamma(T_s - T_g) + \varepsilon_g \rho_g \sum_n \nabla H_r \frac{\delta C_r}{\delta t}$	(5)
	$\frac{\partial}{\partial t}(\varepsilon_s \rho_s H_s) + \nabla \cdot (\varepsilon_s \rho_s u_s H_s) = \nabla \cdot (\varepsilon_s \lambda_s \nabla T_s) + \gamma(T_g - T_s)$	(6)
Variation of the chemical species	$\frac{\partial}{\partial t}(\varepsilon_g \rho_g C_{g,i}) + \nabla \cdot (\varepsilon_g \rho_g u_g C_{g,i}) = \nabla \cdot (\varepsilon_g \Gamma_i \nabla C_{g,i}) + \hat{R}_i$	(7)
The rate equation for the generic reaction	$\hat{R}_{i,r} = -k_r \cdot \rho_p \cdot (\rho \alpha_i) \cdot \phi(t) \cdot F(N) \cdot F(A)$	(8)
Decay model based on coke content	$\Phi(t) = e^{-\alpha t}$	(9)
Alkaline nitrides	$F(N) = \frac{1}{1 + k_N C_N t_C / F_{c/o}}$	(10)
Polycyclic aromatic adsorption	$F(A) = \frac{1}{1 + k_A (C_A + C_R)}$	(11)
Arrhenius' equation	$k_r = k_r^0 \exp\left(\frac{E_r}{RT}\right)$	(12)
Arrhenius equation (any temperature and dependent on the hold up of solids)	$k_c(T, \varepsilon_s) = k_{r,550^\circ C}(\rho, \varepsilon_s) \exp\left[-\frac{E_r}{R} \left(\frac{1}{T} - \frac{1}{550^\circ C}\right)\right]$	(13)
Residence time distribution via scalar (CFD)	$\frac{\partial \phi}{\partial t} + \nabla \cdot (v\phi) = \nabla \cdot \left(\rho D_\phi + \frac{\mu_s}{S_{cl}}\right) \nabla \left(\frac{\phi}{\rho}\right) + S_\phi$	(14)
	$Q(t) = \int_A V_{out} C_{out} dA$	(145)
	$E(t) = \frac{Q(t)}{\int_0^\infty Q(t) dt}$	(15)
	$A(t) = \int_0^t E(t) dt$	(16)
	$t_m = \int_0^\infty t E(t) dt$	(17)

3. The residence time distribution via CFD

Computational fluid dynamic techniques, with the use of the tracer or scalar and quick reply analysis, have been evidenced as an effective method to investigate the Residence Time Distribution (RTD) (Song et al., 2011). The CFD technique involves solving, in an Eulerian frame, the continuity, the momentum and the

energy equations in the transient state-run and guaranteeing that the simulation time is adequate to show that the variables have a cyclic behavior. Then the scalar tracer is added in the riser at the inlet via a user defined function. The scalar has properties identical to the actual phase in the reactor system. The tracer concentration is taken as a scalar and the transport equation is solved; the RTD function can be built by monitoring the tracer in time at the riser outlet. The scalar transport equation to calculate the residence time of catalyst is given by equations 14 to 18.

4. Simulation

4.1 Geometry and Grids Generation

An industrial riser was considered. The geometries built are meshed using tetrahedral grid refined with prisms on the surfaces; a mesh with 800 thousand control elements was built and used in this work. The dimensions of the industrial classic riser were taken from Alvarez-Castro et al., (in press). Vaporized gasoil mixed with water vapor is injected into the base of the reactor and a side entrance is used for feeding in the hot catalyst – 7 wt. % of the total water vapor is feed with catalyst. The nonslip condition at the walls was used for both phases. Details of geometry in the inlet and outlet regions are shown in Figure 1.

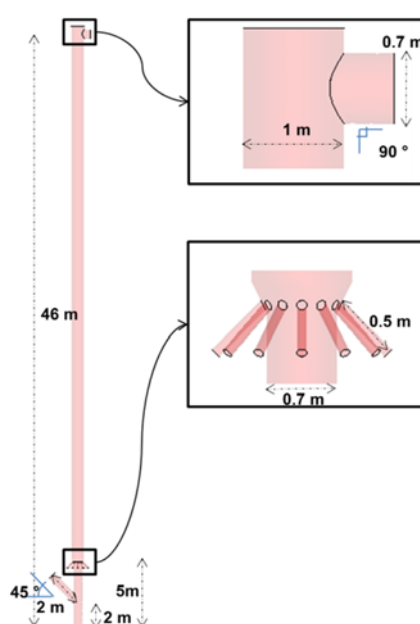


Figure 1: Riser geometry

4.2 Simulation Setting-up

The transient model used in this work considers a three-dimensional gas-solids continuous flow, and chemical reactions with heat transfer. It is assumed that the feed enters the riser vaporized; According to Nayak et al., (2005), 400 kJ/kg is the heat required for the evaporation of the liquid droplets and assumed in the simulations. Then the gas velocity is increased due to the molar expansion caused by cracking reactions. Spatial derivatives of the mass, momentum, energy, species conservation equations were calculated using a finite volume method to discretize the governing equations. It was also necessary to couple 12 lumps kinetic model and inactivation of catalyst particles to represent the catalytic cracking behavior and a scalar function to represent the tracer into the riser. Transient expressions were estimated via the second-order backward Euler method. The convective terms were interpolated through a high resolution scheme. A CFD code using CFX as tool to solve routines was implemented.

4.3 Convergence

A time step of 10^{-3} seconds (Courant number less than one) was used in order to guarantee that the results were independent of the time step selected. Approximately twelve days were necessary to estimate an equivalent process time (15 s) that was adequate to show that the behavior of the variables was cyclical. Then two additional days were required to calculate the period of time (40 s) necessary for adding the tracer and

building a RDT curve for reactive flow. The RSM convergence residuals of less than 10^{-4} were used as the condition for advancing in time. The simulations were carried out using a parallel code with 8 partitions on computers with Xeon 3 GHz dual core processors.

5. Results and Discussion

Figure 2 shows a catalyst distribution for the riser, in a volume rendering. The first seven meter height of riser is the more difficult region to describe since in this zone the feed particle (solid catalyst) and reagents (gasoil) get in contact. It can be seen that the solids (dense region) agglomerate at the center of the wall; from the profile one can analyze the regions where the catalyst has a longer residence time in the equipment in relation to the vertical axis.

In order to compare the product yields' predictions, with experimental data reported in the literature, comparisons were made with Chang et al., (2012) as presented in Figure 3. The results show good agreement between simulation and experimental data.

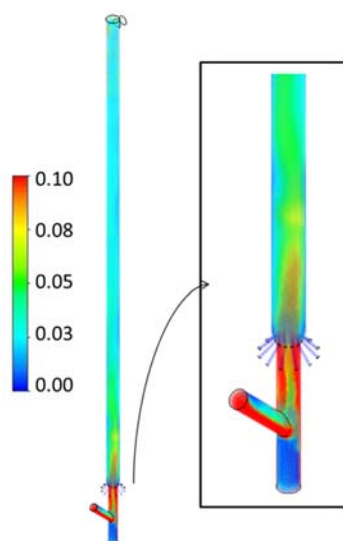


Figure 2: Catalyst volume fraction profile

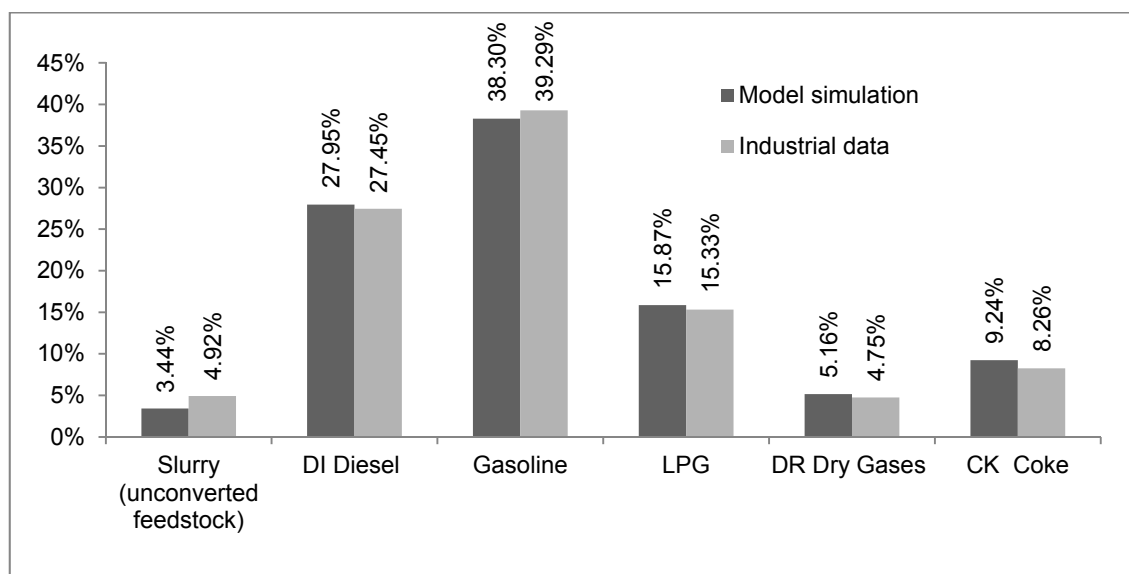


Figure 3: Validation of the product yield of model simulation against industrial data

5.1 Residence time

The residence time strategy was carried out considering the profile of velocity after fifteen seconds, when the velocity profiles becomes constant. After that, the particle tracer was added in the inlets in one second. The transport equation (scalar) was solved without diffusion and then the tracer behavior was measured at the riser outlet. Figure 4 shows the residence time distribution curve. Once the tracer is added to the velocity field obtained after 15 s of operation (i.e. when a = a stabilized field is obtained).

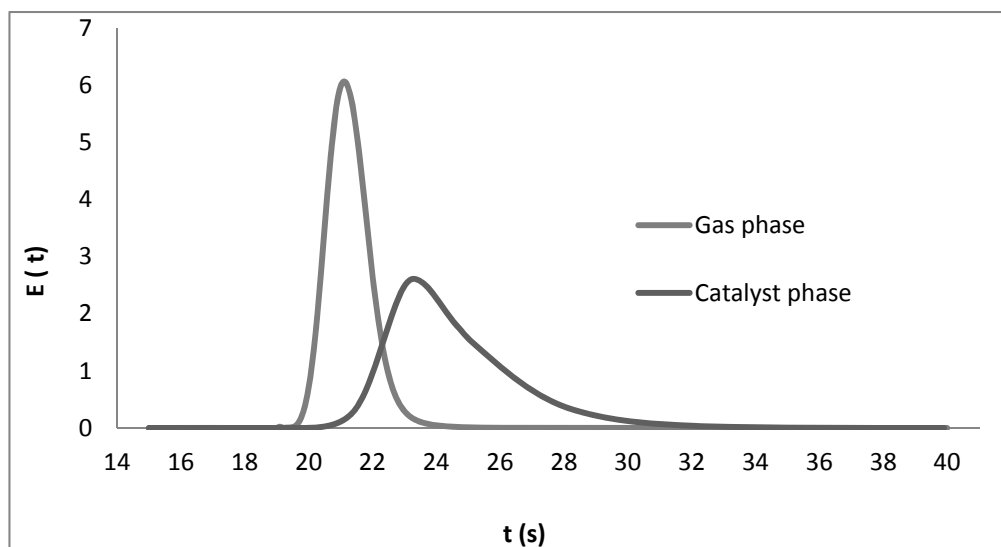


Figure 4: Residence time distribution curve for catalyst and gas phases

The accumulated residence time distribution curve is presented in Figure 5. It can be observed that the average residence time of the gas and catalyst is about 5.2 s and 7s respectively, which is in accordance with the data from fluid catalytic cracking handbook, table 11.2 "Depending on the degree of catalyst back-mixing in the riser, the Catalyst residence time is usually 1.5-2.5 times longer than the hydrocarbons" (Sadeghbeigi, 2012b).

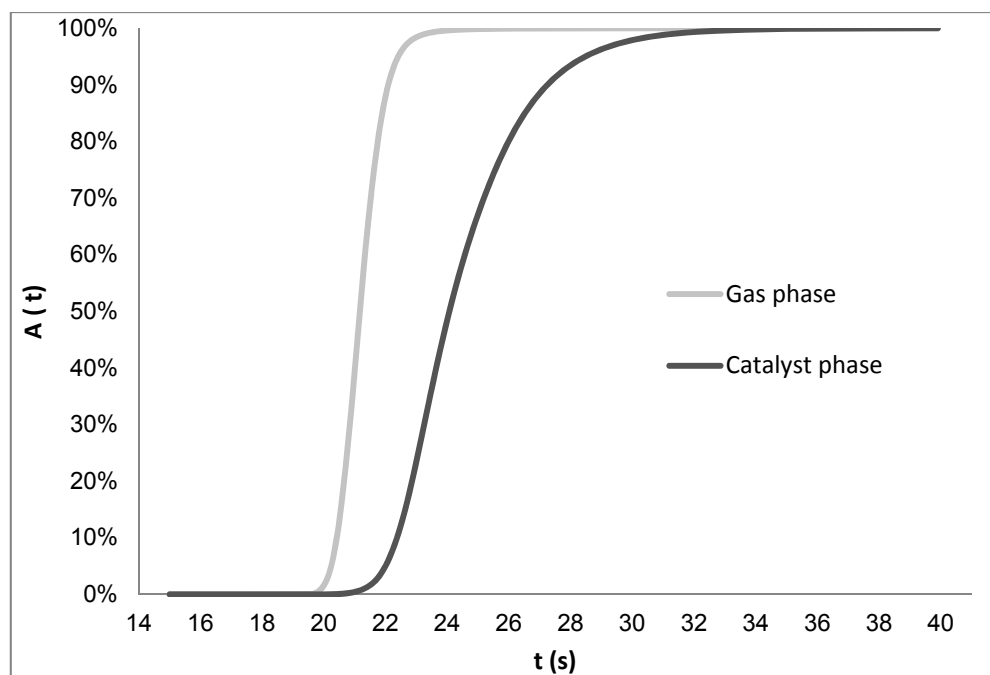


Figure 5: Accumulated residence time distribution curve for catalyst and gas phases

6. Conclusions

The simulations from the model showed good prediction when the results were compared with the kinetic industrial data; it also showed a better hydrodynamic behavior, which avoids the core-annulus effect and improves homogenization.

Scalar or Tracer technique has shown to be an appropriate practice to compare the residence times for different operating conditions. Good agreement between riser residence time and product yields was observed, which allows for concluding that the method presented is employable to estimate important parameters in riser designs and selectivity of products process.

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