

# MODELING AND SIMULATION OF INDUSTRIAL FCC RISERS

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## ABSTRACT

Risers are considered vital parts in Fluidized Catalytic Cracking (FCC) conversion units. It is inside the riser reactor that the heavy hydrocarbon molecules are cracked into lighter petroleum fractions such as liquified Petroleum gas (LPG) and gasoline. The FCC process is considered a key process in the world petroleum industry, since it is the main responsible for the profitable conversion of heavy gasoil into commercial valuable products. This work presents a simplified transient model to predict the response of a FCC riser reactor, i.e., the fluid flow, temperature and concentrations of the mixture components throughout the riser and at the exit. A bi-dimensional fluid flow field combined with a 6 lumps kinetic model and two energy equations are used to model the gasoil mixture flow and the cracking process inside the riser reactor. The numerical results are in good agreement with experimental data, as a result, the model can be utilized for design, and optimization of FCC units. The simulation herein presented shows the applicability of the proposed method for the numerical simulation and control of industrial riser's units.

**Keywords:** petroleum refining, numerical simulations, FCC riser.

## NOMENCLATURE

$A_{gs}$	specific surface area of the particulate based on the unit reactor volume, $m^2/m^3$
$C_c$	coke concentration, $kg_{coke}/kg_{cat}$
$C_i$	lump concentration, $kmol/m^3$
$C_p$	specific heat, $kJ/kg K$
$E$	activation energy, $kJ/kmol$
$h$	gas-particulate heat transfer coefficient, $kJ/m^2 s K$
$K$	reaction pre-exponential constant, $m^3/kg_{cat} s$ or $m^6/kmol kg_{cat} s$
$\dot{m}$	mass flow, $kg/s$
$M$	molecular weight, $kg/kmol$
$n$	reaction order
$N$	the number of lumps
$p$	the pressure, Pa
$r, z$	cylindrical coordinates, m
$R$	universal gas constant, $kJ/kmol K$
$t$	time, s
$T$	temperature, K
$v_r, v_z$	fluid velocities, $m/s$
$Y$	mass fraction

## Greek symbols

$\Delta H$	reaction enthalpy, $kJ/kg$
$\varepsilon$	porosity
$\phi$	catalyst deactivation function
$\varphi$	phase volume fraction

$\mu$	viscosity, $N. s/m^2$
$\rho$	the fluid density, $kg/m^3$
$\Omega_i$	reaction term, $kmol/m^3 s$

## Subscripts

ad	adsorption
cat	catalyst-phase
gas	gas-phase
$i, j$	component index
st	steam-phase
vgo	feedstock kinetic lump

## Superscripts

in	input
k	volume index

## INTRODUCTION

The importance of the FCC unities for the petroleum industry is growing steadily as the demand for the utilization of heavy oil increases. Therefore, there is great interest of the petroleum refining industry in the development of new technologies, which may increase the conversion, and also the quality, of the gasoil into noble products like gasoline and LPG. For these reasons, several works have been found in the technical literature related to the catalytic cracking of petroleum fractions. Such studies can be divided in two major

research segments: the fluid flow and the catalytic cracking reaction schemes, both of great importance for the FCC process modeling. It can also be observed in the literature, that there exist countless types of models for both the fluid flow and cracking kinetics, varying from simple models to three dimensional and three phase models.

This work focuses its attention on the riser reactor. It is inside the riser reactor that all the cracking reactions responsible for the heavy gasoil conversion into lighter petroleum fractions take place. The hot catalyst ( $\sim 700^{\circ}\text{C}$ ) coming from the regenerator, enters at the bottom of riser and is brought into contact with a liquid stream of gasoil ( $\sim 240^{\circ}\text{C}$ ) flowing from a number of nozzles and, almost instantaneously, is vaporized. This inlet zone is characterized by the presence of turbulence and high temperature and concentrations gradients. This turbulent zone is important, but it happens only in the few first meters of the riser, and in some models the presence of turbulence is not considered in the riser simulation. Another simplification assumed in the majority of the riser's models is the hypothesis that the gasoil injected at the bottom of the riser "well mixed" with the catalyst. This assumption originates from the observation that the increase in the complexity of the simulation model normally does not increase, in the same order of magnitude, the precision of the model to predict the conversion of gasoil inside the riser.

In general, the fluid flow models can be classified in three categories (Martignoni, 1998). Firstly, the one-dimensional models, that are normally simple to formulate and to solve. They are more suitable when the interest is to explore the influence of operating conditions, test a kinetic model or when the simulation includes not only the riser, but also other equipments like the regenerator and the stripper. The simplest kind of these models is the homogeneous version, where both the gasoil and the catalyst are moving at the same velocity and the gasoil is assumed to enter the riser completely vaporized (Ali and Rohani, 1997; Blasetti and Lasa, 1997; Cerqueira, et al., 1997; Jacob et al., 1976; Juárez et al., 1999). The heterogeneous version considers different velocities for the gas and the particulate, resulting in different residence times for the gasoil and the catalyst inside the riser. Gupta and Rao (2001) developed a one-dimensional-three-phase flow model, where the riser was axially divided in a number of compartments where energy and mass balances are performed for each one of the phases at each compartment. It is also considered the coexistence of the three phases interacting through the change of mass and energy. The work of Gupta and Rao (2001) focuses its attention on the atomization effect in the conversion of the gasoil. Martignoni and Lasa (2001), developed a one-dimensional model where a pseudo-three-phase flow is assumed.

The second type comprises the semi-empirical models, which are usually described as core-annulus models. Normally

the particle fall velocity and particle concentration are determined empirically. These models cannot predict results for different operational conditions from those of the model parameter estimation. However, the models have a simple formulation and the numerical solution is easily obtained (Derouin et al., 1997; Patience et al., 1992).

More detailed than the above discussed models, are those that consider the riser reactor as bi or three-dimensional. These models are based on phenomenological concepts and use a simultaneous solution of the conservation equations of mass, momentum, energy and species for both the gas and particulate phases (Gao et al., 1999; Mathiesen, et al., 1999). The physical properties are not necessarily assumed to be constant, and additional equations must be set for them. Turbulent models are normally used to describe the fluid flow and in some formulations, the granular kinetic theory is used to determine the physical characteristics of the particle flow (Neri and Gidaspow, 2000; Tsuji et al., 1997). More recent works have already included in the formulation a third flow-phase, which was added to incorporate the effect of feed vaporization at the entrance region of the riser (Gao et al., 2001, Chang, S.-L. and Zhou, 2003). This class of models is clearly more accurate than the two types already discussed, and can be used as a design tool regardless of having or not experimental support. However, they are very complex, difficult to formulate, and in some situations their numerical solution have not been properly developed yet.

The catalytic cracking kinetics is also of great importance for the correct prediction of mass fractions concentrations at the riser's output section. Just like it was shown for the fluid flow, there are many kinetic models in the literature for the modeling of the cracking reactions in a FCC riser reactor. The important thing to be considered in a simulation is to recognize what is the main goal of the work, and then select the most appropriate kinetic model for that specific use. The simple models, with just a few number of lumps, are usually more suitable for specific simulations, where the kinetic model is developed for a particular type of feedstock and/or catalyst. Examples of this kind of models can be found in the works of Weekman (1968), Blasetti and Lasa (1997), Pitault *et al.* (1994) and Cerqueira *et al.* (1997). These simple models that describe the cracking kinetics with 3, 4 or 5 lumps have the disadvantages that, some of them, are unable to predict some key FCC products independently.

More complex models, with a larger number of lumps, can also be found in the literature. The most known of them is the 10 lumps model proposed by Jacobi *et al.* (1976). A variation of this model is the 12 lumps model proposed by Oliveira (1987) which add to the 10 lumps model of Jacobi *et al.* (1976) two more gaseous lumps. These more "sophisticated" models have basically two advantages in comparison with the model with less lumps: a single group

of kinetic constants can be used for various feedstocks and all the most important FCC products can be predicted separately. However, they also have the disadvantage that a large number of kinetic constants must be estimated, and since each lump represents a differential equation in the mathematical model, the complexity of the numerical solution also increases.

In the present work, a bi-dimensional fluid flow field combined with a 6 lumps kinetic model, and two energy equations are used to simulate the gas oil cracking process inside the riser reactor

### MATHEMATICAL MODEL

A general sketch of the problem is shown in Fig. 1. The geometry and the input of the catalyst, steam and gasoil at the bottom of the riser, as well as the output at the top are schematically represented. In Fig. 1, H is the height of the riser, R is the riser's radius, and the cylindrical coordinates system is represented by the z and r directions. The input variables for the model are the mass flow and temperatures of the catalyst, steam and gasoil. These variables determine the operational conditions of the unit.

As already discussed, in an industrial riser, the catalyst and the lift steam are injected at the bottom of the riser; while the gas oil and atomization steam enter the riser through injection nozzles in a higher radial section. However, like the majority models found in the literature, it has been assumed here that all the matter (particulate, gas oil and steam) is introduced at the bottom of the riser.

Although the system consists of a multiphase problem, it is modeled as a well-mixed single phase flow. The flow is assumed to be bi-dimensional, and incompressible, with constant physical properties. The mass and momentum conservation equations for a Newtonian fluid are given by

$$\frac{\partial v_r}{\partial r} + \frac{v_r}{r} + \frac{\partial v_z}{\partial z} = 0 \quad (1)$$

$$\rho \left( \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + v_z \frac{\partial v_r}{\partial z} \right) = -\frac{\partial p}{\partial r} + \mu \left( \frac{\partial^2 v_r}{\partial r^2} + \frac{1}{r} \frac{\partial v_r}{\partial r} - \frac{v_r}{r^2} + \frac{\partial^2 v_r}{\partial z^2} \right) \quad (2)$$

$$\rho \left( \frac{\partial v_z}{\partial t} + v_r \frac{\partial v_z}{\partial r} + v_z \frac{\partial v_z}{\partial z} \right) = -\frac{\partial p}{\partial z} + \mu \left( \frac{\partial^2 v_z}{\partial r^2} + \frac{1}{r} \frac{\partial v_z}{\partial r} + \frac{\partial^2 v_z}{\partial z^2} \right) \quad (3)$$

where, r and z are the cylindrical coordinates [m], p the pressure [Pa],  $\rho$  the fluid density [ $\text{kg}/\text{m}^3$ ],  $v_r$  and  $v_z$  the fluid velocities [m/s], t the time [s], and  $\mu$  the viscosity [ $\text{N} \cdot \text{s}/\text{m}^2$ ].

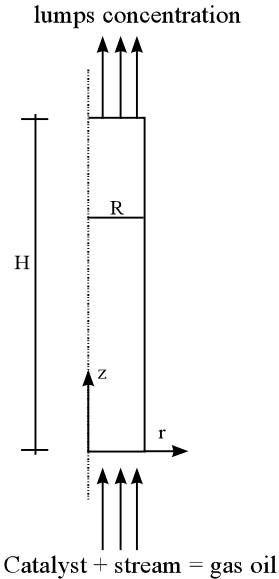


Figure 1. Problem sketch.

For the catalytic cracking reaction simulation, a 6 lump kinetic model (Petrobras six (2001)) was adopted (Fig. 2). In this model the primary reactions (gasoil conversion into products) are of second order, while all other reactions are first order. The fifteen kinetic constants are necessary to describe the catalytic cracking of gasoil, as presented in Fig. 2.

Even though the kinetic model is built with only 6 lumps, it is still possible to predict separately the gasoline and LPG lumps, which are currently considered as the key FCC products.

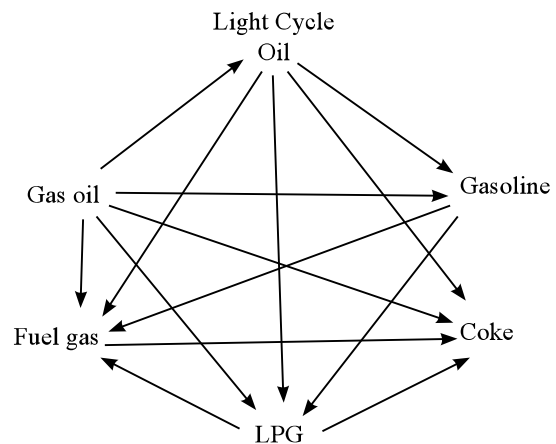


Figure 2. Lumped kinetic scheme.

The proposed set of species equations is as follows:

$$\frac{\partial C_i}{\partial t} + v_r \frac{\partial C_i}{\partial r} + v_z \frac{\partial C_i}{\partial z} = \Omega_i \quad (4)$$

where  $\Omega_i$  is the reaction term given by

$$\Omega_i = \left[ \sum_{j=1}^{i-1} M_j K'_{i,j} (C_j^*)^{n_{j,i}} - \sum_{j=i+1}^N M_j K'_{i,j} (C_i^*)^{n_{i,j}} \right] \quad (5)$$

$$\phi = (1 - \varepsilon) \frac{\rho_{cat}}{M_i}$$

$$C_i^* = \frac{1 - \varepsilon}{\varepsilon} \rho_{cat} K'_{ad,i} C_i \quad (6)$$

$$K'_{i,j} = K_{i,j} e^{\left( \frac{-E_{i,j}}{RT_{cat}} \right)} \quad (7)$$

$$K'_{ad,i} = K_{ad,i} e^{\left( \frac{-E_{ad,i}}{RT_{cat}} \right)} \quad (8)$$

$$\phi = e^{(-406.4 C_c)} \quad (9)$$

$$C_c = \frac{M_{coke} C_{coke}}{C_{cat}^{in}} \quad (10)$$

where,  $C_i$  is the lump concentration [kmol/m<sup>3</sup>],  $\Omega_i$  the reaction term of lump  $i$  [kmol/m<sup>3</sup> s],  $C_c$  the coke concentration, [kg<sub>coke</sub>/kg<sub>cat</sub>],  $E$  the activation energy, [kJ/kmol],  $K$  the reaction pre-exponential constant [m<sup>3</sup>/kg<sub>cat</sub> s or m<sup>6</sup>/kmol kg<sub>cat</sub> s],  $M$  the molecular weight [kg/kmol],  $n$  the reaction order,  $N$  the number of lumps,  $R$  the universal gas constant [kJ/kmol K],  $T$  the temperature [K],  $\varepsilon$  the porosity, and  $\phi$  the catalyst deactivation function. The subscripts “ad” and “cat” represent adsorption and catalyst, respectively. The superscript “in” means input.

Finally, to complete the formulation, two more equations are necessary, the catalyst and the gas energy equations. Even though a one-phase model was presented in the fluid flow formulation, two energy equations are necessary to characterize a temperature gradient between gas and particulate. In the reaction term (Eq. (5)), the catalyst temperature is used to calculate the reaction kinetics constants, while for the heat exchange between the particulate and gaseous phases, a second energy equation (gas equation) is necessary. The two energy equations are written as follows

$$\begin{aligned} & \rho_{cat} C_{p,cat} \left( \frac{\partial T_{cat}}{\partial t} + v_r \frac{\partial T_{cat}}{\partial r} + v_z \frac{\partial T_{cat}}{\partial z} \right) = \\ & h A_{gs} (T_{cat} - T_{gas}) + \\ & \left[ (\Delta H_{vgo}) \Omega_{vgo} M_{vgo} + (\Delta H_{coke}) \Omega_{coke} M_{coke} \right] \end{aligned} \quad (11)$$

$$\begin{aligned} & (\varphi_{vgo} \rho_{vgo} C_{p,vgo} + \varphi_{st} \rho_{st} C_{p,st}) \\ & \left( \frac{\partial T_{gas}}{\partial t} + v_r \frac{\partial T_{gas}}{\partial r} + v_z \frac{\partial T_{gas}}{\partial z} \right) = \\ & - h A_{gs} (T_{cat} - T_{gas}) \end{aligned} \quad (12)$$

where, the not yet defined variables are:  $\varphi$  is the phase volume fraction,  $C_p$  the specific heat [kJ/kg K],  $\Delta H$  the reaction enthalpy [kJ/kg],  $h$  the gas-particulate heat transfer coefficient [kJ/m<sup>2</sup> s K],  $A_{gs}$  the specific surface area of the particulate based on the unit reactor volume [m<sup>2</sup>/m<sup>3</sup>]. The subscripts “cat”, “gas” and “st” indicate catalyst-phase, gas-phase and steam, respectively.

The presented kinetic model showed in Fig. 2 is actually able of capture the major conversion kinetic characteristics of gasoil into light products. However, for a better fitting between the presented mathematical model results and the available experimental data (Petrobras Six, 2001), it was necessary to solve an inverse parameter estimation problem. In this procedure, six fitting parameters of the mathematical model were adjusted by the solution of a non-linear system of algebraic equations where the outputs of the mathematical model were compared to the experimental data. The inverse problem method and also the validation of the present formulation are presented in detail in Souza *et al.*, (2004).

Next, the versatility of the present model is illustrated through its application on the simulation of a industrial size FCC riser.

## EXAMPLE OF AN INDUSTRIAL FCC RISER SIMULATION

This section brings a complete simulation of an industrial FCC riser which was performed with the mathematical method presented in section 0. Table 1 shows the operational conditions and some geometrical and physical parameters of the simulations. This data was obtained from Gao *et al.*, (2001).

The finite differences method was used for the discretization of the geometry shown in Fig 1, and the resulting non-linear system of algebraic equations was solved with the Newton-Raphson method. For the presented simulation it was used a bi-dimensional mesh, in cylindrical coordinates, with 1560 volumes.

Normally, for industrial applications, the main goal of a FCC riser simulation is to predict, for a particular set of operational conditions, the mass fraction of each component (gasoline, LPG, Light Cycle Oil, etc) at the riser output section. If this prediction is possible, the set of input parameters can be fitted in such a way that the conversion of a specific product can be maximized. The procedure can be conducted without, or with just a few number of experimental tests in the unity, leaving the bulk of the tests to be simulated with a computer code, and making possible a fast, easy and low cost adjustment of the unit to the fluctuations of the market needs.

Table 1. General operational characteristics of the FCC unit.

<b>Geometry</b>	
Height(m)	32.8
Diameter(m)	0.6
<b>Feedstock</b>	
Gasoil mass flow (kg/h)	12744
Gasoil input temperature (°C)	320
Steam mass flow (kg/h)	442.4
Steam input temperature (°C)	320
Catalyst mass flow (kg/h)	62445.6
Catalyst input temperature (°C)	567
Catalyst/oil ratio	4.9
Input pressure (bar)	2.5
<b>Physical parameters</b>	
Catalyst density (kg/m <sup>3</sup> )	1560
Catalyst specific heat (kJ/kg K)	1.097
Gasoil density (kg/m <sup>3</sup> )	22
Steam density (kg/m <sup>3</sup> )	0.7
Steam specific heat (kJ/kg K)	2.0
Gas phase viscosity (kg/m s)	2.×10 <sup>-5</sup>
Heat transfer coefficient between the phases (kJ/s K)	1×10 <sup>3</sup>

The mass fractions output, and also their profiles along the height of the riser obtained with the present simulation are shown in Fig. 3. It is seen in that figure that the cracking reactions of the gasoil are more intensive in the first few meters of the riser, (where the concentrations gradients are higher) and, after that input region, they are almost complete, and the concentrations profiles practically do not change anymore till the end of the riser.

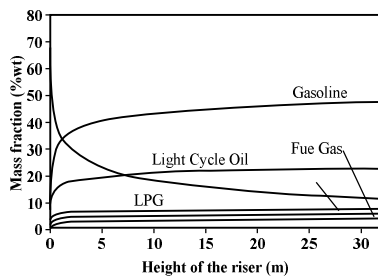


Figure 3. Mass fraction profiles along the riser.

The temperature profiles for the gas phase (gasoil and steam) and for the solid phase (catalyst) are shown in Fig. 4. It can be seen in Fig. 4 that the method is able to predict the heat transfer between the two phases. At the bottom of the riser ( $H = 0$  m), the catalyst is at 560 °C and the gasoil is at 320 °C. As in the case of the lump profiles, the initial condition is drastically modified in the first few meters of the riser and both temperatures reach a common value, which will remain almost the same till the end of the riser. The point where the curves get together is a

direct function of the gas-particulate heat transfer coefficient ( $h$ ), while the final temperature at the end of the riser is a function of the cracking reactions and mass balance between the phases.

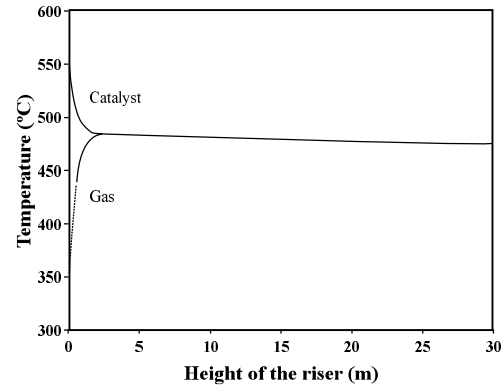


Figure 4. Average temperature profiles along the riser.

The bi-dimensional fields of concentration for the lumps gasoil, gasoline and LPG are shown in Fig. 5. The concentrations (mass fractions) of each lump at each control volume are plotted, i.e., they are calculated for each control volume as the mass flow, of the specific lump divided by the total mass flow rate in the volume. Hence, the bi-dimensional field for the concentrations is calculated by the following equation

$$Y_i^k = \frac{\dot{m}_i^k}{\dot{m}_{\text{total}}^k} \quad (13)$$

where,  $Y_i^k$  and  $\dot{m}_i^k$  are the mass fraction and gas mass flow rate of component  $i$  inside the volume  $k$  and  $\dot{m}_{\text{total}}^k$  is the total gas mass flow rate in the control volume  $k$ .

Fig. 5 presents the influence of the riser wall on the gasoil conversion. For each cross-section of the riser, the velocity in the  $z$  direction varies from approximately two times the mean section velocity at the center of the riser to zero at the wall. This velocity profile induces a higher concentration of the gasoil at the center of the riser in such way that, near the wall, the concentration of gasoil tends to zero, and all gasoil that remains in that region is totally converted into products. It should be remembered that the maximum conversion near the wall is not associated with the maximum mass flow, actually it is the opposite, i.e., the maximum mass flow of gasoil occurs in the center of the riser.

The same phenomena of maximum conversion in the region near the riser wall can also be observed experimentally in an industrial unit, but in this case, it happens for a different reason. In an actual industrial riser, the catalyst behavior differs from the physical assumption of solid and fluid in one phase flowing in the riser. Near the wall, the shock of the solid particles with the wall makes the particulate lose part of its energy, and its velocity direction abruptly changes with the shock. This phenomenon increases the catalyst concentration near the wall and, depending



on the operating conditions of the unity (mass flow ratio between the phases, mainly) it may cause the back slip of the catalyst on the wall. With this, the porosity near the wall tends to decrease, which means that, like in the mathematical model presented here, the gasoil concentration is higher in the center of the riser, and the conversion is higher in the region near the wall.

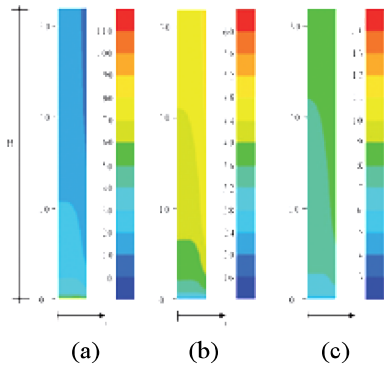


Figure 5. Lumps concentrations along the riser for: (a) gasoil, (b) gasoline and (c) LPG.

The radial concentration (mass fraction) profiles in four different transversal sections of the riser are shown in Fig. 6. It is seen that these profiles are almost uniform along the radii of the riser, showing a small variation, as already discussed in relation to Fig. 5, in the region near the wall, where the gasoil conversion is higher.

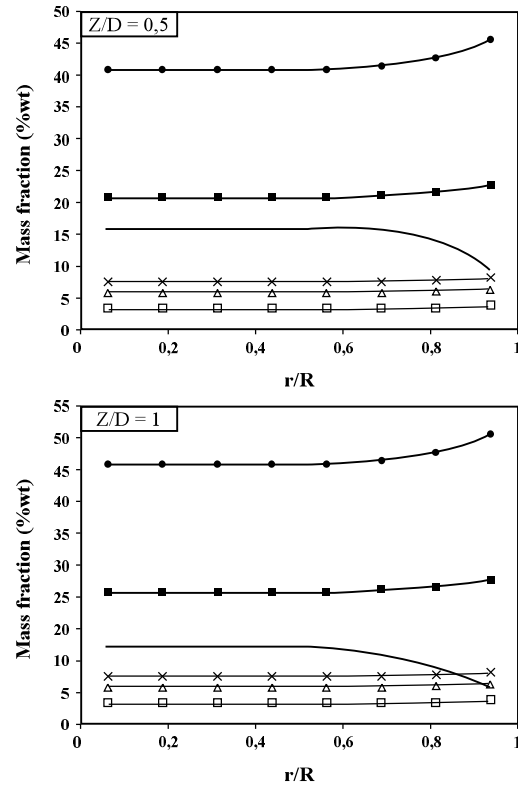


Figure 6. Radial mass fraction profiles for various cross sections along the riser.

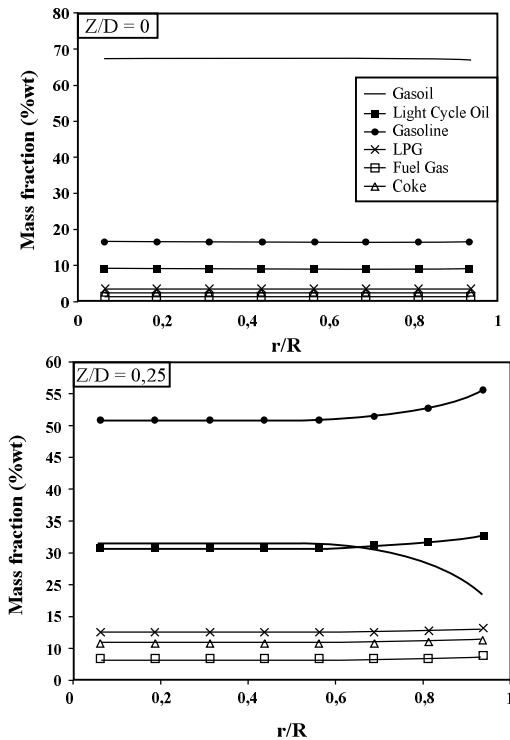


Figure 7. Bi-dimensional temperature profiles: (a) gaseous phase (b) solid phase.

The bi-dimensional fields for the solid and gas phases are presented in Fig. 4. The same phenomena of higher concentration gradients observed only in the first few meters of the riser (Fig. 5) are also present for the temperatures fields. The average temperature profile shown in Fig. 4 is confirmed with the bi-dimensional temperature profiles. It is important to emphasize that the temperature gradients rely on two different phenomena: the heat transfer between the phases and the endothermic cracking reactions of the gasoil.

## CONCLUSIONS

A simplified mathematical model for the numerical simulation of the fluid flow and the cracking reactions of the gasoil inside of FCC risers is presented in this work. The present formulation can be considered simple and easy to solve numerically if compared with the more sophisticated tri-dimensional and two-phase models available in literature. However, it is, still capable of determining with good quantitative and qualitative precision, the variables of interest for the oil refining industry: the mass concentrations and temperature of the key FCC products at the output section of the riser.

The simulations presented illustrated the applicability of the proposed model for the numerical simulation of an actual size industrial FCC unity. The average mass fraction and temperature profiles along the height of the riser were presented and discussed. For the gasoil (vgo) and the two main products of the FCC riser, gasoline and LPG, the bi-dimensional fields of the mass fractions were plotted. The temperature profiles and bi-dimensional fields for both phases were also presented. The presented results demonstrated that the model can be used as a tool for design, control and optimization of FCC units.

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