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A TWO-PHASE ONE-DIMENSIONAL MODEL FOR SIMULATION OF FCC RISERS

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Abstract. *The FCC (Fluidized Catalytic Cracking) is one of the most important processes in a petroleum refinery plant. The numerical modeling of this process has been performed by several authors who have proposed different mathematical models and reported them in the literature. With the constant increase of computational capabilities, such models have become even more complex and with wider application. The different models address both fluid flow and cracking kinetic, varying from simple one phase and one-dimensional models to three-dimensional and three-phase models. Therefore, there is no common ground regarding the most adequate formulation, and advantages and drawbacks may be identified in each available model. In the present work, a relatively complex model reported in the literature is reproduced. Even though it is a one dimensional model, it includes many physical phenomena, like the dependence of the fluid properties on temperature and the transport equations formulation for both phases (gas and particulate). In a following stage, some simplifications in the mathematical formulation are included to the model and the results obtained with both formulations (with and without simplifications) are compared. The main goal of the present work is to establish a relationship between each included physical phenomenon and its real influence on the capability of the model to predict the products formation inside the riser reactor.*

Keywords*. FCC, Catalytic cracking, Finite differences, Fluid flow*

1. Introduction

The FCC (Fluidized Catalytic Cracking) is a key process for the petroleum refinery industry. With this process, heavy hydrocarbon molecules can be broken into lighter ones, and products of commercial interest such as gasoline and LPG are obtained in large scale and with relatively low costs. Another advantage of the FCC process is that the gasoil (feedstock), is a sub-product of the atmospheric and vacuum distillation and other petrochemical processes. This "sub-product" (gasoil), with a low commercial value, is then transformed into a high aggregated value products. The environmental advantages may also be cited; since industrial sub-products may be used as the feedstock for the FCC process, the amount of industrial trash discarded to the environment may be considerably diminished. Other important issue to be considered, is that the most important variables of the process, as mass flow and input temperature of the feedstock, among others, can be easily controlled, allowing a flexible adjusting of the production to the market variations.

The numerical modeling of the FCC (Fluidized Catalytic Cracking) has been reported in the literature by several authors. Some of these models simulates the whole unity, and are built with a mathematical formulation where the riser, the stripper and the regenerator were all considered in the simulation. Other simple models concentrates its analysis only on a specific equipment, developing for it a more detailed formulation. In this work, only the riser will be considered.

There are different kinds of models for the FCC riser. These models address its formulation for the fluid flow, for the cracking kinetic, or both of them. The complexity of these models may vary from a simple one phase and one-dimensional model to a three-dimensional and three-phase model. Depending on its industrial application, Souza, (2006) proposed that the different FCC models may be used for: (i) the development of a major model where the simulations of the entire conversion FCC unit is considered; (ii) testing or studying of specific catalytic cracking phenomena, such as catalyst deactivation, adsorption, kinetic models etc.; (iii) the search for better operating conditions (unit optimization), and (iv) phenomenological studies of the physical problem.

For the first type of model, the simulation is performed not only for the riser, but also for other equipments like the regenerator and the stripper. It is very important to have a fast solution for the riser model. This kind of model is normally used in the development of control systems, where the most desired feature is a low computational time solution. In these applications, it is not necessary an exact determination of the values of the variables, but only to determine qualitatively correct the system response to changes in the operating conditions. Examples of these kind of

models are the works of Han and Chung (2001) and Ali *et al*. (1997). The second type encompasses models used when the main goal is to study a specific physical phenomenon of the gasoil catalytic cracking, such as analysis of a catalyst deactivation function (Cerqueira *et al.* 1997a), the coke formation in the cracking process (Cerqueira *et al.* 1997b), the adsorption phenomena in the catalytic cracking [Martignoni, and Lasa, 2001) and the building of kinetic models (Ancheyta *et al.,* 1999). The third type of models strives for unit optimization. In this case, it is necessary to have a fast and sufficiently precise model that will be used to run several simulations searching for the best values for the input variables (mass concentrations, temperatures, etc.). The fourth and last type refers to models which try to include all important physical phenomena (Gao *at al.*, 2001; Chang and Zhou, 2003). These models are generally three-dimensional with two or three phases flow. The conservation equations are written for each phase of the fluid flow and the physical properties are not necessarily assumed constant. Turbulent models are normally used to describe the fluid flow.

Based on the great number of models, with different levels of complexities shown in the above paragraph, it is reasonable to conclude that there is no common ground regarding about the most adequate formulation for the FCC modeling. The four types of models discussed above may be used as a reference for choosing the most adequate model for a specific need, therefore great difference in the complexity may be observed among the models classified in a same case of application. For example, the one-dimensional models of Han and Chung (2001) and Ali *et al*. (1997) were considered both of first type, but conceptually they are completely different. While the Ali *et al*. (1997) formulates the riser as an one phase mixture fluid flow model, Han and Chung (2001) uses a two-phase model for the fluid flow simulation.

In the present work, part of the Han and Chung (2001) work is reproduced. In this model, an one-dimensional formulation for the riser, the regenerator and the stripper is presented, therefore only the riser formulation is reproduced in this first simulation. This model includes many physical phenomena, like the dependence of the fluid (and particle) properties (specific heat, viscosity, etc.) on temperature and the transport equations formulation for both phases (gas and particulate). These phenomena are normally simplified in simpler models.

At this moment, the species conservation, gasoil energy equation and catalyst energy equation are already implemented. The specific heat of the gasoil dependence on the temperature and the feedstock was the first property calculation added to the model. Two simulations were performed: one with the full specific heat temperature and feedstock dependence and another with a fixed average value for the gas phase specific heat. The comparison of the results showed a small difference in the products mass fraction predictions at the riser output section. The momentum equations for the gasoil and the catalyst are also already implemented and working, therefore they where not validated yet. The comparison solution between the two-phase model and the one-phase model will be performed in a following work.

2. Mathematical model

Figure 1 shows a schematic diagram of the studied system, with its simple geometry, where H is the length of the riser in the flow direction. Regenerated catalyst and gasoil enter the system from the bottom of the riser, whereas the product lumps and the deactivated catalyst leave it from the top of the riser.

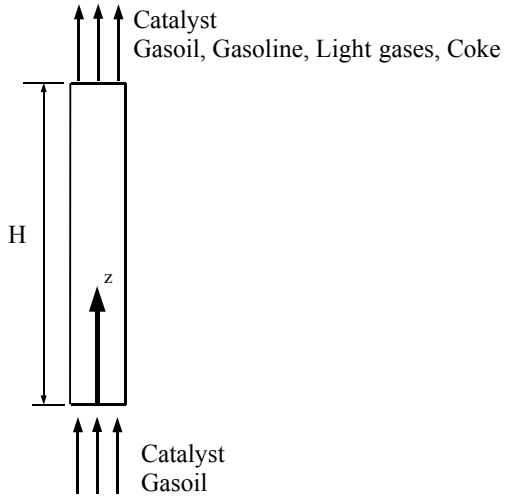


Figure 1 – Problem sketch

In this first simulation, only the riser reactor model will be simulated. The present formulation also considers the following assumptions: incompressible, laminar, one-dimensional flow and homogeneous mixture. The gasoil density

and bed porosity were also considered constants, but the gas phase specific heat was considered as to be a function of the bet temperature.

The kinetic model that will determine the products mass fraction profiles along the riser was based on a 4-lumps, as shown in Fig. 2. All the pre-exponential constants (k_{ij}) of the kinetic model and heat of reactions (ΔH) are available in Han and Chung (2001).

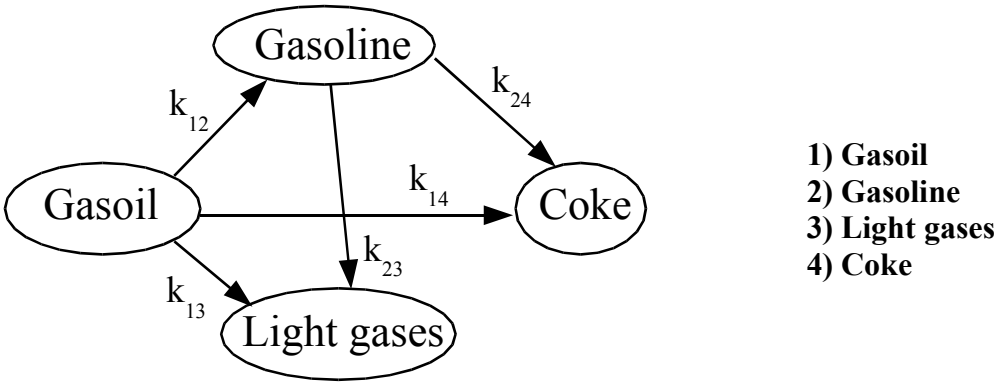


Figure 2 – Lumped kinetic model

According with Han and Chung (2001), the lumps mass fraction profiles along the riser reactor can be predicted by

$$\frac{\partial y_i}{\partial z} = \frac{\rho_c \epsilon_c A \phi_c}{\dot{m}_g} \Omega_i \quad \text{with i = 1 to 4} \tag{1}$$

where

$$\begin{aligned}
\Omega_1 &= -(k_{12} + k_{13} + k_{14})\, y_1^2 \\
\Omega_2 &= k_{12}\, y_1^2 - k_{23}\, y_2 - K_{24}\, y_2 \\
\Omega_3 &= k_{13}\, y_1^2 + k_{23}\, y_3 \\
\Omega_4 &= k_{14}\, y_1^2 + k_{24}\, y_3
\end{aligned} \tag{2}$$

In Eqs. (1-2) y is the lump mass fraction, ρ the density, ϵ the volume fraction, ϕ the catalyst deactivation function, z the axial coordinate, A the riser cross section area, $\dot{m}$ the mass flow rate, Ω the reaction term and k the pre-exponencial constants. The sub-indexes c, and g, indicates catalyst and gas, respectively.

The temperature profiles for the gasoil and catalyst are determined by the following energy equations

$$\frac{\partial T_c}{\partial z} = \frac{A h_p}{\dot{m}_c Cp_c}\left(T_g - T_c\right) \tag{3}$$

$$\frac{\partial T_g}{\partial z} = \frac{A}{\dot{m}_g Cp_g}\left[h_p\left(T_g - T_c\right) + \rho_c \epsilon_c \Omega_T\right] \tag{4}$$

where

$$\Omega_T = -\phi_c\left(\Delta H_1 k_{12} y_1^2 + \Delta H_2 k_{13} y_1^2 + \Delta H_3 k_{14} y_1^2 + \Delta H_4 k_{23} y_2 + \Delta H_5 k_{24} y_2\right) \tag{5}$$

In Eqs. (3-5), T is the temperature, $h_p = h\ A_p$ the interface heat transfer coefficient between gas phase and catalyst phases, Ω_T energy reaction term, C_p the specific heat and ΔH heat of reaction.

The Han and Chung (2001) work considers all physical properties as functions of temperature, pressure or feedstock. In the present stage of development of this work, only the gaseous phase specific heat dependency with the feedstock and temperature was incorporated to the model.

The gas-phase heat capacities of gasoil and gasoline lump are calculated as (Lee and Kesler, 1988):

$$Cp_g = \beta_1 + \beta_2 T + \beta_3 T^2 \tag{6}$$

where

$$\beta_1 = -1.492343 + 0.124432\,K_f + \beta_4\left(1.23519 - \frac{1.04025}{Sg}\right) \tag{7}$$

$$\beta_2 = -7.53624\times10^{-4}\left[2.9247 - \left(1.5524 - 0.05543\,K_f\right) + \beta_4\left(6.0283 - \frac{5.0694}{S_g}\right)\right] \tag{8}$$

$$\beta_3 = 1.356523\times10^{-6}\left(1.6946 + 0.0884\,\beta_4\right) \tag{9}$$

$$\beta_4 = \left[\left(\frac{12.8}{K_f}\right)\left(1 - \frac{10}{K_f}\left(S_g - 0.885\right)\left(S_g - 0.7\right)\times10^4\right)\right]^2 \quad \text{for } 10 < K_f < 12.8 \tag{10}$$

$\beta_4 = 0$ for all others cases

The density S_g and K_f are defined as

$$S_g = \frac{141.5}{\mathrm{API} + 131.5} \tag{11}$$

$$K_f = \frac{\left(1.8\,T_{Me}\right)^{1/3}}{S_g} \tag{12}$$

where T_{Me} is the mean average boiling temperature.

For the light gases lumps, the specific heat is calculated by

$$Cp_g = 0.2457 + 5.3\times10^{-3}\,T - 2.1527\times10^{-6}\,T^2 \tag{13}$$

3. Results

The ordinary differential equation system formed by Eqs. (1), (3) and (4) was solved with a fourth-order Runge-Kutta algorithm (Kincaid, 1991). Fig. 3. shows the computational domain with the appropriated boundary conditions for the problem. For the transport equation of the kinetic model (Eq. (1)), at the input section of the riser, it is considered that only gasoil is entering. Therefore the mass fraction of gasoil is set to 1, while for the other three lumps the mass fractions are set to zero. The catalyst and gasoil (gas) temperatures are a known operating condition at the input section of the riser, thus a prescribed value is set to this variables in the mathematical model. The operating conditions for all simulations are presented in Table 1.

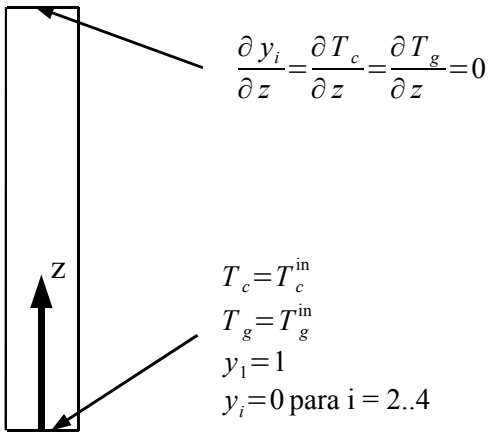


Figure 3 – Boundary conditions and computational domain

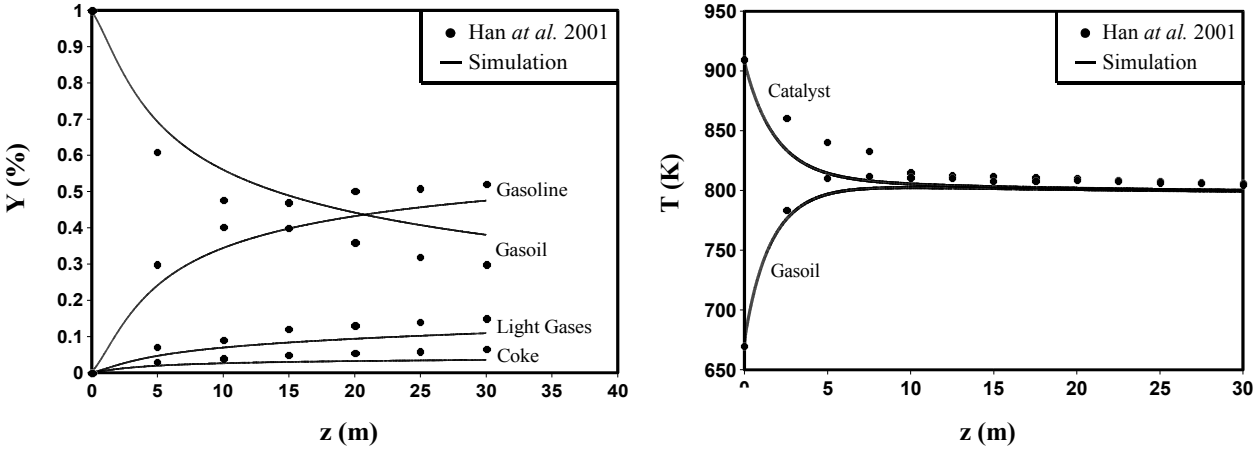
At the riser output section, it was considered that the mass fractions of the lumps are no longer varying, and the derivative in the flow direction is set to zero for each lump. The same boundary condition is prescribed for both gas phase and catalyst temperatures at the top of the riser, as also shown in Fig. 3.

Table 1: General operating conditions for all simulations

Geometry	
Length (m)	30
Diameter (m)	1,1
Feedstock	
Gas oil mass flux (kg/s)	50
Catalyst mass flux (kg/s)	350
Physical parameters	
Catalyst density (kg/m^3)	1410
Catalyst specific heat (kJ/kg K)	1,15
Catalyst input temperature (°K)	910
Gasoil specific heat (kJ/kg K)	4.5*
Gasoil input temperature (°K)	670
Heat exchange coefficient between phases (kJ/s K)	1 x 10^2

* for the simulations with constant gas phase specific heat.

The comparison of the Han and Chung (2001) results and those obtained with the present formulation are shown in Fig. 4. Even though, at this stage of the simulations both models are considerably different, a qualitative agreement between the results for both the mass fractions and temperatures profiles along the riser may be observed in Fig. 4.



(a) (b)

Figure 4 – Comparison between the model and the Han and Chung (2001) results

The differences between the two models do not allows a quantitative validation of the present program, therefore the good qualitative results obtained are sufficient for the analysis performed in this paper.

The main goal of the present paper is to analyze the influence of the dependence of the specific heat of the gas phase with the temperature. This dependence of the gas phase specific heat on the temperature is added to the model by the Eqs. (6-12). This set of equations also incorporates to the model the dependence of the gasoil specif heat with the feedstock, therefore this influence will not be explored in the present work.

The set of equations needed to incorporate the gas phase specific heat dependence on the temperature (Eqs. (6-12)) also include some complications to the simulation solution. Even though only algebraic equations are added to the model, this equations are dependent of the gas phase temperature and for this reason, also included in the differential system of equations to be solved (Eqs. (1, 3-4)). The model will be considerably simplified if were set a constant average value for the gas phase specific heat, and if no significant differences between the two solutions were observed, this simplification should be the best option for the simulation.

In order to quantify this influence, the program develop with the model presented in this work was run with and without the specific heat dependence on the temperature. Fig. 5. shows the comparison of both results for the mass fraction and temperature profiles along the riser.

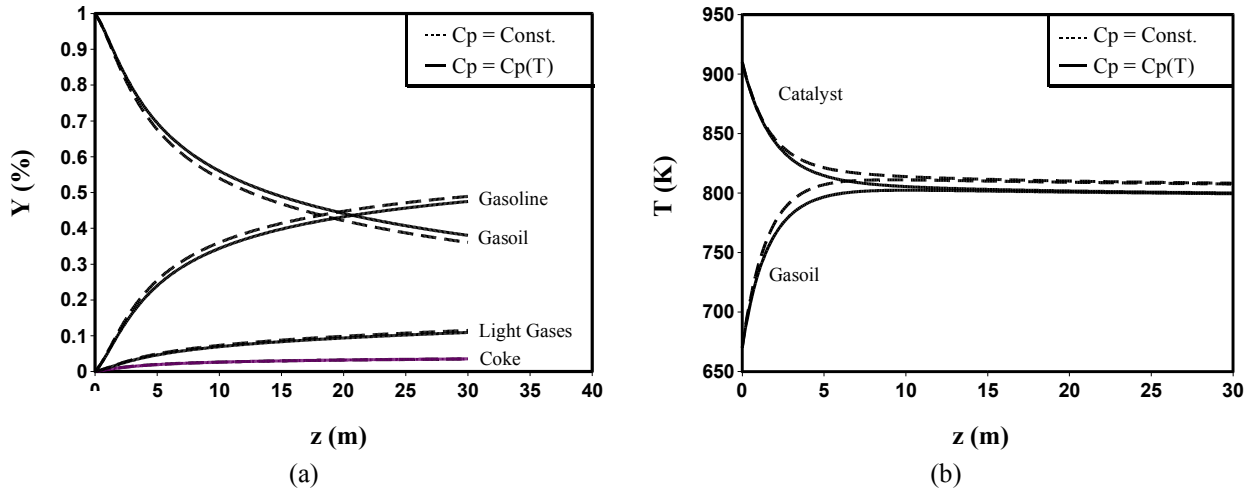


Figure 5 – Mass fraction and temperature profiles along the riser: (a) Cp = *constante*, (b) *Cp = CP(T)*

As can be seen in Fig. 5, a small deviation between the results obtained with the two simulations can be observed. Comparing Figs. 5a and 5b, it can be notice that at the input section of the riser (up to 5m approximately) no significant deferences may be observed between the two simulation. In this region, with high catalyst temperature and low gasoil temperature, both mass fraction and temperature profiles are almost identical. After this input section, a small deviation between the profiles for both mass fractions and temperatures are observed, therefore this difference remains less than 7%. Table 2 shows the comparison between the mass fraction predictions at the riser output section of the riser. Table 2 shows that only a small difference between the predicted mass fractions of the lumps were found.

Table 2: Gas phase specific heat influence on the mass fraction at the riser output section

Y	**For Cp = constant**	**For Cp = Cp(T)**	**%error** $\left\lvert\frac{Cp-Cp(T)}{Cp}\right\rvert$
Gasoil	0,3600	0,3803	5,64%
Gasoline	0,4893	0,4751	2,90%
Light Gases	0,1149	0,1092	4,96%
Coke	0,0352	0,0354	0,57%

4. Conclusions

In this work, a simplified fluid flow and kinetic model for a FCC riser was used to study the influence of gas mixture specific heat on the product profiles along the riser reactor. Two simulation were performed: one with a constant value for the specific heat of the gas phase and another with the specific heat formulated as a function of the gas phase temperature. The results obtained with this comparison showed that the difference between the two models remains less than 7%, what considering the difficult and uncertainness of the corrected prediction of these profiles when they are compared with experimental data, the use of such a complex formulation for the specific heat mixture calculation may not aggregate significant improvement to the model prediction. Since the two models were not compared with the experimental data, but only among them, and the difference between the two predictions is quite small, it is not possible to concern about the best formulation (with or without specific heat dependence on temperature), but only about their advantages and disadvantages. The constant specific heat formulation has a more simplified mathematical model, and consequently an easy and fast solution, while the temperature dependent formulation is more phenomenological corrected and may be the best choice for theoretical studies of the physics of catalytic cracking phenomenal inside the riser reactor, but according with the results obtained in this work do not increase the products profiles prediction along the riser.

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