INTRODUCTION

The Fluid Catalytic Cracking (FCC) process represents nowadays an important segment for the petroleum industry. It is the key process for the profitable conversion of heavy hydrocarbon molecules into products of commercial interest like gasoline, light olefins and LPG. With the FCC process the residual fractions of the atmospheric and vacuum distillation are reprocessed of commercial interest like gasoline, light olefins and LPG. The catalytic cracking of hydrocarbons in a FCC riser is a very complex physical and chemical phenomenon, which combines a three-dimensional, three-phase fluid flow with a heterogeneous catalytic cracking kinetics. Several researchers have carried out the modeling of the problem in different ways. Depending on the main objective of the modeling it is possible to find in the literature very simple models while in other cases, when more accurate results are necessary, each equipment is normally treated separately and a set of differential and algebraic equations is written for the problem. The riser reactor is probably the most important equipment in a FCC plant. All cracking reactions and fuel formation occur during the short time (about 4-5s) that the gas oil stays in contact with the catalyst inside the riser. This work presents a simplified model to predict the, temperature and concentrations in a FCC riser reactor. A bi-dimensional fluid flow field combined with a 6 lumps kinetic model and two energy equations (catalyst and gas oil) are used to simulate the gas oil cracking process. Based on the velocity, temperature and concentration fields, it is intended, on a next step, to use the second law of thermodynamic to perform a thermodynamic optimization of the system.

ABSTRACT

The catalytic cracking of hydrocarbons in a FCC riser is a very complex physical and chemical phenomenon, which combines a three-dimensional, three-phase fluid flow with a heterogeneous catalytic cracking kinetics. Several researchers have carried out the modeling of the problem in different ways. Depending on the main objective of the modeling it is possible to find in the literature very simple models while in other cases, when more accurate results are necessary, each equipment is normally treated separately and a set of differential and algebraic equations is written for the problem. The riser reactor is probably the most important equipment in a FCC plant. All cracking reactions and fuel formation occur during the short time (about 4-5s) that the gas oil stays in contact with the catalyst inside the riser. This work presents a simplified model to predict the, temperature and concentrations in a FCC riser reactor. A bi-dimensional fluid flow field combined with a 6 lumps kinetic model and two energy equations (catalyst and gas oil) are used to simulate the gas oil cracking process. Based on the velocity, temperature and concentration fields, it is intended, on a next step, to use the second law of thermodynamic to perform a thermodynamic optimization of the system.
cracking reactions. The complexity of chemical structure of the gas oil makes it very difficult to describe its kinetics at a molecular level. Therefore, the modeling of such complex process can be simplified by lumping large numbers of chemical compounds with similar behavior. Weekman and Nace, 1970, presented the oldest and also simplest three-lump model to predict the catalytic cracking reactions. Other examples of simple models are the four-lump model proposed by Blasetti and Lasa, 1997, and the five-lump model propose by Juárez et al., 1999. These simple models that describe the cracking kinetics with 3, 4 or 5 lumps have the advantage that just a few kinetic constants must be estimated for each feedstock, but depending on the simplicity of the model, the key FCC products cannot be predicted separately. More sophisticated models, normally with more than 10 lumps, have basically two advantages: a single group of estimated kinetic constants can be used for various feedstock and all the most important FCC products can be predicted separately. The disadvantages of these models are that a large number of kinetic constants must be estimated and as each lump represents a differential equation in the mathematical model, the complexity of the numerical solution may increase exponentially. Examples of these models are the classical 10 lumps model presented by Jacob et al., 1976, the 12 lumps model presented by Cerqueira et al., 1997a and the 19 lumps model presented by Pitault et al., 1994.

In the present work, a 2-D fluid flow field combined with a 6 lumps kinetic model and two energy equations (catalyst and gas oil) are used to simulate the gas oil cracking process inside the riser reactor. Next the mathematical model and some preliminary results are presented.

MATHEMATICAL MODEL

A general simple problem sketch is shown in Fig. 1. The geometry and the catalyst, gas oil and steam inputs are schematically represented. In Fig. 1, H is the length of the riser in the flow direction and R the riser’s radius.

Although heavy gas oil, steam and particulate catalyst are injected simultaneously in the riser, in this treatment, the moving matter inside the riser is approximated by an equivalent well mixed fluid with an average set of properties. The fluid flow is assumed bi-dimensional, incompressible and with constant properties. The mass and momentum conservation equations for a Newtonian fluid is given by

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v_r)}{\partial r} + \frac{\partial (\rho v_z)}{\partial z} = 0
\]

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

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

where, \( r \) and \( z \) are the cylindrical coordinates, \( m; p \) the pressure, \( Pa; \rho \) the fluid density, \( kg/m^3 \); \( v_r \) and \( v_z \) the fluid velocities, \( m/s \); \( t \) the time, \( s \); and \( \mu \) the viscosity, \( N.s/m^2 \).

The dependence of the velocity field on the spatial variation of the equivalent fluid average properties will be investigated and, if necessary, added to the model in a follow up study.

For the catalytic cracking reaction simulation, a 6 lump model (Fig. 2) provided by Petrobras Six, 2001, was adopted.

Equation (4) combined with Eqs. (5)-(9) represents the kinetic model set of equations. Even though this kinetic model is constructed with only 6 lumps, it is still possible to predict the key FCC products separately. Another important thing to be noticed is that the adsorption is also included in the kinetic model.
PRELIMINARY RESULTS

A preliminary step before solving the set of differential equations (Eqs. (1)-(4), (11) and (12)) was to solve a simplified one-dimensional, steady state problem. This was made to evaluate the kinetic model behavior and to test the model sensitivity to operating conditions changes. A fourth order Runge-Kutta method was used to solve the simplified set of differential equations given by

\[ \varepsilon V_{in} \frac{\partial C_i}{\partial Z} = \Omega, \]

where the new variables are: \( V_{in} \) – mixture average input velocity, m/s; \( \varepsilon \) - mass flux, kg/s, and \( A \) – riser cross section area, m².

The problem sketch for the one-dimensional model is similar to that shown in Fig. 1, with the only difference that the gas oil is injected at the bottom of the riser. The FCC riser characteristics and operating conditions are presented in Table 1.

The temperature and concentrations solutions for the one-dimensional model are shown in Fig. 3. This simple model was already able to predict the dependence between the catalyst temperature and the gas oil conversion. It is possible to see in Fig. 3 that, as expected, the gas oil consumption and products formation are greater when the catalyst temperature is high and that it is at the bottom (first few meters) of the riser where the majority of the reactions occur. Another important phenomena observed in Fig. 3 is that at high temperatures the rate of formation of light cycle oil is higher than the rate of gasoline formation.

| Table 1. Riser characteristics and operating conditions |
|-----------------|-----------------|
| **Geometry**    | **Feedstock**   |
| Length (m)      | 18              |
| Diameter (m)    | 0.0508          |
| **Physical parameters** | **Catalyst density (kg/m³)** | 1400 |
|                 | **Catalyst specific heat (kJ/kg K)** | 1.09 |
|                 | **Catalyst input temperature (°C)** | 670 |
|                 | **Gas oil density (kg/m³)** | 10 |
|                 | **Gas oil input temperature (°C)** | 200 |
|                 | **Water vapor density (kg/m³)** | 0.5 |
|                 | **Water vapor specific heat (kJ/kg K)** | 2.0 |
|                 | **Water vapor input temperature (°C)** | 200 |
Fig. 3 - Runge-Kutta solution

With these results obtained with the one-dimensional Runge-Kutta solution, the same problem (with the gas oil injected at the bottom of the riser) was solved with a bi-dimensional finite differences scheme. The solution grid used had 8 x 70 volumes.

Similar temperature and concentrations profiles were obtained, but now a bi-dimensional concentration and temperature fields are available. The temperature fields for the catalyst and the gas (gas oil + water vapor) are shown in Fig. 4.

The concentration fields for the gas oil, light cycle oil and gasoline are presented in Fig. 5. The bi-dimensional mass fractions are calculated by

\[ Y_i^k = \frac{m_i^k}{m_{total}} \tag{16} \]

where, \( Y_i^k \) and \( m_i^k \) are the mass fraction and mass flux of component \( i \) at volume \( k \), respectively and \( m_{total} \) is the input gas oil mass flux.

The mass fractions of the LPG, fuel gas and coke lumps are presented in Fig. 6.

CONCLUSIONS

There is a lack of agreement among scientists about the most appropriate formulation model for FCC risers. The most complex models are normally suitable for units design, while the simple ones are used for units’ control. The present model was constructed with the main goal of creating a fast and enough accurate computational code, not as simple as the plug flow models, but also not as complex as the three-dimensional and two-phase models. As it was shown in this paper, the proposed model has a
simple incompressible formulation of the fluid flow and a six lump kinetic model to the catalytic cracking reactions. The study presented in this work brings the preliminary results obtained with the proposed FCC riser reactor model. First, a one-dimensional fourth order Runge-Kutta solution was used to test the model. Next, the same solution was obtained with a bi-dimensional finite differences scheme and then, on a third step, a bi-dimensional model with radial injection of gas oil was discussed. The fourth and last step will be the formulation and implementation of a thermodynamic optimization methodology. This optimization will be based on the second law of thermodynamics and the concept of entropy generation minimization (Bejan, 1996).

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