

# HYDORDYNAMIC MODEL OF FLUID CATALYTIC CRACKING (FCC) RISER REACTOR

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## Abstract

While commercial FCC riser reactor converts heavy hydrocarbon petroleum fractions into a slate of more usable products, mass transfer, momentum transfer, heat transfer, catalytic cracking reaction and phase transfer are entangled and occur simultaneously inside the riser reactor. Since the FCC process is in nature strong inter-coupled with multiphase flow hydrodynamics, in order to predict accurate behavior of the riser reactor, all these processes need to be comprehensive modeled. Unfortunately most of published literature focused too much on the FCC process itself without paying enough attention to significant influence on the cracking kinetics from multiphase flow hydrodynamic, such as local catalyst concentration, local catalyst velocity and even catalyst average size. The aim of this work is to develop a generic modeling approach which can fully incorporate multiphase flow hydrodynamics with FCC process. The emphasis of this model is to develop a framework to simultaneously simulate the multiphase flow hydrodynamics, cracking reaction and their inter-coupling characteristics in riser reactor. This modeling approach opens up a new dimension for making generic models suitable for the analysis and control studies of FCC units. Predictions of the model will compare with the yield pattern of industrial scale plant data reported in literatures.

**Keywords:** Fluid Catalytic Cracking, Multiphase flow hydrodynamics, Cracking Kinetics, Riser Reactor

## Introduction

Fluid catalytic cracking (FCC) is one of the most important refinery unit operations. It is the primary conversion process in the modern refinery industry. FCC riser reactor is designed to use acidic catalyst to decompose heavy oil, such as vacuum gas oil, into more valuable lighter hydrocarbons at certain range. The hydrocarbon feed enters reactor riser through feed atomizing nozzles and comes in contact with the hot catalyst coming from the regenerator. The feed gets vaporized and cracks down to the lighter molecules as it travels upwards along with the catalyst. As a result of cracking, the velocity of the vapors increases along the riser height. Coke, the byproduct of cracking reactions, gets deposited on the catalyst surface thus causing the catalyst to loose its activity. The cracked hydrocarbon vapors are separated from the deactivated catalyst in a separator;

Efforts are continuously made to improve the process in order to increase the productivity of the refinery industry and also to reduce pollutant emissions to the environment. However detailed modeling of the riser reactor is a challenging task for theoretical investigator not only due to complex hydrocarbons in the FCC feed but also because of the involvement of different types of reactions taking place simultaneously.

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Numerous articles are found on catalytic cracking reaction in the published literature. Most of them are based on representation of oil in few lumps (like 4 lumps, 10 lumps, 14 lumps and so on). Weekman and Nace [1] were first to develop a three-lump cracking model to study gasoline production of a FCC unit; the three lumps considered were gas oil, gasoline and light gases plus coke lumps. These models led to a relationship between the gasoline yield and the gas oil conversion. However, because light gas and coke are taken as one lump, the coke yield cannot be determined separately. Since these studies, more complex kinetic models for the FCC process have been developed. These include: the four-lump model [2]; the five-lump model [3, 4]; the six-lump model [5]; and the ten-lump model [6]. All these models considered isothermal plug flow in the riser reactor.

However, when a gas vertical riser transports the particles, both experimental and theoretical studies have shown they are non-uniformly distributed all over the cross-section of the riser. Momentum transfer, heat transfer, mass transfer, and catalytic cracking reaction are interrelated and occur simultaneously in commercial FCC riser reactor. To predict accurate behavior of the riser reactor, all these processes need to be modeled. In recent years, many efforts have been made in order to develop a comprehensive mathematical model which can incorporate chemical reaction kinetic, multiphase hydrodynamic and their inter-coupling process [7, 8, 9]. Unfortunately most of published literature didn't pay enough attention to significant influence on the cracking kinetics from multiphase flow hydrodynamic, such as local catalyst concentration, local catalyst velocity and even catalyst average size, which are believed to place significant effect on the reaction kinetics.

The aim of this work is to develop a generic modeling approach which can fully incorporate multiphase flow hydrodynamics with FCC reaction kinetics. The emphasis of this model is to develop a framework to simultaneously simulate the multiphase flow hydrodynamics, cracking reaction and their inter-coupling characteristics in riser reactor. In order to avoid the mathematical complexities, four lump kinetic schemes are being used in this work. This modeling approach opens up a new dimension for making generic models suitable for the analysis and control studies of FCC units. Predictions of the model will compare with the yield pattern of industrial scale plant data reported in literatures.

## **Model description**

The aim of this work is to develop a modeling approach which can incorporate gas-solid multiphase flow hydrodynamics with FCC process with the consideration of the effects of local temperature and catalyst local concentration. In order to simplify the equation derivation, following commonly used assumption were made.

1. It is assumed that the small amount of steam and by-product  $H_2$  are neglected in the mixture of vapor, so all the gas phase will only composed by the components in the four-lump model.
2. it is assumed that, at the riser inlet, hydrocarbon feed comes in contact with the hot catalyst coming from the regenerator and instantly vaporizes (taking away latent heat and sensible heat from the hot catalyst). The vapor thus formed moves upward in thermal equilibrium with the catalyst. Under this assumption, the complex multiphase flow which includes gas, solid and liquid become gas-solid flow.
3. There is no loss of heat from the riser and the temperature of the reaction mixture (hydrocarbon vapors and catalyst) falls only because of the endothermicity of the cracking reactions.
4. Deal gas law is assumed to hold while calculating gas phase density variation on account of molar expansion due to cracking and gas phase temperature.

5. Temperature of gas phase and solids phase is assumed to be identical, and heat and mass transfer resistances are assumed as negligible. In this way, it is much easier to calculate total energy balance inside the riser reactor.
6. In addition, all coke (one of the productions of the cracking reaction) is assumed to attach on the catalyst particles surface and the change of catalyst particles dimension is neglected.

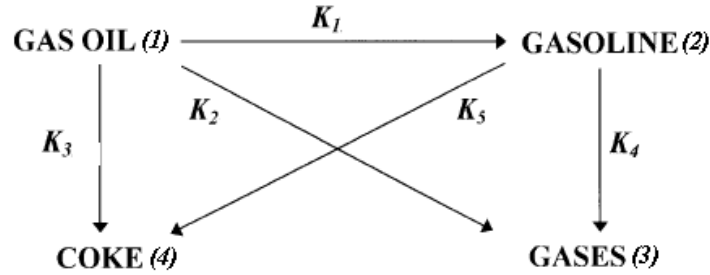


Fig. Four-lump model for gas oil cracking reactions.

Figure 1 gives the typical four-lump model used in our modeling approach. It is assumed that the vacuum gas oil is cracked into the most desired gasoline, by-products of gases and coke. Since the FCC reactor is operating at high temperature, the secondary cracking reaction occurs for gasoline to form coke and gases. There is no inter-reaction between coke and gases.

The solid catalyst and gas oil was fed from the bottom of the riser reactor and the governing equations are discussed below.

The mass balance of gas and solid phase can be described by equation (1) & (2).

$$\text{Solid phase: } \frac{d(\alpha_s \rho_s U_s)}{dz} = (r_3 + r_5)M_4 \quad (1)$$

$$\text{Gas phase: } \frac{d(\alpha_g \bar{\rho}_g U_g)}{dz} = -(r_3 + r_5)M_4 \quad (2)$$

Here the average gas density can be calculated from the ideal gas law as:

$$\bar{\rho}_g = \frac{P \cdot \sum_{i=1}^3 (C_i \cdot M_i)}{RT \sum_{i=1}^3 C_i} \quad (3)$$

The term in the left hand side of the above equations represents the coke mass amount, which is the mass transfer between gas and solid phases when coke deposits on the surface of the catalyst solid. Based on the force balance of each control volume, the momentum equation of solid and gas phase can be derived as,

$$-\frac{dP}{dz} = \bar{\alpha}_g \rho_g g + \bar{\alpha}_g \rho_g u_g \frac{du_g}{dz} + F_D \quad (4)$$

Which shows that, pressure gradient is balanced for gravitational force, acceleration of gas phase and particle-fluid interfacial force between gas and solids.

The momentum equation of solids phase can be expressed based on (5);

$$F_D = \bar{\alpha}_s \rho_s g + G_s \frac{dU_s}{dZ} + \gamma \quad (5)$$

The particle-fluid interfacial force balance for gravitational force, solids acceleration and the solids axial compact momentum due to inter particle collisions. In equation (4),  $F_D$  is the drag force per unit volume. It is obtained by multiplying the drag force on a single particle by the number of particle per unit volume. In this model, Richard-Zaki equation is still utilized to consider the averaged drag force.

$$F_D = \frac{18\mu}{d_s^2} \cdot \frac{\alpha_s}{(1-\alpha_s)^4} \cdot (U_g - U_s) \quad (6)$$

In the solids acceleration regime, the stabilized wake effect becomes too important [24, 24], which leads to reduction in drag force of trailing particles of collision pair. Hence, the modified drag force may be expressed by:

$$F'_D = k_1 F_{D0} \quad (7)$$

$K_1$  is the coefficient of wake effect of the neighboring particles on the particle-fluid interfacial force [22], which is represented as,

$$k_1 = 1 - (1 - A) \exp \left[ B \cdot \left( \sqrt[3]{\frac{\pi}{6\bar{\alpha}_s}} - 1 \right) \right] \quad (8)$$

where

$$A = 1 - \exp(-0.483 + 3.45 \times 10^{-3} \text{Re} - 1.07 \times 10^{-5} \text{Re}^2) \quad (9)$$

$$B = -0.115 - 8.75 \times 10^{-4} \text{Re} - 5.61 \times 10^{-7} \text{Re}^2 \quad (10)$$

Then the corrected drag force should be:

$$F'_D = K_1 \cdot F_D \quad (11)$$

With the assumption of instantaneous vaporization of the Gas Oil, the steady-state continuity equations for the components and lumps in the gas phase can be written as equations (12), (13) and (14);

$$U_g \frac{dC_1}{dz} + C_1 \frac{dU_g}{dz} = -(k_1 + k_2 + k_3)C_1 \quad (12)$$

$$U_g \frac{dC_2}{dz} + C_2 \frac{dU_g}{dz} = mk_1 C_1 - (k_4 + k_5)C_2 \quad (13)$$

$$U_g \frac{dC_3}{dz} + C_3 \frac{dU_g}{dz} = nk_2 C_1 + qk_4 C_2 \quad (14)$$

While the continuity equation for the coke on the catalyst is represented by

$$U_s \frac{dC_4}{dz} + C_4 \frac{dU_s}{dz} = k_3 C_1 + k_5 C_2 \quad (15)$$

where m, n and q stand for the molar expansion of each component, which means, during the cracking process, each molar of reactant will become m, n or q molar of productions.

The temperature dependence of kinetic parameters appearing in Equation (12)~(15) was described by the Arrhenius expression:

$$k_i = \left(\frac{C}{O}\right)_L \cdot \Phi_s k_i \cdot e^{\frac{E_j}{R} \left(\frac{1}{T_0} - \frac{1}{T}\right)} \quad (16)$$

Instead of using a uniform catalyst to oil ratio, a local catalyst to oil ratio, which is directly coupled with local catalyst concentration and reactant concentration, is used in this approach. This local catalyst to oil ratio can be represented as,

$$\left(\frac{c}{o}\right)_L = \frac{\alpha_s \rho_s g}{C_1 M_1} \quad (17)$$

Besides, the catalyst activity coefficient  $\Phi_s$  represents catalyst deactivation because of coke deposition. This coefficient depends on the coke concentration on the catalyst, and following correlation proposed by Pitault et al.[10] will be adopted in this model.

$$\Phi_s = \frac{B+1}{B + \exp(A \cdot wt_{coke} \%)} \quad (18)$$

and

$$wt_{coke} \% = \frac{y_{coke} \cdot W}{m_c} \times 100 \quad (19)$$

Since it has been assumed that the gas phase is always in thermal equilibrium with the solid catalyst all along the riser, and neglecting the heat transfer resistance between the catalyst and gas phases, the evolution of the temperature along the riser is obtained from the enthalpy balance equation,

$$\left(\alpha_s \rho_s C_{p,s} U_s + M_{coke} C_{coke} C_{p,coke} U_s + \alpha_g \bar{\rho}_g \bar{C}_{p,g} U_g\right) \frac{dT}{dz} = -r_1 \cdot \Delta H_r \quad (20)$$

The energy equation represents the combined change of internal energy of gas and solid phase. In summary, for a complete description of this gas-solid flow coupled reaction model, we have totally 10 independent equations ((1), (2), (3),(4), (5), (12), (13), (14), (15), (20)) for totally 10 independent variables ( $\alpha_s, U_s, U_g, C_1, C_2, C_3, C_4, \bar{\rho}_g, T$ ), hence, the problem is closed.

## Results and discussion

In this proposed model, the material balance equations were combined with reaction kinetics and the hydrodynamic model equation to obtain the moles of each lumps at the any height level of the riser, thus, this model can not only predict the yield pattern along the riser height, but also can give the prediction the temperature, pressure, phase velocity and phase concentration along the whole riser. As a preliminary study of the proposed model, we used one operating case reported in literature [11]. The following table 1 gives the basic parameters of the operating conditions.

Table 1 Operating condition of industrial FCC riser reactors

| Parameter                           | Derouin et al.<br>(1997) |
|-------------------------------------|--------------------------|
| Catalyst flux (kg/m <sup>2</sup> s) | 470                      |
| CTO                                 | 5.5                      |
| VGO feed rate (kg/s)                | 85                       |
| Feed temperature (K)                | 650                      |
| Catalyst inlet temperature (K)      | 960                      |
| Riser inside diameter (m)           | 1                        |
| Riser height (m)                    | 35                       |
| Droplet diameter (μm)               | 100                      |

Figure 2 gives the model prediction of axial profile of the gas and solid velocities. It is interesting to notice that, because of the molar expansion of the cracking reaction, the gas velocity keeps increasing along the whole riser, which also causes the increase of the solid velocity due to the gas-solid interacting force.

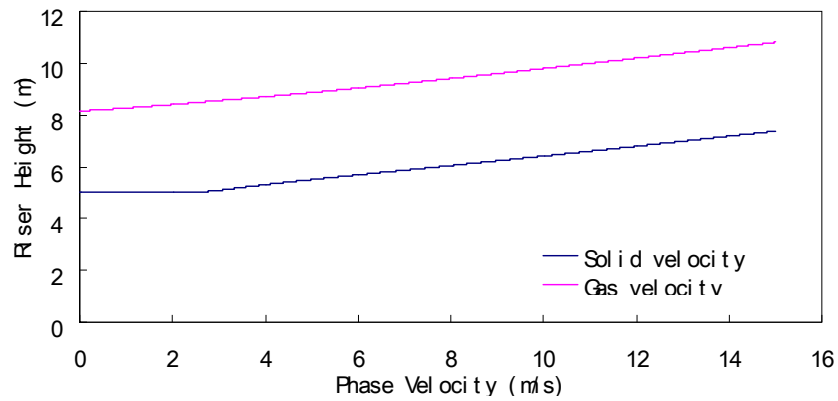


Fig. 2 Model prediction of axial profile of gas and solid velocity

Fig. 3 demonstrates the average gas density change tendency along the riser. With the VGO cracking into Gasoline and gas oil, the averaged gas density also decreases since the averaged molecular weight decrease. However the figure 3 also illustrates the fact that with the increase of the riser height, the average gas density change gradient also decreases. It shows that at the lower part of the riser, the cracking reactions are much more violent than those in the upper part of the riser, which is because that in the lower part of the riser, the temperature, reactant molar concentration and contact area with catalyst all present large values.

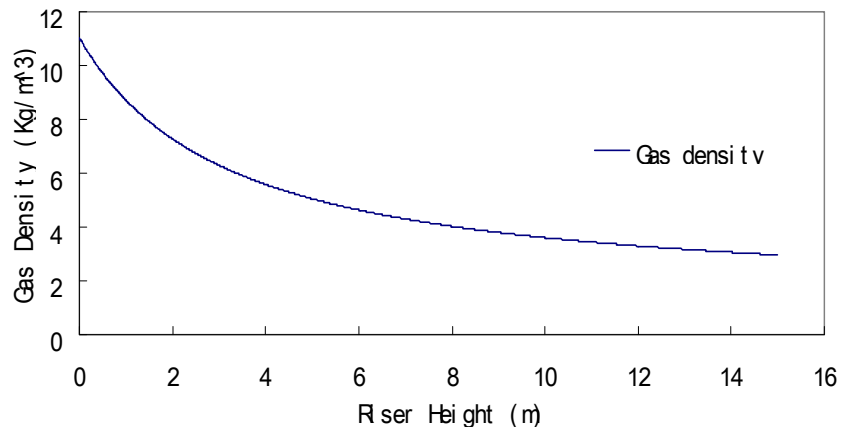


Fig. 3 Model prediction of average gas density

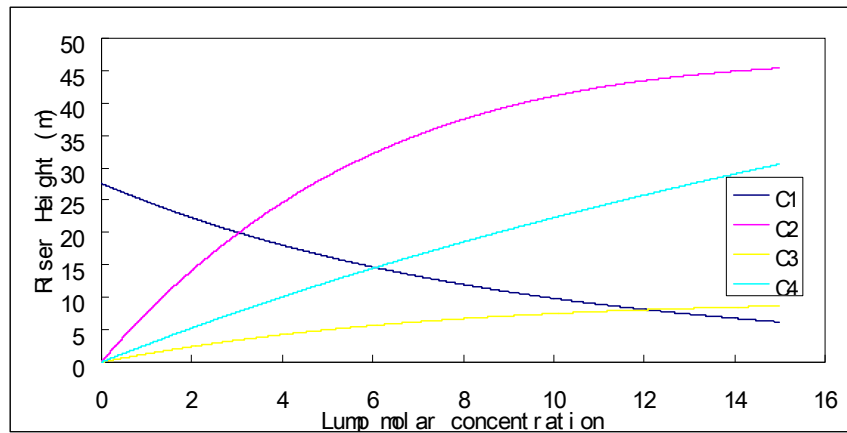


Fig. 4 Model prediction of axial profile of lump molar concentration

In Fig. 4, it shows the model prediction of molar concentration changes of all four lumps. Based on the figure, we can notice with the gas oil keep cracking into other productions, its molar concentration decreases along the riser, and all other three lumps, including gasoline, gases and coke molar concentration increase. Based on the model prediction, we can not only predict the production yield at the exit of riser, but also find the detailed concentration profile at any height of riser.

## Conclusion

A comprehensive mechanistic model is proposed in this paper, which describes the mechanism to consider the inter-coupling between gas-solid flow hydrodynamic with chemical reaction kinetics. The emphasis of this model is to develop a framework to simultaneously simulate the multiphase flow hydrodynamics, cracking reaction and their inter-coupling characteristics in riser reactor. In order to avoid the mathematical complexities, four lump kinetic schemes are being used in this work. This modeling approach opens up a new dimension for making generic models suitable for the analysis and control studies of FCC units. Predictions of the model are compared with the yield pattern of industrial scale plant data reported in literatures.

## Nomenclatures

|                   |   |
|-------------------|---|
| $C_i$             | molar concentration of lumps                              |
| (c/o)             | catalyst oil ratio [g cat/g oil]                          |
| $d_s$             | average size of solid particles                           |
| $F_D$             | drag force  |
| $G$               | flow flux   |
| $k_i$             | rate constant for the cracking of $i$ th pseudo-component |
| $M_i$             | molecular weight of component $i$                         |
| $M_{\text{coke}}$ | molecular weight of coke                                  |
| $P$               | pressure  |
| $r_i$             | rate of disappearance of $i$ th pseudo-component          |
| $R$               | ideal gas constant  |
| $T$               | gas and solid temperature                                 |
| $U_s$             | solid velocity  |
| $U_g$             | gas velocity  |
| $w_{\text{coke}}$ | concentration of coke on catalyst surface                 |

|                |                              |
|----------------|------------------------------|
| $\Delta H_r$   | heat of reaction             |
| $\rho_s$       | solid density                |
| $\bar{\rho}_g$ | average density of gas phase |
| $\alpha_s$     | solid volume fraction        |
| $\alpha_g$     | solid volume fraction        |
| $\varepsilon$  | catalyst porosity            |
| $\gamma$       | Solid momentum dissipation   |
| $\mu$          | viscosity                    |

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