Modelling and simulation of gas-solid flows in riser reactors

S.A. Coutinho¹, J.J.N. Alves¹, W.P. Martignon² & M. Mori³

¹ Department of Chemical Engineering, Federal University of Campina Grande, Brazil
² Superintendence of Oil Shale Industrialization, Petrobras S.A-Brazilian Petroleum Company, Brazil
³ Department of Chemical Process, State University of Campinas, Brazil

Abstract

In the processing of the petroleum, the catalytic cracking unit is of basic importance. In this unit, the fractions of low aggregate value are transformed into fractions of high commercial value. This work presents numerical results of the fluid dynamics of gas-solid flow in risers. The two-phase flow model, which treats the gas and particulate phases as two continuum fluid phases, was used. The effects of the riser geometry and the stress model for particulate phase in the particle concentration were obtained. The predicted results by using the Kinetic Theory of Granular Flows Model (KTGF), which was implemented in the CFX software by the authors, were compared with that obtained by assuming that the particulate phase as inviscid fluid. The results were analyzed in terms of particle concentration in the riser. The results shows that the predicted results obtained by using the KTGF are in better agreement with the experimental information from the literature. The results also show that both mathematical model and geometrical effects are important to predict particle distribution inside the riser.

1 Introduction

The main reactor of the circulating fluidized catalytic cracking (FCC) consists of a vertical tube (riser), which can present characteristics, such as: high particle concentration at the wall and descending movement in the area of high particle concentration that directly affects the conversion and the selectivity in gasoline,
Computational Methods in Multiphase Flow

while is the main product of interest. Those fluid dynamic characteristics are depending of operational conditions and riser geometry. The simulation of the fluid dynamics behavior, and of the reaction kinetic, is of basic importance in the development and optimization of the process. One question is how to predict the fluid dynamic characteristics of the gas solid flows? This work show the answer is: including geometrical effects and using adequate models. In this work the kinetic theory of granular flows (KTGF) model was implemented in the commercial software CFX 4.4, product of AEA TECHNOLOGY and the results obtained shows that geometry and mathematical model affects the predicted particle distribution inside the reactor and are of crucial importance to predict correctly the pattern flows inside the riser reactor.

2 Mathematical model

The two-phase flow model, in which both the gas and particles are treated as two continuums phases, was used in this work. In this model there is one solution field for each phase separately. The mathematical model is based on the mass and momentum conservations. These are the continuity equations and momentum equations for each phase [1].

Gas phase continuity equation

$$\frac{\partial [\rho_g \varepsilon_g v_g]}{\partial t} + \nabla \cdot \left[ \rho_g \varepsilon_g v_g \right] = 0$$  \hspace{1cm} (1)

Gas phase linear momentum

$$\frac{\partial [\rho_g \varepsilon_g v_g]}{\partial t} + \nabla \cdot \left( \rho_g \varepsilon_g (v_g \cdot v_g) - \mu_g^{\text{eff}} (\nabla v_g + (v_g)\nabla) \right) =$$

$$- \varepsilon_g \nabla P_g + \beta_{gs} (v_s - v_g)$$  \hspace{1cm} (2)

In the Equations (1) and (2) \(v_g\) and \(\varepsilon_g\) are the vector velocity and the volumetric fraction of the gas phase, respectively. \(P_g\) is the pressure and \(\rho_g\) is the density of gas. The gas phase effective viscosity, \(\mu_g^{\text{eff}}\), is calculated from the sum of molecular (\(\mu_g^{\text{lam}}\)) and turbulent (\(\mu_g^{\text{turb}}\)) viscosities:

$$\mu_g^{\text{eff}} = \mu_g^{\text{lam}} + \mu_g^{\text{turb}}$$ \hspace{1cm} (3)

The gas phase viscosity, \(\mu_g^{\text{lam}}\), is a physical property of air, and the turbulent viscosity of the gas phase is dependent of the kinetic energy of turbulent movement,
K, and its dissipation rate, \( \varepsilon \), is calculated from the Komogorov-Prandtl relation [2]:

\[
\mu^\text{turb}_g = 0.09 \frac{\rho_g k^2}{\varepsilon^k}
\]  

(4)

The standard \( k-\varepsilon \) model was used. In this model the turbulent kinetic energy and its dissipation rate are calculated from their conservation equations [1]:

\[
\frac{\partial (\varepsilon_g \rho_g k)}{\partial t} + \nabla \cdot [\rho_g \varepsilon_g \mathbf{v}_g k] = \nabla \cdot [\varepsilon_g \Gamma_k \nabla k] + \varepsilon_g \left( \mu^\text{eff}_g \nabla \mathbf{v}_g \cdot \left( \nabla \mathbf{v}_g + (\nabla \mathbf{v}_g)^T \right) - \frac{2}{3} \nabla \cdot \mathbf{v}_g \left( \mu^\text{eff}_g \nabla \cdot \mathbf{v}_g + \rho_g k \right) \right)
\]

(5)

\[
\frac{\partial (\varepsilon_g \rho_g \varepsilon)}{\partial t} + \nabla \cdot [\rho_g \varepsilon_g \mathbf{v}_g \varepsilon] = \nabla \cdot [\varepsilon_g \Gamma_\varepsilon \nabla \varepsilon] - \varepsilon_g C_2 \rho_g \frac{\varepsilon^2}{k}
\]

\[
\varepsilon_g C_1 \left( \mu^\text{eff}_g \nabla \mathbf{v}_g \cdot \left( \nabla \mathbf{v}_g + (\nabla \mathbf{v}_g)^T \right) - \frac{2}{3} \nabla \cdot \mathbf{v}_g \left( \mu^\text{eff}_g \nabla \cdot \mathbf{v}_g + \rho_g k \right) \right)
\]

(6)

The parameters in the \( K-\varepsilon \) model are:

\[
\Gamma_k = \frac{\mu^\text{turb}_g}{\sigma_k}, \quad \Gamma_\varepsilon = \frac{\mu^\text{turb}_g}{\sigma_\varepsilon}, \quad \sigma_k = 1.00, \quad \sigma_\varepsilon = 1.30, \quad C_1 = 1.44, \quad C_2 = 1.92.
\]

Particulate phase continuity equation [1]:

\[
\frac{\partial [\rho_s \varepsilon_s]}{\partial t} + \nabla \cdot [\rho_s \varepsilon_s \mathbf{v}_s] = 0
\]

(7)

Particulate phase linear momentum:

\[
\frac{\partial [\rho_s \varepsilon_s \mathbf{v}_s]}{\partial t} + \nabla \cdot \left( \varepsilon_s \left( \rho_s \varepsilon_s \mathbf{v}_s \mathbf{v}_s - \mu^\text{eff}_s \left( \nabla \mathbf{v}_s + (\nabla \mathbf{v}_s)^T \right) \right) \right) =
\]

\[
- \varepsilon_s \nabla P_g + \beta_g \left[ \mathbf{v}_g - \mathbf{v}_s \right] + \nabla \cdot \left( - P_s + \left( \frac{\varepsilon_s - 2 \mu_s}{3} \right) (\nabla \cdot \mathbf{v}_s) \right)
\]

(8)
202 Computational Methods in Multiphase Flow

In the Equations (7) and (8) \( \mathbf{v}_s \) and \( \varepsilon_s \) are the vector velocity and the volumetric fraction and the pressure of the particulate phase, respectively. \( \rho_s \) is the density of particles.

In the KTGF the transport properties of the particulate phase are dependent on the granular temperature \( (\theta = 1/3(\text{fluctuating component of particle velocity})^2) \) for which a transport equation is derived from the kinetic theory of granular flows [3][4][5][6]:

\[
\frac{3}{2} \left[ \frac{\partial (\varepsilon_s \rho_s \theta_s)}{\partial t} + \nabla \left[ \rho_s \varepsilon_s \mathbf{v}_s \theta_s \right] \right] = \nabla \left[ \Gamma \nabla \theta_s \right] + \tau_s : \nabla \mathbf{v}_s - \gamma_2
\]  

(9)

In the KTGF,

\[
\tau_s = \left( -P_s + \left( \varepsilon_s - \frac{2\mu_s}{3} \right) \nabla \cdot \mathbf{v}_s \right) I + \mu_s \left( \nabla \mathbf{v}_s + (\nabla \mathbf{v}_s)^T \right)
\]  

(10)

is the tensor stress in particulate phase.

\[
\gamma_2 = 3 \left( 1 - e^2 \right) \varepsilon_s^2 \rho_s \varepsilon_s \left[ \frac{4}{d_p} \sqrt{\frac{\theta_s}{\pi}} - \nabla \cdot \mathbf{v}_s \right] \theta_s
\]  

(11)

is the dissipation rate of pseudo-thermal energy - kinetic energy of the fluctuating motion of the particulate phase - due to particle-particle collisions, where “\( e \)” is the coefficient of restitution particle-particle, that have its value between zero, for perfectly inelastic collisions, and one, for perfectly elastic collisions. \( d_p \) is the particle diameter.

\[
P_s = \varepsilon_s \rho_s \left[ 1 + 2(1 + e) \varepsilon_s \rho_0 \right] \theta_s
\]  

(12)

is the effective pressure on the particle phase due to particle-particle contact,

\[
g_0 = \frac{3}{5} \left[ 1 - \left( \frac{\varepsilon_s}{\varepsilon_{s,\text{max}}} \right)^{1/3} \right]^{-1}
\]  

(13)

is the radial distribution function, where \( \varepsilon_{s,\text{max}} \) is the maximum particle concentration (packed bed).
\[ \xi_s = \frac{4}{3} \varepsilon_s^2 \rho_s d_p g_0 (1 + e) \sqrt{\frac{\theta_s}{\pi}}, \] (14)

is the bulk viscosity of the particle phase (or second coefficient of viscosity of the particulate phase),

\[ \mu_s = \frac{10 \rho_s d_p}{96(1 + e) g_0} \left[ 1 + \frac{4}{5} (1 + e) g_0 \varepsilon_s \right]^2 \sqrt{\pi \theta_s} + \frac{4}{5} \varepsilon_s^2 \rho_s d_p g_0 (1 + e) \sqrt{\frac{\theta_s}{\pi}}, \] (15)

is the effective viscosity of the particulate phase, and

\[ \Gamma_T = \frac{150 \rho_s d_p}{384(1 + e) g_0} \left[ 1 + \frac{6}{5} (1 + e) g_0 \varepsilon_s \right]^2 \sqrt{\pi \theta_s} + 2 \varepsilon_s^2 \rho_s d_p g_0 (1 + e) \sqrt{\frac{\theta_s}{\pi}}, \] (16)

is the diffusion coefficient of pseudo-thermal energy.

If the particle phase is assumed to be inviscid all parameters dependent of the granular temperature are zero.

The coefficient of momentum transfer between the gas and particulate phases, \( \beta \), was calculated from [7]:

\[ \beta = \left( \frac{17.3}{Re} + 0.336 \right) \frac{\rho_g |v_g - v_s| \varepsilon_s}{d_p \varepsilon_s^{-2.8}} \] (17)

2.1 Boundary conditions

Except for pressure that is obtained by extrapolation from the flow domain, the following boundary conditions were specified: 1) at the inlet all variables have their values specified; 2) at the tube center the symmetry condition (only for symmetric case); 3) at the exit the continuity condition (derivation zero with relation to \( z \)); and 4) at the wall the non-slip condition was specified for the two velocity components of the gas phase. The turbulent kinetic energy and its dissipation rate are calculated from the well-known wall functions [1]. For the particulate phase the impermeable wall condition, \( \varepsilon_{s,w} = 0 \), is applied for the normal velocity component. Using the inviscid model for particulate phase the slip condition was applied to parallel velocity component of the particulate phase. Using KTGF model, the parallel velocity component is obtained from a balance of momentum transfer between the particles and the wall [8]:

\[ -\mu_s \frac{\partial v_{s,n}}{\partial \eta} \bigg|_W = \frac{\Phi_w \sqrt{3} \pi \rho_s \varepsilon_s \theta^{1/2} v_{s,\phi} \left| v_{s,n} \right|_W}{6 \varepsilon_{s,max} \left[ 1 - \left( \frac{\varepsilon_s}{\varepsilon_{s,max}} \right)^{1/3} \right]^{1/3}} \] (18)
204 Computational Methods in Multiphase Flow

Where \( \eta \) is the coordinate normal to the wall, \( \phi \) is the coordinate parallel to the wall, and \( \Phi_w \) is the friction factor particle-wall, which have its value between 0 and 1. The granular temperature at wall is obtained from the flow of the pseudo-thermal energy to the wall - balance at wall - ,

\[
-\Gamma \frac{\partial \theta}{\partial \eta} \bigg|_w = \gamma_w - \nu_{s, \phi} \tau_{\phi 2} \bigg|_w ,
\]

(19)

Where,

\[
\gamma_w = \frac{\sqrt{3\pi} \varepsilon_s \rho_s \theta^{3/2} \left(1 - \varepsilon_w^2\right)}{4 \varepsilon_{s, \text{max}} \left[1 - \left(\varepsilon_s / \varepsilon_{s, \text{max}}\right)\right]} ,
\]

(20)

is the dissipation rate of pseudo-thermal energy due to inelasticity of the particle-wall collisions.

In case of using the inviscid model for particle phase, a null derivative was applied at wall to obtain the particle concentration and in case of using the KTGF model, the particle concentration at the wall is calculated from a radial momentum balance at the wall, for the fully developed region:

\[
\frac{\partial}{\partial \eta} \left( \varepsilon_s \theta \right) \bigg|_w - \varepsilon_s \theta \bigg|_w = \gamma \frac{\partial \varepsilon_s}{\partial \eta} \bigg|_w
\]

(21)

The right hand side term in the equation 16 limits the particle concentration to the maximum value physically possible, were \( \gamma = \gamma(\varepsilon_s, T) \) is obtained by applying the limit of \( \varepsilon_{s, \text{max}} \rightarrow \varepsilon_{s, \text{max}} \) when \( \theta \bigg|_w \rightarrow 0 \) [9].

3 Numerical method

We have one system of non-linear, differential partial equations that can be solved numerically. In this work the software CFX 4.4 that uses the finite volume method (FVM) with collocated grid was used for discretization of the system of equations. The momentum conservation equation for each phase is used to calculate the velocity components of each phase. In the finite volume method the calculation domain is divided into non-overlapping finite volumes in which the conservation equations are integrated [1][10][11].

4 Results

The CFX 4.4 software was used to simulate the gas-solid flow. The software used has not the KTGF in the full version implemented. The KTGF like described in the mathematical model was implemented in the CFX 4.4 software.
and results obtained by using the KTGF (account for particle-particle interactions), were compared with that obtained by assuming the particulate phase as inviscid phase (no particle-particle interactions) for a symmetrical riser. Also, using the inviscid model for particulate phase results obtained for asymmetrical and symmetrical riser were compared to verify the effect of riser geometry. The characteristics of the studied case are given in table 1 [12]. Experimental data from the literature shows a radial distribution of particle concentration, that, for this studied case, at the axial position of 9 m above the entrance, the volumetric particle fraction change from 2% at the centerline to approximately 30% near the wall [12].

Table 1: characteristics of the system.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>R, m</td>
<td>0.152</td>
</tr>
<tr>
<td>H, m</td>
<td>10.0</td>
</tr>
<tr>
<td>v_{c0}, m/s</td>
<td>3.78</td>
</tr>
<tr>
<td>( \rho_p ), kg/m^3</td>
<td>1.22</td>
</tr>
<tr>
<td>( \mu_p ), kg/m.s</td>
<td>4.0x10^{-3}</td>
</tr>
<tr>
<td>( \varepsilon_\phi )</td>
<td>0.0218</td>
</tr>
<tr>
<td>v_{c0}, m/s</td>
<td>2.62</td>
</tr>
<tr>
<td>( \rho_x ), kg/m^3</td>
<td>1714</td>
</tr>
<tr>
<td>d_{p}, \mu m</td>
<td>76</td>
</tr>
<tr>
<td>( \varepsilon_{s, max} )</td>
<td>0.65</td>
</tr>
<tr>
<td>( \varphi )</td>
<td>1.0</td>
</tr>
<tr>
<td>e</td>
<td>1.0</td>
</tr>
<tr>
<td>e_w</td>
<td>0.9</td>
</tr>
<tr>
<td>( \Phi )</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Figure 1: Particle distribution predicted with inviscid model for particle phase and asymmetrical riser (3D).

Figure 1 presents predicted particle distribution inside the riser reactor when the inviscid model was used for particulate phase (riser 3D). The results shown a non uniform and asymmetrical profile of particle concentration inside the riser. The maximum value of volumetric fraction of particles predicted was equal to approximately 12 % at wall and near the riser entrance.
206 Computational Methods in Multiphase Flow

Figure 2 presents predicted particle distribution inside the riser reactor when the inviscid model was used for particulate phase (riser 2D). The results show a flat profile of particle concentration inside the riser and the maximum value of volumetric fraction of particles predicted was equal to 2.18% near the riser entrance.

Figure 2: Particle distribution inside the symmetrical riser by using the inviscid model for particulate phase.
Figure 3 shows the particle distribution predicted when the KTGF model was used to calculate particle phase effective viscosity and particle-particle interactions are account (riser 2D). We can see that, when the KTGF was used to estimate effective stress between particles, the predicted results are, qualitatively, in better agreement with the experimental data that the results obtained when the inviscid model was used. In this case a maximum of particle concentration of 59% was predicted at wall and near the riser entrance as indicated in Figure 3.

5 Conclusions

The results shown that the KTGF, which was implemented in the CFX 4.4 software by the authors, is a model able to predict the gas solid patterns flow in risers. The results also shown that if the particle-particle iterations inside the riser are not considered in the model, bad results are predicted when compared with experimental observations of the literature. The results also show that
geometrical effects are important in particle distribution, but the non-uniform particle distribution is consequence principally of the stress particle-particle inside the riser, while the asymmetrical distribution is consequence of riser asymmetry.

References