Modular Simulation of Fluidized Bed Reactors

By Rouzbeh Jafari, Rahmat Sotudeh-Gharebagh, and Navid Mostoufi*

Simulation of chemical processes involving nonideal reactors is essential for process design, optimization, control and scale-up. Various industrial process simulation programs are available for chemical process simulation. Most of these programs are being developed based on the sequential modular approach. They contain only standard ideal reactors but provide no module for nonideal reactors, e.g., fluidized bed reactors. In this study, a new model is developed for the simulation of fluidized bed reactors by sequential modular approach. In the proposed model the bed is divided into several serial sections and the flow of the gas is considered as plug flow through the bubbles and perfectly mixed through the emulsion phase. In order to simulate the performance of these reactors, the hydrodynamic and reaction submodels should be integrated together in the medium and facilities provided by industrial simulators to obtain a simulation model. The performance of the proposed simulation model is tested against the experimental data reported in the literature for various gas-solid systems and a wide range of superficial gas velocities. It is shown that this model provides acceptable results in predicting the performance of the fluidized bed reactors. The results of this study can easily be used by industrial simulators to enhance their abilities to simulate the fluidized bed reactor properly.

1 Introduction

Fluidized beds have been used as industrial reactors in the processes involving catalytic and gas-solid reactions for more than 50 years. In spite of the extensive research efforts on fluidization during these years, many features of such reactors which strongly influence their performance have only recently begun to be understood. The uncertainties associated with scale-up and modeling of fluidized beds is a significant obstacle in the widespread use of fluidized beds in chemical industries [1].

Two types of phenomena, i.e., physical and chemical, coexist in the fluidized beds. The physical phenomenon corresponds to the bed hydrodynamics, i.e., properties of bubble and emulsion phases. The chemical phenomenon corresponds to the chemical changes occurring in each phase. In order to model a fluidized bed properly, one has to consider two submodels describing these two phenomena: the hydrodynamic submodel which explains the physical phenomena, and the reaction submodel which describes the chemical reactions occurring in the bed.

Fluidized beds are hydrodynamically more complex than other gas-solid contactors, mainly fixed and moving bed reactors. Thus, it is important to understand and characterize the parameters influencing the hydrodynamics of fluidized beds [1,2]. Various hydrodynamic models are presented in the literature. Hydrodynamic models are divided into three general categories, i.e., single-, two- and three-phase models. A large number of these models are developed based on the two-phase concept of fluidization. In this category of models, the fluidized bed is divided into two sections, i.e., bubble phase (rich in gas) and emulsion phase (rich in solids). Early two-phase models employed quite simple assumptions, such as the existence of solid-free bubbles and the emulsion phase to be at minimum fluidization condition [1]. However, the existence of solid particles in bubbles has been shown both experimentally [3,4] and theoretically [5,6]. The emulsion phase also does not remain at the minimum fluidization condition and may contain a higher amount of gas at higher gas velocity [4,7]. A fluidized bed may operate at several fluidization regimes, mainly bubbling, turbulent and fast fluidization regimes. Most of the hydrodynamic models available in the literature are applicable only to one of these regimes. Recently, there have been few attempts to develop hydrodynamic models which could be employed at various fluidization regimes [8–10].

Numerous methods have been introduced in the literature for fluidized bed reactor modeling and simulation. Weiss et al. [11] simulated a fluidized reactor by dividing it into 11 serial blocks, each of them being a continuously stirred tank reactor (CSTR) for both gas and solid phases. Basu et al. [12] developed a model in which a plug flow regime for both the gas and solids is assumed. Lee and Hyppanen [13] presented a model which considers the CSTR and plug flow reactor (PFR) for gas phase and solid phase in the reactor riser, respectively. Sotudeh-Gharebagh et al. [14] simulated the circulating fluidized bed combustor by ASPEN PLUS by combining some standard blocks and user-written kinetic subroutine. Alizadeh et al. [15] simulate the polymerization fluidized bed

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reactor using CSTRs in series. El-Halwagi et al. [16] also presented the three-phase model for fluidized bed reactor simulation by PFRs and CSTRs for bubble, cloud and emulsion phases. These models either have not yet been implemented in the industrial process simulation programs or have used simplified hydrodynamic assumptions. The hydrodynamics of such reactors become very important when highly exothermic reactions take place in the reactor.

Various process simulation programs, such as ASPEN PLUS, PRO/II, HYSYS, CHEMCAD, DESIGN II and INDISS, are available and are employed for process simulation purposes by industrial entities. All these programs have been developed based on the sequential modular approach, i.e., they consist of different standard modules which could be combined together to represent the whole process. These process simulators are generally not strong in reactor modules and only contain standard, ideal reactors, such as PFR and CSTR. In spite of their vast use in the chemical industries, a fluidized bed reactor module is not offered in these programs.

In this work, a fluidized bed reactor model is presented by combining the standard reactor modules available in the process simulation programs. These standard modules have to be combined in a logical way to represent the reality in the fluidized bed reactors. Furthermore, the model has to be easily applicable in all process simulation programs.

2 Model Implementation

A fluidized bed reactor is a nonideal reactor, i.e., it cannot be considered as either a PFR or a CSTR. It has been tried by some researchers to model such nonideality by the tanks-in-series model (e.g., [11,15,16]). However, these models ignore the main aspect of gas-solid fluidization, i.e., coexistence of bubble and emulsion phases in the reactor. The movement of gas through the bubbles in the fluidized bed could be considered as plug flow while it could be considered as completely mixed in the emulsion phase. Therefore, while the whole reactor could be axially divided into several sections, each section itself may be considered to be consisting of two ideal reactors: a PFR to represent the gas flow through the bubbles and a CSTR to represent the gas flow through the emulsion. Such an approach is closer to the reality than the previous models which consider each section as a CSTR. A schematic diagram of the \( n \)th stage of the proposed model is illustrated in Fig. 1. It is assumed that first the reaction takes place in each reactor of each stage and then the mass transfer occurs at the exit of the reactors between the effluents.

Additional assumptions considered in developing the model are:
- The bubbles reach their equilibrium size quickly above the distributor. Therefore, the bubble diameter is assumed to be constant along the bed height.
- The hydrodynamics of both phases could be characterized by the dynamic two-phase (DTP) model [9]. It has been shown that this model could estimate the hydrodynamic parameters of the fluidized bed properly, compared to other hydrodynamic models [17–19].
- The reactor operates at isothermal conditions. As a result, the hydrodynamic parameters of the bed, physical properties of components and reaction rate constants are considered to be constant throughout the bed.
- Radial gradients within the bed are neglected.

As mentioned before, the bed is divided into a number of equal-volume stages, each consisting of two phases, i.e., bubble and emulsion. The generalized steady-state mass balance equation for either bubble or emulsion phases in a reacting stage is:

\[
\frac{\text{bulk flow in}}{\text{bulk flow out}} - \frac{\text{mass transfer}}{\text{dissappearance by chemical reaction}} = 0 \quad (1)
\]

By applying Eq. (1) to the system shown in Fig. 1 for the reactant \( A \), the mass balances in the \( n \)th stage for bubble and emulsion phases are given by the following equations\(^1\):

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\(^1\) List of symbols at the end of the paper.
Bubble phase:
\[ C_{Ab(i-1)} U_b A_b - A_b \varepsilon_b \int_{z_i}^{z_{i-1}} r_{A(i)} dz - K_{be} (C_{Ab(i)} - C_{Ab(i-1)}) V_{b(i)} - C_{Ab(i)} U_b A_b = 0 \]

Emulsion phase:
\[ C_{Ae(i-1)} U_e A_e - r_{A(i)} V_{CSTR(i)} + K_{be} (C_{Ab(i)} - C_{Ab(i-1)}) V_{e(i)} \left( \frac{\delta}{1-\delta} \right) - C_{Ae(i)} U_e A_e = 0 \]

The hydrodynamics and mass transfer coefficients needed to solve these equations are given in Tab. 1. Number of divisions, \( n \), in these equations is the parameter of the model that has to be determined from the experimental data.

### 3 Results and Discussion

As has been mentioned in the previous section, the bed height is divided into a number of divisions with equal

<table>
<thead>
<tr>
<th>Table 1. Hydrodynamic and mass transfer equations of the model.</th>
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<tbody>
<tr>
<td><strong>Bubble diameter</strong> [25]</td>
</tr>
<tr>
<td>[ D_b = D_{bo} - (D_{bn} - D_{bo}) \exp \left( -0.15 h_{bf} \frac{A_{Dh}}{D_f} \right) ]</td>
</tr>
<tr>
<td>[ D_{bo} = 0.8713 \left( \frac{A(U_o - U_{mf})}{N_D} \right)^{0.4} ]</td>
</tr>
<tr>
<td>[ D_{bn} = 1.6377 \left( A(U_o - U_{mf}) \right)^{0.4} ]</td>
</tr>
<tr>
<td><strong>Bubble velocity</strong> [26]</td>
</tr>
<tr>
<td>[ U_b = U_o - U_e + u_{br} ]</td>
</tr>
<tr>
<td>[ u_{br} = 0.711 \sqrt{gD_b} ]</td>
</tr>
<tr>
<td><strong>Bubble to emulsion mass transfer coefficient</strong> [1]</td>
</tr>
<tr>
<td>[ \frac{1}{K_{be}} = \frac{1}{K_{ce}} + \frac{1}{K_{bc}} ]</td>
</tr>
<tr>
<td>[ K_{ce} = 6.77 \left( \frac{D_{Ah} u_{br} e_c}{D_b} \right) ]</td>
</tr>
<tr>
<td>[ K_{bc} = 4.5 \left( \frac{U_e}{D_b} \right) + 5.85 \left( \frac{D_{Ah}}{D_b} \right)^{0.5} \left( \frac{g}{D_b} \right)^{0.25} ]</td>
</tr>
<tr>
<td><strong>Bubble phase fraction</strong> [9]</td>
</tr>
<tr>
<td>[ \delta = 1 - A_{f(1)} - A_{f(2)} \exp \left( \frac{-(U_o - U_{mf})}{A_{f(3)}} \right) ]</td>
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<tr>
<td><strong>Bubble phase voidage</strong> [9]</td>
</tr>
<tr>
<td>[ \varepsilon_b = A_{void-b(1)} + A_{void-b(2)} \exp \left( \frac{-(U_o - U_{mf})}{A_{void-b(3)}} \right) ]</td>
</tr>
<tr>
<td><strong>Emulsion phase voidage</strong> [9]</td>
</tr>
<tr>
<td>[ \varepsilon_e = A_{void-e(1)} + A_{void-e(2)} \exp \left( \frac{-(U_o - U_{mf})}{A_{void-e(3)}} \right) ]</td>
</tr>
<tr>
<td><strong>Volume of the ( i )th stage</strong></td>
</tr>
<tr>
<td>[ V_{(i)} = \frac{V_i}{n} ]</td>
</tr>
<tr>
<td><strong>Volume of bubble phase in each stage</strong></td>
</tr>
<tr>
<td>[ V_{b(i)} = V_{(i)} \delta ]</td>
</tr>
<tr>
<td><strong>Volume of emulsion phase in each stage</strong></td>
</tr>
<tr>
<td>[ V_{e(i)} = V_{(i)} (1 - \delta) ]</td>
</tr>
<tr>
<td><strong>Volume of PFR in each stage</strong></td>
</tr>
<tr>
<td>[ V_{PFR(i)} = V_{b(i)} \varepsilon_b ]</td>
</tr>
<tr>
<td><strong>Volume of CSTR in each stage</strong></td>
</tr>
<tr>
<td>[ V_{CSTR(i)} = V_{e(i)} \varepsilon_e ]</td>
</tr>
</tbody>
</table>
volumes. This number is a parameter of the model developed in this work and has to be determined from the experimental data. Several sets of the experimental reaction data carried out in fluidized bed reactors are available in the literature. Five series of experimental data sets are employed in this work. These data are as follows:

- Grace and Sun [20] carried out ozone decomposition reaction in a fluidized bed. Air was used as the fluidizing gas and the reaction is first order with respect to ozone.
- Fryer and Potter [21] carried out ozone decomposition reaction in a fluidized bed. Air was used as the fluidizing gas and the reaction is first order with respect to ozone.
- Shen and Johnstone [22] carried out catalytic oxidation of nitrous oxide in excess of oxygen. Oxygen was the fluidizing gas and the reaction is first order with respect to nitrous oxide.
- Massimilla and Johnstone [23] carried out oxidation of ammonia in excess of oxygen. Oxygen was the fluidizing gas and the reaction is first order with respect to ammonia.
- Heidel et al. [24] carried out ethylene hydrogenation in excess of hydrogen. Hydrogen was the fluidizing gas and the reaction is first order with respect to ethylene.

All reactions considered in this work are first order with respect to one of the reactants. Thus, the kinetics used in this work can be described by:

$$-r_A = KC_A$$

(4)

The properties and operating conditions of these data are given in Tab. 2. These data sets are employed in this work to estimate the number of divisions of the fluidized reactor at different operating conditions.

In each case, the bed height is initially divided into a number of equal zones. The model equations (Eqs. (2) and (3)) are then solved and the results of such solution were compared with the corresponding experimental data. The number of divisions which would best fit the experimental data was chosen to be the total number of stages in that case. It was found that in the case of slower reactions and higher gas velocities a larger number of stages are required to simulate the fluidized bed reactor accurately as compared to the faster reactions and lower gas velocities for which the reactor could be simulated even with a single stage. In fact, a higher gas velocity enhances the solids mixing and also makes the gas pass faster through the bed, thus, the whole bed could be simulated as a smaller number of stages shown in Fig. 1. Similarly, a smaller number of stages would be needed if a faster reaction is to be carried out in the reactor. Based on this discussion, it is proposed that the number of stages is a function of the following dimensionless number:

$$J = \frac{HaU_0}{U_{mf}}$$

(5)

A faster reaction (higher Ha) and/or higher superficial gas velocity (higher $U_0$) both have the same effect on the newly defined dimensionless number (higher J) and would result in a smaller number of stages to be employed in the simulation (smaller n). The minimum fluidization velocity is added to Eq. (5) to represent the effect of the properties of the solids in the number of stages in the proposed model. The values of the number of stages obtained at different operating conditions are summarized in Tab. 3 as a function of the dimensionless number J.

**Table 3. Number of stages.**

<table>
<thead>
<tr>
<th>$J$</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>$J &lt; 11.1$</td>
<td>1</td>
</tr>
<tr>
<td>11.1 $J &lt; 5.62$</td>
<td>2</td>
</tr>
<tr>
<td>5.62 $&lt; J &lt; 0.63$</td>
<td>3</td>
</tr>
<tr>
<td>$0.63 &lt; J$</td>
<td>4</td>
</tr>
</tbody>
</table>

In order to determine the validity of a hydrodynamic model, it is necessary to check it at the circumstances that the hydrodynamics would be predominant. The reactions considered in this work could be considered as fast reactions. In such a condition, the performance of the reactor is more influenced by the hydrodynamics than the kinetics. In fact, since the extent of the mixing in the reactor is represented by its hydrodynamics, the hydrodynamics of the bed becomes the limiting step in the conversion of the reactant(s) in the case of fast reaction rate. Therefore, the performance of the reactor would be
mainly characterized by its hydrodynamics at the conditions of the experimental data employed in this work.

Results of the model presented in this work are compared with the experimental conversion of ozone in the fluidized bed reactor reported by Grace and Sun [20] at different superficial gas velocities and various reaction rate constants in Fig. 2. The parity plot of calculated against experimental conversions is also given in Fig. 3. It could be seen in these figures that the proposed model is in good agreement with the experimental results in predicting the fluidized bed reactor performance for different reaction rate constants and a wide range of superficial gas velocities.

![Figure 2](image1.png)  
**Figure 2.** Fluidized bed reactor conversion as a function of superficial gas velocity at different reaction rate constants (E: experimental [20], C: calculated).

![Figure 3](image2.png)  
**Figure 3.** Comparison of experimental data of Grace and Sun [20] with calculated results employing sequential modular approach.

Results of the model presented in this work are compared with the data reported by Fryer and Potter [21] in terms of the conversion of ozone at different reaction rate constants and various superficial gas velocities in Fig. 4. The parity plot of calculated against experimental conversions is also given in Fig. 5. Similar to the previous case, these figures show that there is a good agreement between the proposed model and the experimental results in predicting the fluidized bed reactor performance for different reaction rate constants and superficial gas velocities. However, by increasing the reaction rate constant, the model prediction deviates from the experimental data. According to the discussions made earlier, in the case of fast reactions the hydrodynamics becomes the limiting step in characterizing the reactor performance. In this case, the deviation could be contributed to the fact that the constants of the DTP model are evaluated for a particle which is slightly different from the catalyst employed by Fryer and Potter [21] in terms of particle properties, even though both are Geldart B particles.

The conversions calculated based on the model developed in this work are compared with the data reported by Shen and Johnston [22], Massimilla and Johnston [23] and Heidel et al. [24] in the parity plots given in Figs. 6, 7 and 8, respectively. As illustrated in these figures, the agreement between the model
prediction and experimental data is satisfactory. However, the under- or overprediction of the conversion in some cases shown in these figures should be mainly attributed to the fact that the number of stages, \(n\), may assume only integer values.

### 4 Conclusions

A new hydrodynamic model is developed for fluidized bed reactors based on the sequential modular approach. The proposed model is a combination of the tanks-in-series model for nonideal reactors and the two-phase concept of fluidization. According to this model, the fluidized bed is divided into a number of equal-volume stages in which the gas in bubbles moves as plug flow and the gas in emulsion is completely mixed. The number of stages was evaluated from the data available in the literature and found to be a function of \(Ha\), \(U_0\) and \(U_{mic}\). Since the proposed model consists only of the ideal reactors, which are available in the commercial process simulation programs, it is possible to introduce the nonideal fluidized bed reactors in such programs by this model. The model is easy to use in all process simulation programs which are also developed based on the sequential modular approach. The comparison between the model results and the experimental data indicates that the proposed model is able to predict the real performance of the fluidized bed reactors satisfactorily over a wide range of superficial gas velocities (i.e., bubbling and turbulent regimes of fluidization) both Geldart A and Geldart B types of particles. A more reliable prediction of the reactor performance would be achieved if the parameters of the DTP model are evaluated specially for the catalyst employed in the process.

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### Symbols used

- \(a_i\) [m\(^2\)] interphase area per unit volum
- \(A\) [m\(^2\)] cross-sectional area
- \(A_{k(1)}\) constant of dynamic two-phase model
- \(A_{k(2)}\) constant of dynamic two-phase model
- \(A_{k(3)}\) constant of dynamic two-phase model
- \(A_{vol-kr(1)}\) constant of dynamic two-phase model
- \(A_{vol-kr(2)}\) constant of dynamic two-phase model
- \(A_{vol-kr(3)}\) constant of dynamic two-phase model
\( A_{\text{Void-d}} \) [-] constant of dynamic two-phase model
\( A_{\text{Void-e}} \) [-] constant of dynamic two-phase model
\( A_{\text{Void-f}} \) [-] constant of dynamic two-phase model
\( C_A \) [kmol/m³] concentration of component A
\( D_{AB} \) [m²/s] diffusion coefficient
\( D_b \) [m] bubble mean diameter
\( D_{b0} \) [m] bubble initial diameter
\( D_{bm} \) [m] bubble maximum diameter
\( d_p \) [m] particle diameter
\( d_t \) [m] reactor diameter
\( G \) [m/s²] acceleration of gravity
\( H \) [m] bed height
\( H_a \) [-] Hata number \((KD_{AB}^{0.5}d_b/K_{bc})\)
\( h_{rif} \) [m] bed height at minimum fluidization condition
\( J \) [-] dimensionless number \((HaU_b/U_{mf})\)
\( K \) [s⁻¹] reaction constant
\( K_{bc} \) [s⁻¹] bubble to cloud mass transfer coefficient
\( K_{bc} \) [s⁻¹] bubble to emulsion mass transfer coefficient
\( K_{ee} \) [s⁻¹] cloud to emulsion mass transfer coefficient
\( N_D \) [-] number of orifices in unit area of grid
\( N \) [-] total number of stages
\( P \) [P] reactor operating pressure
\( r_A \) [kmol/m³s] reaction rate based on component A
\( T \) [K] reactor operating temperature
\( U_b \) [m/s] bubble velocity
\( \theta_b \) [m/s] bubble rise velocity
\( U_e \) [m/s] superficial velocity at onset of fluidization
\( U_e \) [m/s] emulsion gas velocity
\( U_{mf} \) [m/s] minimum fluidization velocity
\( U_0 \) [m/s] superficial gas velocity
\( V_b \) [m³] bubble phase volume
\( V_{CSTR} \) [m³] CSTR volume
\( V_c \) [m³] emulsion phase volume
\( V_{PFR} \) [m³] PFR volume

Greek symbols
\( \rho_s \) [kg/m³] solid density
\( \epsilon_b \) [-] bubble phase voidage
\( \epsilon_e \) [-] emulsion phase voidage
\( \delta \) [-] bubble phase fraction

Subscripts
B bubble phase
E emulsion phase
I section no.

References