

MATHEMATICAL MODELING OF COAL-FIRED  
FLUIDIZED BED COMBUSTORS

by

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## Mathematical Modeling of Coal-Fired Fluidized Bed Combustors

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This article compares two models published in the literature. [Rajan and Wen, *AIChE J.* 26:642-655 (1980); Preto, *Studies and Modeling of Atmospheric Fluidized Bed Combustion of Coal*, Ph.D. thesis, Queen's University at Kingston, 1986]. Their performance is tested against experimental data for different operating conditions. The importance of the different assumptions is analyzed and discussed. For the conditions analyzed in the present article the model of Rajan and Wen more closely follows the experimental trends. However, some deficiencies were detected and an improved version of this model is presented. Special attention is devoted to the computation of the carbon loading and bed expansion ratio.

### NOMENCLATURE

$A_t$	cross section area of the bed ( $m^2$ )
$A_0$	area of the cross section by each nozzle opening ( $m^2$ )
$D_b$	bubble diameter (m)
$D_g$	gas diffusivity ( $m^2 s^{-1}$ )
$D_t$	bed diameter (m)
$g$	acceleration due to gravity ( $m s^{-2}$ )
$h$	height above the distributor (m)
$K_{be}$	mass transfer coefficient ( $s^{-1}$ )
$U_b$	absolute bubble velocity ( $m s^{-1}$ )
$U_e$	velocity of air through the emulsion phase ( $m s^{-1}$ )
$U_{mf}$	minimum fluidization velocity ( $m s^{-1}$ )
$U_0$	superficial velocity ( $m s^{-1}$ )
$V_0$	volumetric flow rate from a single nozzle opening ( $m^3 s^{-1}$ )

### Greek

$\epsilon_b$	bubble fraction in the bed
$\epsilon_c$	fraction of cloud-wake and bubble in the bed
$\epsilon_e$	void fraction in the emulsion phase

$\epsilon_{mf}$  void fraction at minimum fluidization

### INTRODUCTION

Fluidized bed combustion is now generally recognized as a clean and inexpensive method for coal combustion, capable of efficiently burning a wide variety of solid fuels in an environmentally acceptable manner. Research on fluidized bed combustors (FBC) has proceeded for a number of years. In the 1970s the demand for theoretical models became urgent as the technique developed towards commercial applications. At present several mathematical models are available, although still at an early stage of development. Attempts to develop mathematical models have produced many advances in predicting details and qualitative performance but little success in setting up reliable design relationships. The present models rely on empirical and semiempirical expressions obtained from experiments, often under narrow parameter ranges and for cold models.

Several mathematical models on FBC have been reported in the literature [1]. However, most of

these are mainly concerned with some specific subprocess or developed for a specific application. In the present article, we compare the performance of two models [2, 3] that consider the most important phenomena occurring in FBC but with different degrees of complexity. An improved version of ref. 2 is presented and the results are compared with those of the original model. The improved version performed better for both pilot-scale and industrial fluidized bed conditions.

## THE MODELS OF RAJAN AND WEN [2] AND PRETO [3]

### Description of the Models

The mathematical models of Rajan and Wen [2] and Preto [3] were compared against experimental data acquired in a pilot scale FBC. Both models include all the significant processes occurring in FBC but with different degrees of complexity. Rajan and Wen have extensively tested their model. It is a comprehensive model that includes most FBC processes and it is both detailed and complex. The model of Preto was developed in a modular approach. Although generally simpler, it includes a homogeneous gas phase reaction description with more detail, using a Gibbs function minimization technique considering ten gas species. The volatiles distribution is a function of the turnover and devolatilization times. The model is applied in a unique computer program that is different from the application of the model of Rajan and Wen [2], which is done at two levels, each with a different degree of complexity. The hydrodynamic submodel is further developed in the model of Rajan and Wen and the considerations of nonuniform bubble size, temperature, and carbon concentration in the bed constitute more elaborate approximations. In this model a complete inventory of the solid material is performed, while in Preto's model the balance of solid material is much simplified, with elutriation rates calculated from simple correlations.

### Results

The performance of each model is examined for a pilot scale fluidized bed coal combustor for several

sets of operating conditions, based on published experimental data [4, 5]. Both sets of experiments were performed in the same combustor at Sheffield University. The combustor, constructed from stainless steel, is 1.83 m high and has a square cross section of  $0.3 \times 0.3$  m. Some of the properties of materials and the operating conditions are reported in Table 1. The bed height is kept constant at 0.6 m.

### Carryover Losses

The correlation of Merrick and Highley [6] in the model of Rajan and Wen for the calculation of elutriation rate overpredicts this value [7, 8]. In the present work the constant in the original correlation (130) was replaced by the value 1, as suggested in ref. 2.

Figure 1 illustrates the effect of temperature on measured and predicted values of carryover losses. The influence of temperature can be assessed by comparing four different bed operating temperatures ( $770^\circ$ ,  $820^\circ$ ,  $870^\circ$ , and  $920^\circ\text{C}$ ), for a crushed coal with excess air of 20%, from the data of Brikci-Nigassa [4]. The superficial velocity increases with temperature from 0.8 to 0.9 m/s. The model of Rajan and Wen predicts the elutriation rates for sand and char reasonably well and their variation with temperature. The elutriation rate of sand increases with bed temperature, due to the increase of gas velocity, whereas that of char decreases because the carbon loading decreases due to the augmentation of the reaction rate. The model of Preto assumes that the elutriation rate is a proportion of the feed rate, slightly dependent on the superficial velocity. For the elutriation of char, although attrition of it is considered, only a slight variation with temperature was predicted.

Figure 2 illustrates the effect of excess air on the measured and predicted values of carryover losses for the crushed coal [4], with a bed temperature of  $820^\circ\text{C}$  and a superficial velocity of 0.83 m/s. The excess air is defined as the percentage of air in excess or deficit of the stoichiometric theoretical air. The variation in the excess air was obtained by changing the coal feed rate from 2.26 to 3.02 g/s, keeping the air feed rate constant. The carryover losses decrease with excess air because the char



**TABLE 1**  
Considered Operating Conditions

	Brikci-Nigassa [4]	Gibbs et al. [5]
Mean surface diameter of inerts feeds (mm)	0.69	0.62
Mean surface and mean weight diameter of coal feeds (mm)	0.17 0.57	0.20 0.65
Temperature range (°C)	770-920	800
Excess air range (%)	-10 +22	-10 +10
Superficial velocity (cm/s)	80 - 90	90
Elementar analysis of coal (d.b.)		
C	80.2	62.0
H	5.0	3.7
O	6.0	7.8
N	2.3	1.5
S	1.8	1.7
Proximate analysis of coal		
Volatiles	33.0	33.4
Ash	6.0	19.8
Moisture	1.6	6.8

concentration in the bed is lower for higher values of excess air. The predictions of both models are close to the measurements. The elutriated material represents the main loss of efficiency of the FBC, as it is not recovered. When the excess air increases, the equivalent heat losses vary from 18% to 12.5% of the total heat.

**Carbon Loading**

Despite the lack of experimental evidence, the influence of some operating conditions in the carbon loading and the ability of the models to predict this influence, were investigated. Based on the experimental conditions of Brikci-Nigassa [4],

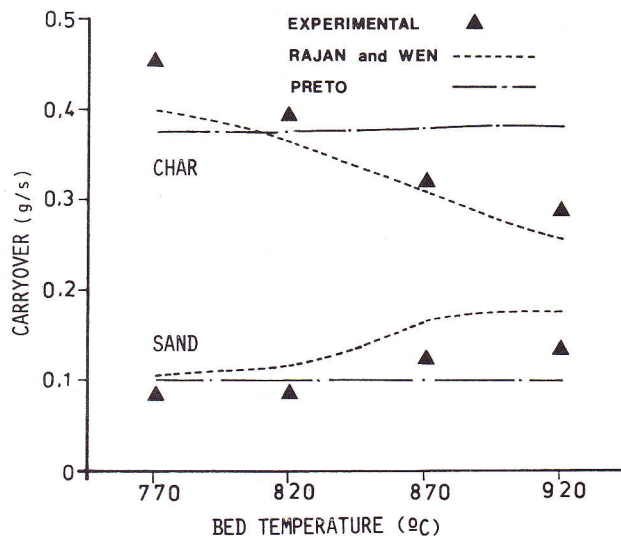


Fig. 1. Variation of sand and char carryover with temperature.

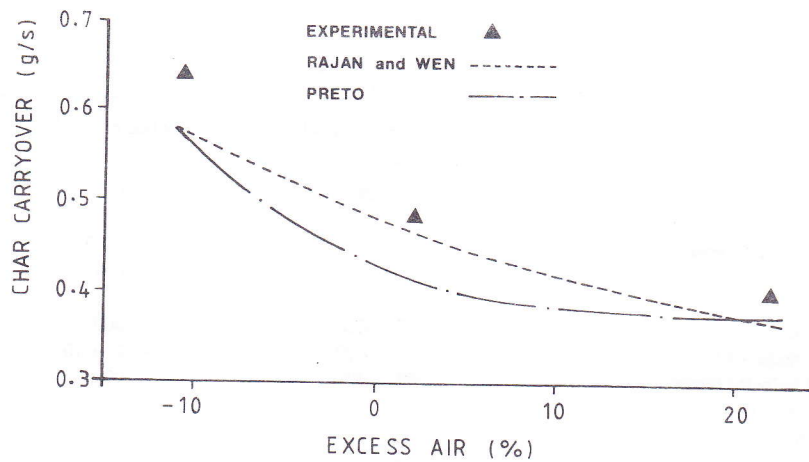


Fig. 2. Variation of char carryover with excess air.

the effect of temperature is analyzed in Table 2. The expected—a decrease of carbon loading with increasing temperature—is obtained with both models.

Based on the experimental data of Gibbs et al. [5], the calculated values of carbon concentration in the bed are shown in Table 3. The tests were performed for a bed temperature of 800°C, superficial velocity of 0.9 m/s, and excess air from -10% to 10%. Both models show the expected trend, the decrease of carbon loading increasing the excess air. The model of Rajan and Wen always predicts larger values of carbon concentration, due to its lower mass transfer coefficient.

### Gas Concentrations Along the Bed

Figure 3 compares species concentrations along the bed predicted by the two models with the

experimental results of Gibbs et al. [5] for a bed temperature of 800°C, a superficial velocity of 0.9 m/s, and an excess air of -10%. The carryover losses for this case were well predicted by both models.

The model of Rajan and Wen predicts the steep variation of the gas concentrations near the distributor more accurately than does the model of Preto. The model of Preto considers a larger mass transfer and emulsion fraction, leading to a higher oxygen concentration in the emulsion phase throughout the bed. In the model of Rajan and Wen, due to the lower value of the mass transfer coefficient, the oxygen in the emulsion phase is only high close to the distributor. Preto predicts a more uniform volatiles release throughout the bed in comparison with Rajan and Wen, whose model predicts volatiles release mainly in the feedport region. In the former model the temperature is

TABLE 2

Influence of Bed Temperature on the Predicted Carbon Concentration

Experimental Conditions	Temperature (°C)	Models Used	
		Rajan and Wen [2]	Preto [3]
Brikci-Nigassa [4]	770	10.0	1.14
	820	5.4	0.94
	870	2.3	0.82
	920	1.1	0.68

TABLE 3

Influence of Excess Air on the Predicted Carbon Concentration

Experimental Conditions	Excess Air (%)	Models Used	
		Rajan and Wen [2]	Preto [3]
Gibbs et al. [5]	-10	6.6	3.4
	0	4.3	3.0
	10	3.0	1.9

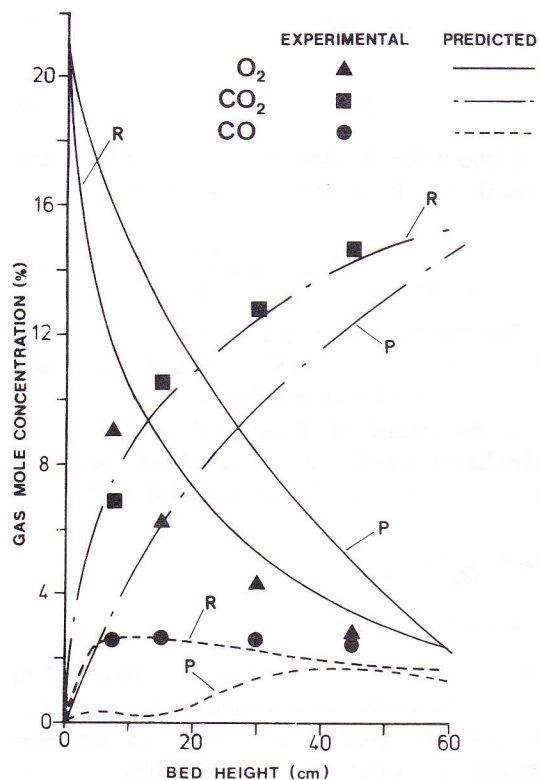


Fig. 3. Gas species concentrations along the bed. Case R—model of Rajan and Wen; case P—model of Preto.

kept constant along the bed, whereas in that of Rajan and Wen, the temperature of particles is calculated at each location, leading to larger combustion rates near the distributor. For these reasons, Rajan and Wen predict that the combustion occurs mainly near the distributor whereas Preto predicts a more uniform distribution throughout the bed. The model of Preto predicts a low CO concentration near the distributor, as a result of the high concentration of oxygen in the emulsion phase.

#### Bed Expansion Ratio

The bed expansion ratio was calculated for the experimental conditions of Gibbs et al. [5] using both models. The model of Rajan and Wen predicts a large value for the bed expansion ratio (2.08) when compared with the value (1.71) obtained from a correlation previously published [9]. This is because their model predicts a low

value for the bubble velocity, leading to a large bubble fraction and a large expansion ratio. In the model of Preto the expansion ratio (1.36) is calculated from an experimental correlation obtained by Preto for a larger bed than the present one as well as those considered by Babu et al. [9]. The range of applicability of the correlation of Babu et al. includes the present conditions, although the data are based on beds of mostly small uniform particles.

#### Discussion

For the conditions analyzed here the model of Rajan and Wen follows the experimental trends more closely. The influence of more detailed description of the homogeneous gas phase reaction and volatiles evolution in the model of Preto could not be assessed in the present test cases. However, some discussion arises in the analysis of the results of the model of Rajan and Wen.

The bed expansion ratio is overpredicted by this model as a consequence of deficiencies in the hydrodynamic model. The superficial velocity through the emulsion phase is considered equal to the minimum fluidization velocity, and the upper limit for the bubble fraction was fixed at 0.7. This value is higher than the maximum value derived when bubbles are considered as spheres in a cubic array ( $\pi/6$ ). Glicksman et al. [10] derive a relation between the superficial velocity through the emulsion phase and the bubble fraction. In the model of Rajan and Wen the influence of bed diameter on bubble velocity is not considered. Werther and Hegner [11] indicate that bubbles of equal size rise faster in fluidized beds of larger diameter, due to the formation of bubble tracks and solid circulation patterns.

The value of carbon concentration in the bed obtained from the model of Rajan and Wen is large compared to the usual values presented in literature [12]. This is a consequence of the assumed low mass transfer, which controls the overall combustion rate. Chavarie and Grace [13] presented a literature review of mass transfer models, in which they conclude that pure diffusive models underpredict mass transfer coefficients.

The model of Rajan and Wen was hence



modified in the hydrodynamic and mass transfer submodels.

## THE MODEL OF RAJAN AND WEN MODIFIED

### Description of the Model

#### Original Model

In its original form, the model of Rajan and Wen calculates the bubble size and bubble growth from the model of Mori and Wen [14], with the bubble velocity described by Davidson and Harrison [15] and the bubble fraction described by Kunii and Levenspiel [16]. Mori and Wen established a correlation to predict the bubble diameter in freely bubbling fluidized beds and account for the effect of bed diameter on the bubble size.

$$\frac{D_{bm} - D_b}{D_{bm} - D_{bo}} = \exp(-0.3 h/D_t), \quad (1)$$

where  $D_{bo}$  is the initial bubble diameter and  $D_{bm}$  is the maximum bubble diameter obtained from coalescence. These diameters are calculated from the correlations:

$$D_{bo} = 0.872[A_0(U_0 - U_{mf})]^{2/5}, \quad (2)$$

$$D_{bm} = 1.64[A_t(U_0 - U_{mf})]^{2/5}. \quad (3)$$

The range of applicability of this correlation is narrow, not covering the cases of large particles and large values of superficial velocities. The conditions considered previously under Results were at the upper limit of the range of applicability of the Mori and Wen model [14]. The bubble rising velocity correlation used is described by Davidson and Harrison [15].

$$U_b = U_0 - U_{mf} + 0.711\sqrt{gD_b}. \quad (4)$$

If the bubble velocity (assuming slug regime) is smaller than the bubble rising velocity, slugging conditions are considered:

$$U_b = U_0 - U_{mf} + 0.35\sqrt{gD_t}. \quad (5)$$

As suggested by Horio and Wen [17], to maintain the consistency of the model the bubble

fraction is calculated according to Kunii and Levenspiel [16].

$$\epsilon_b = (U_0 - U_{mf})/U_b. \quad (6)$$

Cloud-wake fraction including bubble is also described by Kunii and Levenspiel [16] by

$$\epsilon_c = \epsilon_b \frac{\alpha}{\alpha - 1}, \quad \text{where } \alpha = \frac{\epsilon_{mf} U_b}{U_{mf}}. \quad (7)$$

The model assumes a maximum value of the cloud-wake volume of 1% of the bed volume and does not allow for slow bubbles.

In the model of Rajan and Wen, the gas interchange coefficient is calculated using the correlation proposed by Kobayashi et al. [18]:

$$K_{be} = \frac{0.11}{D_b}. \quad (8)$$

#### Modified Model

The model of Rajan and Wen was modified in order to overcome the deficiencies pointed out in the previous Discussion section. In the new version, the correlations for the bubble diameter and bubble velocity proposed by Werther and Hegner [11] and Bellgardt et al. [19] were adapted:

$$D_b = 0.015[1 + 27(U_0 - U_{mf})]^{1/3} \times [1 + 6.84(h + h')]^{1.2}, \quad (9)$$

where

$$h' = \left[ \left( \frac{1.3(V_0^2/g)^{0.2}}{0.015[1 + 27(U - U_{mf})]^{1/3}} \right)^{1/1.2} - 1 \right] \times \frac{1}{6.84}. \quad (10)$$

The bubble velocity is given by

$$U_b = U_0 - U_c + \psi\sqrt{gD_b} \quad (11)$$

where  $\psi$  introduces the influence of bed diameter on bubble velocity and is given by

$$\psi = \begin{cases} 0.64 & D_t < 0.1 \text{ m} \\ 1.6 D_t^{0.4} & 0.1 \text{ m} < D_t < 0.1 \text{ m} \\ 1.6 & D_t > 1 \text{ m} \end{cases} \quad (12)$$

These correlations have a broader range of applicability in terms of particle size, temperature, and superficial velocities than the correlations in the original version of Rajan and Wen.

The bubble fraction and superficial velocity through the emulsion phase is calculated in accordance with Glicksman et al. [10]. The superficial velocity through the emulsion phase is given by

$$U_e = U_{mf} \left[ 1 - \frac{\pi}{2} \ln \left( 1 - \frac{6\epsilon_b}{\pi} \right) \right] (1 - \epsilon_b). \quad (13)$$

The void fraction in the emulsion phase, in accordance with the expansion of the emulsion phase, is given by Delvosalle and Vandershuren [20]:

$$\epsilon_e = \epsilon_{mf} (U_e / U_{mf})^{1/6.7}. \quad (14)$$

The bubble fraction is calculated as in the original version by Eq. 6. The cloud-wake was assumed to occupy a maximum of 20% of bubble volume, as suggested by Rowe and Partridge [21].

Sit and Grace [22] found that the interphase mass transfer increases with particle size. This effect is included in a correlation for the mass transfer coefficient [23] considering diffusive and throughflow effects:

$$K_{be} = \left[ 2U_{mf} + 12 \left( \frac{D_g \epsilon_{mf} U_b}{D_b} \right)^{1/2} \right] / D_b. \quad (15)$$

An enhancement factor due to coalescence was applied to the throughflow term. This correlation was adopted in the present version of the model.

## Results and Discussion

The new hydrodynamic submodel takes into consideration the difference between the bubble flow rate and the excess gas flow. Recent experiments [24–27] demonstrate that not all the gas flow above the minimum fluidization condition passes through the bubble phase. Actually, a large fraction of the excess gas leaks to the emulsion phase during bubble formation. Although a complete understanding of bubble formation is missing [28], it has been shown that no bubbles exist in a zone some millimeters immediately above the distribu-

tor [24, 25]. Caram and Hsu [29] for a simple situation explain the leakage of gas during bubble formation and the influence of the operating parameters in terms of deviations from two phase theory.

In Fig. 4 the actual flow rate through the bubble phase divided by the excess gas flow is plotted against the bed height. Experimental observations in three-dimensional beds [24–27] are reproduced in Fig. 4, along with the values obtained with the modified version of the model of Rajan and Wen for two different operating conditions. The test case *S* corresponds to the operating conditions of the gas concentrations profile analysis (Fig. 3). The test case *BW* was for the data of test number 26 of Babcock and Wilcox [30], which correspond to a bed of cross section of 0.98 m<sup>2</sup> operated with a superficial velocity of 2.5 m/s. A strong influence of bed diameter on the deviation from two-phase theory can be seen in Fig. 4. This influence is taken into account in the hydrodynamics. The influence of bed diameter on the model was introduced through the bubble velocity relation with bed diameter and the relationship presented by Glicksman et al. [10]. The leakage of air from bubble to emulsion phase during bubble formation is not included in the model.

The modified version of the Rajan and Wen model was applied to the bed and operating conditions considered in Fig. 3 [5]. Figure 5 shows the gas concentration profiles obtained with the modified version of the model assuming two volatiles distributions. In case *A* the volatiles are considered to be released mainly in the feedport region as in the original model. Case *B* assumes that most of the volatiles are uniformly evolved in the bed, as suggested by Preto [3], who considers the volatiles distribution by comparing characteristic physical times.

In case *A*, the same steep variation in gas concentration as in the original model can be observed. The lower levels of oxygen obtained with the modified version are a consequence of the larger mass transfer and smaller bubble fraction. The volatiles are all consumed in the bed, leading to a lower oxygen concentration there. The presence of oxygen in the emulsion phase leads to low carbon monoxide concentration in the bed. In case



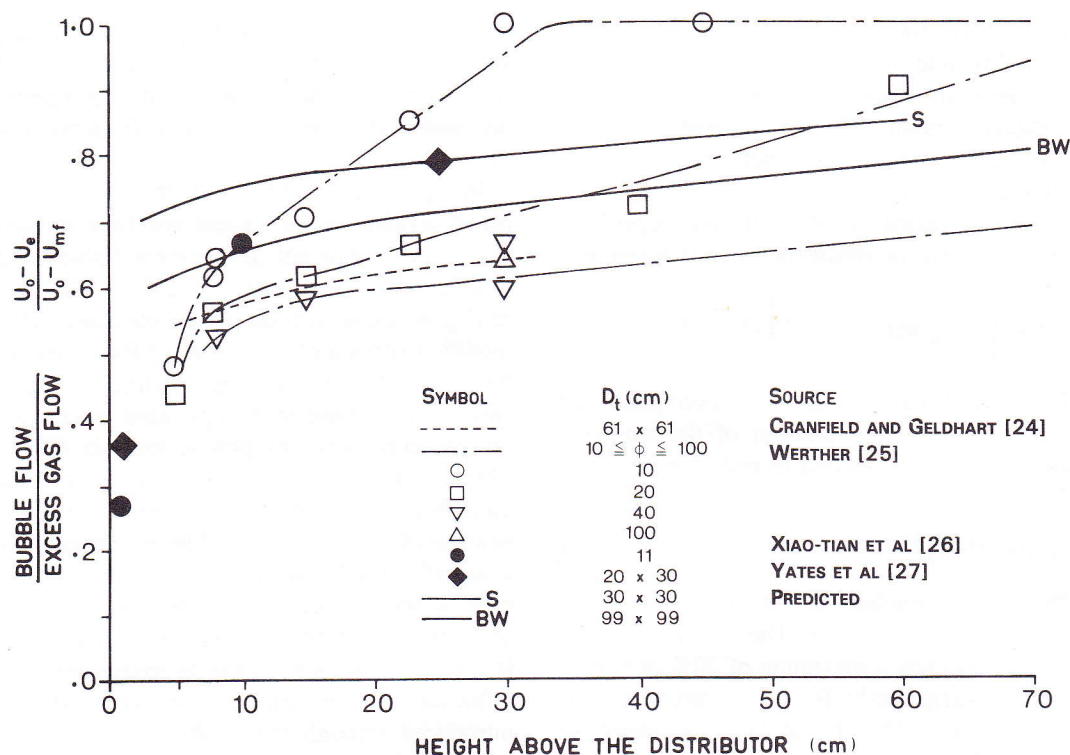


Fig. 4. Deviation from the two-phase theory along the bed height.

B some of the volatiles released in the upper section of the bed are transported to the freeboard, leading to larger oxygen levels. Due to the lower volatiles release near the feedport, the gradient of gas concentration near the distributor is smaller than in the previous case. The gas concentration profiles are reasonably predicted by the modified model [see Fig. 3 (case R) and Fig. 5 (case B)], with the exception of the CO profile, due to the larger oxygen concentration in the emulsion phase. This prediction could be improved by considering the distribution of particle sizes, instead of a mean surface diameter, as in the original and in this modified version of the Rajan and Wen model. Nevertheless, the carbon content in the bed and the bed expansion ratio show considerable improvement in comparison to the original model.

The predicted carbon content in the bed with the modified model is much lower than that with the original model. In the two simulations presented here, with the volatiles mostly released near the feedport and with a more uniform release along

the bed, the calculated carbon concentrations were 1.2% and 0.75% respectively, within the range (0%–2%) found in the literature [12]. These compare with the previous value of 6.6% obtained with the original model.

In order to assess the carbon loading prediction, data from test number 26 of Babcock and Wilcox [30] were used. The bed was operated with a bed temperature of 1100 K and an excess of air of 25%. Table 4 shows the predicted and experimental values of char concentration in the bed. Predictions were from the original and modified model of Rajan and Wen using for the mass transfer coefficient the correlation of Kobayashi et al. [18] and the correlation of Sit and Grace [23].

The values obtained with the modified version of the Rajan and Wen model are much closer to the experimental value. The value of char concentration predicted with the original model decreases substantially when the correlation of Sit and Grace is used. Due to the higher mass transfer coefficient predicted with the Sit and Grace correlation, the availability of oxygen in the emulsion phase

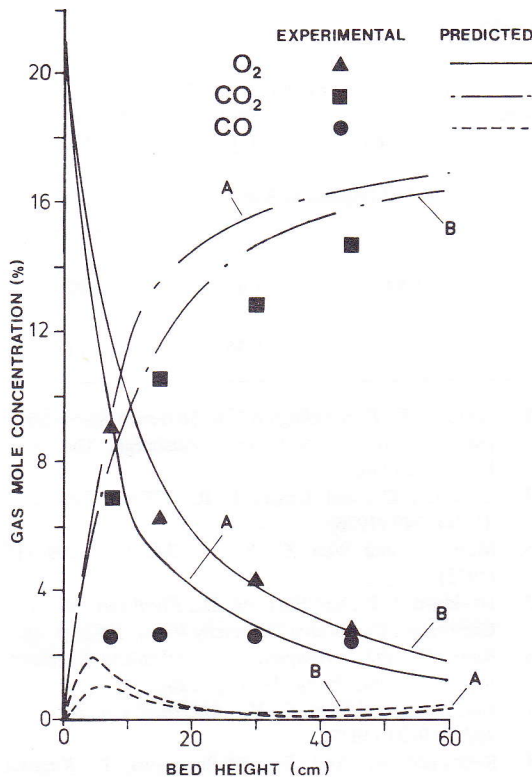


Fig. 5. Gas species concentrations along the bed predicted with the modified model. Case A—volatiles mostly released near the feedport; case B—volatiles mostly uniformly released.

increases, leading to low values of char concentration in the bed. With the modified version of the model the predicted value of the char concentration in the bed, obtained with both correlations, further decreases due to a higher oxygen content in the emulsion phase. This is a consequence of the lower predicted bubble fraction in the bed. The overall reaction rate of char in the bed becomes less dependent on mass transfer. Using both

correlations for mass transfer in the modified model, the values of the char concentration are close to the experimental value. An advantage of the Sit and Grace correlation is that it allows for the influence of particle size on the mass transfer coefficient.

Table 5 shows the predicted values of bed expansion with the original and modified model of Rajan and Wen and with the correlations of Babu et al. [9] and Preto [3] for the operating conditions of the Babcock and Wilcox [30] test case and of Gibbs et al. [5]. The modified model of Rajan and Wen predicts the expansion ratio of the bed more closely to the values presented in the literature [3, 9] than does the original. This is mainly because the modified version includes the influence of bed diameter on bubble velocity, which accounts for the formation of bubble tracks in the bed.

**Conclusion**

Two mathematical models [2, 3] have simulated fluidized bed behavior for different operating conditions and tested the influence of some operating variables. Reasonable agreement has been obtained with the two models. For the conditions analyzed in the present article the model of Rajan and Wen [2] is the one that follows the experimental trends most closely. However, the model of Rajan and Wen [2] was deficient in predicting the bed expansion ratio and of the carbon loading. The modified version of the model that has been presented offers considerable improvement on the computation of the parameters. Nevertheless, for further improvements of the model, experimental data are required with well-defined operating conditions and with simultaneous measurements of all relevant parameters, such as, for example, bed

**TABLE 4**  
Char Concentration in the Bed (% Weight)

	Rajan and Wen		Modified Model		Experimental [30]
	Kobayashi et al. [18]	Sit and Grace [23]	Kobayashi et al. [18]	Sit and Grace [23]	
Char concentration in the bed (% weight)	0.98	0.41	0.16	0.14	0.21



TABLE 5  
Bed Expansion Ratio

Experimental Conditions	Superficial Velocity (m/s)	Models and Correlations Used			
		Rajan and Wen [2]	Modified	Preto [3]	Babu et al. [9]
Bed Expansion Ratio					
Babcock and Wilcox [30]	2.5	3.45	1.84	1.47	1.92
Gibbs et al. [5]	0.9	2.04	1.57	1.36	1.71

composition, gas concentration profiles, and elutriation rates.

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