CHAPTER VII

CORRELATIONS

Correlations for predicting experimental data (average gas hold-ups and specific gas-liquid interfacial area) were developed. In most cases correlations from the literature were used, sometimes it was neccessary to reevaluate the constant parameters in order to obtain the best fit.

The specific gas-liquid interfacial area data were calculated from equation F.13 in APPENDIX F using the experimental values of ϵ_{go} (fraction gas hold-up) and d_s (m). Correlations for $\epsilon_{go}(-)$ or $\epsilon_g(\%)$ and $a_g(m^2/m^3)$ for different systems are presented below.

A. FT Derived Waxes

1. Average Gas Hold-up

Literature correlations by Akita and Yoshida, 1973 and by Bach and Pilhofer, 1978 were used to predict the average gas hold-up for the waxes used in this study (FT-200 wax, Sasol wax, and Mobil wax). The correlation by Bach and Pilhofer provides an excellent fit for the data. Figure 48 compares the values predicted by Bach and Pilhofer's correlation to those obtained by Calderbank *et al.* (1963), by Kuo *et al.* 1985, by Bukur *et al.* (1987), and from this study. This correlation was reevaluated using the experimental data in order to obtain new values for constants, k_1 and k_2 in equation 7.1.

$$\frac{\epsilon_g}{(100-\epsilon_g)} = k_1\left(\frac{u_g{}^3\rho_l{}^2}{\mu_l g(\rho_l-\rho_g)}\right)^{k_2} \qquad (7.1)$$

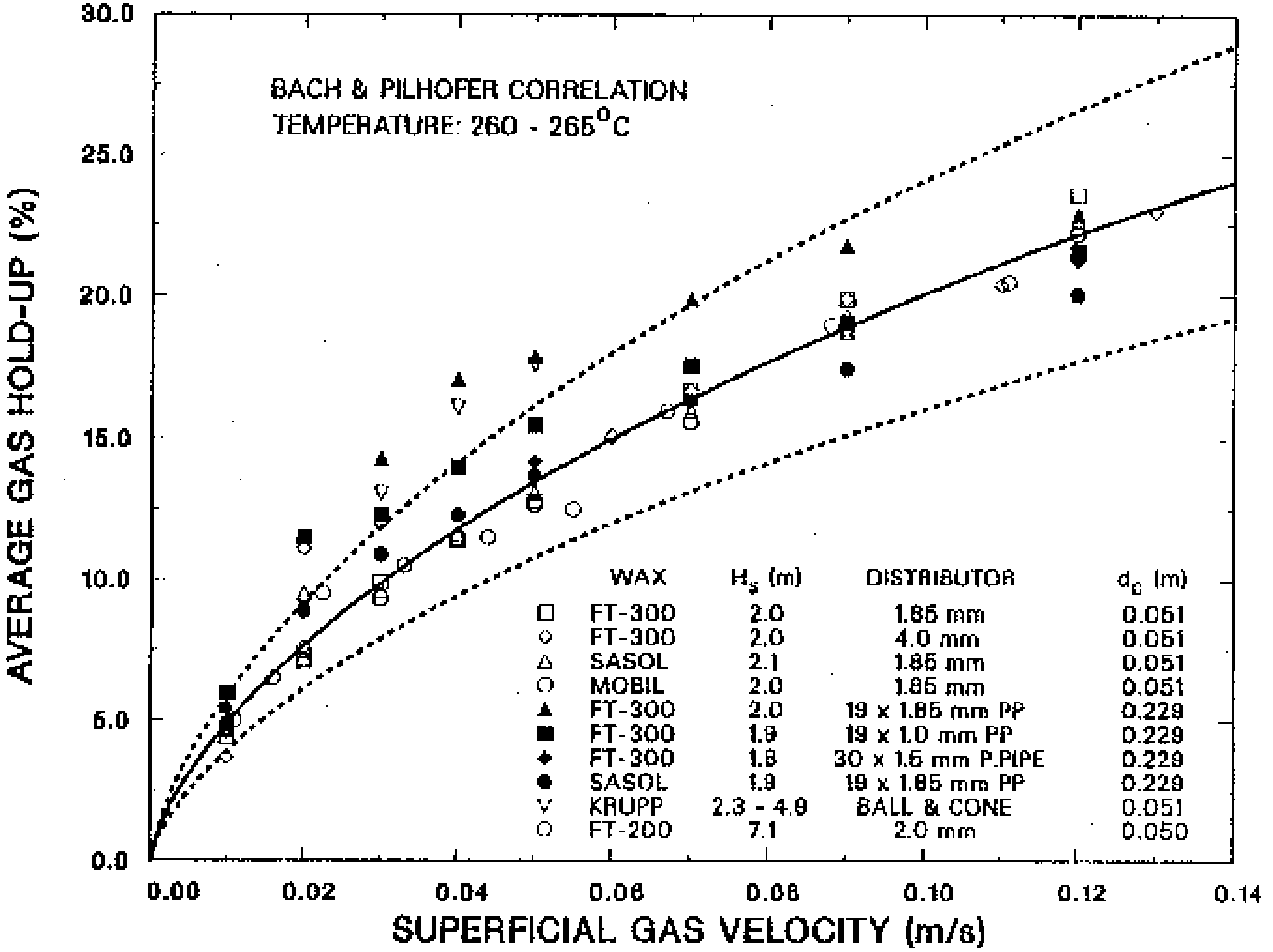

Figure 18. Comparison between experimental hold ups and predictions from Bach and Pilhofer correlation. (solid line Bach and Pilhofer correlation; dashed lines ± 20 % relative deviation from the correlation; ▽ -Calderbank *et al.*, 1983; ○ -Kuo *et al.*, 1985; ◆, ◇, ▲, and ■ -Bukur *et al.*, 1987; remaining data are from the present study).

where ϵ_g is in (%)

The constants k_1 and k_2 were obtained using a NLIN regression procedure in the SAS package, and the statistical results are presented below:

Number of data points: = 349
Mean square error: = 8.14
% of points within ± 30 % = 91.7
Parameter estimates: $k_1 = 0.128$
$k_2 = 0.24$

The new parameters compare very well with the original ones i.e. the new coefficient is 0.128 compared to 0.115 in the original equation and the exponent is 0.24 compared to 0.23 in the original equation.

2. Specific Gas-Liquid Interfacial Area

The specific gas liquid interfacial areas were calculated using the measured hold-up values and the calculated Sauter mean bubble diameters from the DGD technique. The empirical correlation by Deckwer *et al.*, 1982 was used to correlate the experimental data as follows:

$$a_g = k_1 u_g^{k_2} \tag{7.2}$$

The experimental data were divided as follows:

1. Data from experiments with Sasol wax at 200 °C
2. Data from experiments with Sasol wax at 265 °C
3. Data from experiments with Mobil wax at 200 °C
4. Data from experiments with Mobil wax at 265 °C

Using the NLIN procedure the following statistical results were obtained

Liquid		Sasol Wax		Mobil Wax	
Temperature (°C)		200	265	200	265
No. of points		8	20	8	13
Mean Square error		1940	11610	240	1240
% of points within ± 30 % range		87.5	80.0	100.0	100.0
Parameters:	k_1	492	1000	165	300
	k_2	0.26	0.25	0.01	0.01

The correlation for specific gas-liquid interfacial area (m^2/m^3) for Sasol wax at the two temperatures are:

$$a_g = 1000 {u_g}^{0.25} \qquad 0.01 < u_g < 0.12 \text{ m/s} \tag{7.3}$$

at 265 °C and

$$a_g = 492 {u_g}^{0.256} \qquad 0.01 < u_g < 0.12 \text{ m/s} \tag{7.4}$$

at 200 °C.

The change in temperature does not have any significant effect on the exponent, only the coefficient appears to change. The experimental values of the predicted values of interfacial area are compared with the predicted values in Figure 49. Despite the scattering, the correlation provides a reasonably good fit.

The correlation for specific gas-liquid interfacial area (m^2/m^3) for Mobil wax at the two temperatures are:

$$a_g = 300 {u_g}^{0.1} \qquad 0.01 < u_g < 0.12 \text{ m/s} \tag{7.5}$$

at 265 °C and

$$a_g = 165 {u_g}^{0.1} \qquad 0.01 < u_g < 0.12 \text{ m/s} \tag{7.6}$$

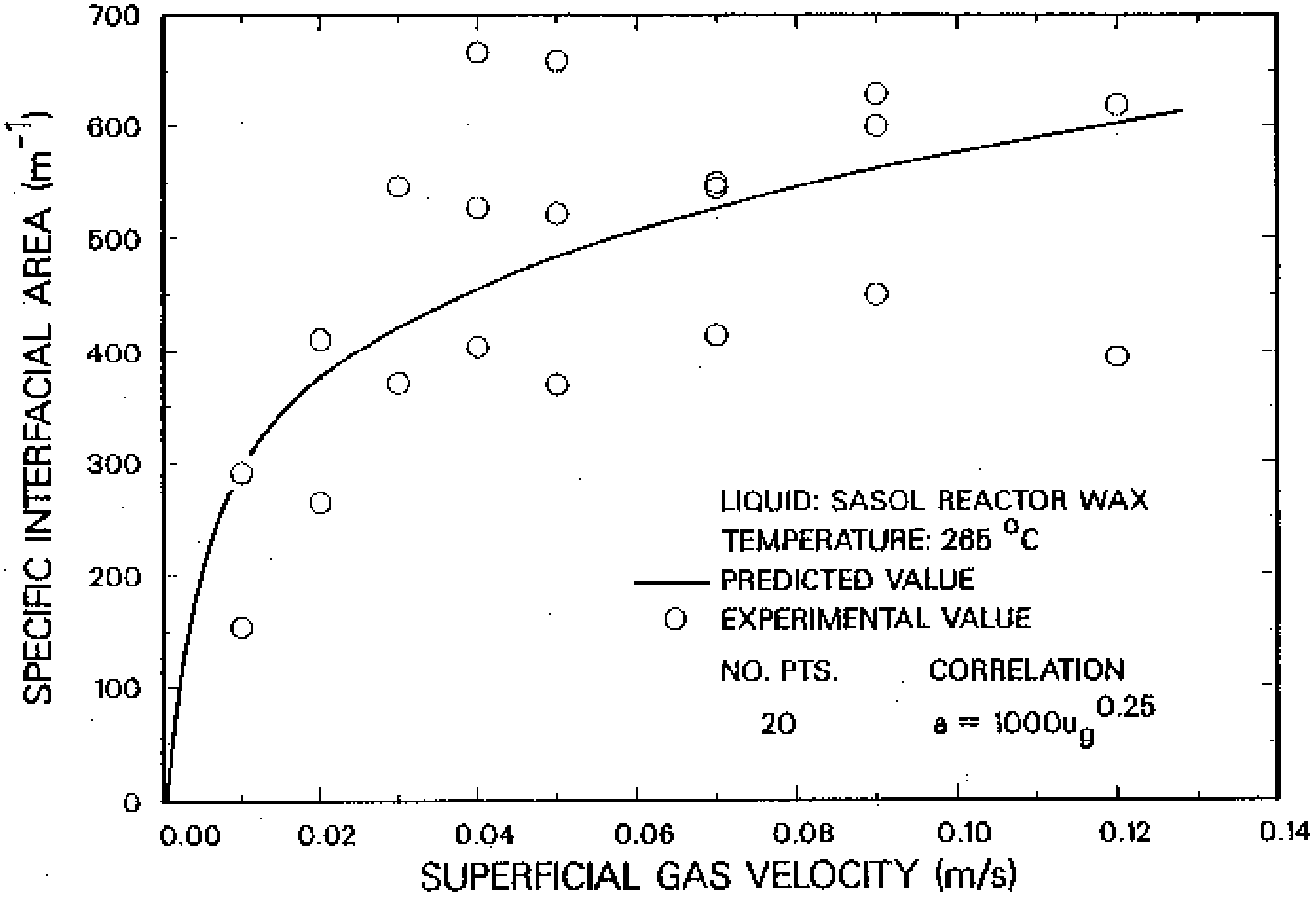

Figure 49. Comparison between experimental specific gas-liquid interfacial area and predictions for Sasol reactor wax.

at 200 °C. Analogous to Sasol wax, temperature has no effect on the value of the exponent. The experimental data are compared with predicted values in Figure 50 which shows to be a good fit.

B. Pure Liquids

1. Average Gas Hold-up

There are various correlations in the literature for calculating the average gas hold-up for different liquid mediums. A comprehensive summary of correlations was presented by Shah *et al.* (1982).

The gas hold-ups obtained in this study were compared with the existing correlations from the literature. The correlations used were either developed from similar systems (type of liquid media) or from a very large pool of data of various systems.

1. Bach and Pilhofer (1978) correlation:

$$\frac{\epsilon_{go}}{(1-\epsilon_{go})} = 0.115\left(\frac{{u_g}^3{\rho_g}^2}{\mu_l g(\rho_l-\rho_g)}\right)^{0.23} \tag{7.7}$$

where ϵ_{go} is fraction gas hold-up. This correlation was developed to fit hold-up values for pure organic liquids. It is recommended for prediction of gas hold-ups in columns ID greater than 0.1 m and superficial gas velocities less than 0.1 m/s. With these ranges, the correlation covers hold-up values in the homogeneous flow regime and the transition to churn turbulent flow regime.

2. Hikita and Kikukawa (1974) correlation:

$$\epsilon_{go} = 0.505\,{u_g}^{0.47}\left(\frac{0.072}{\sigma_l}\right)^{2/3}\left(\frac{0.001}{\mu_l}\right)^{0.05} \tag{7.8}$$

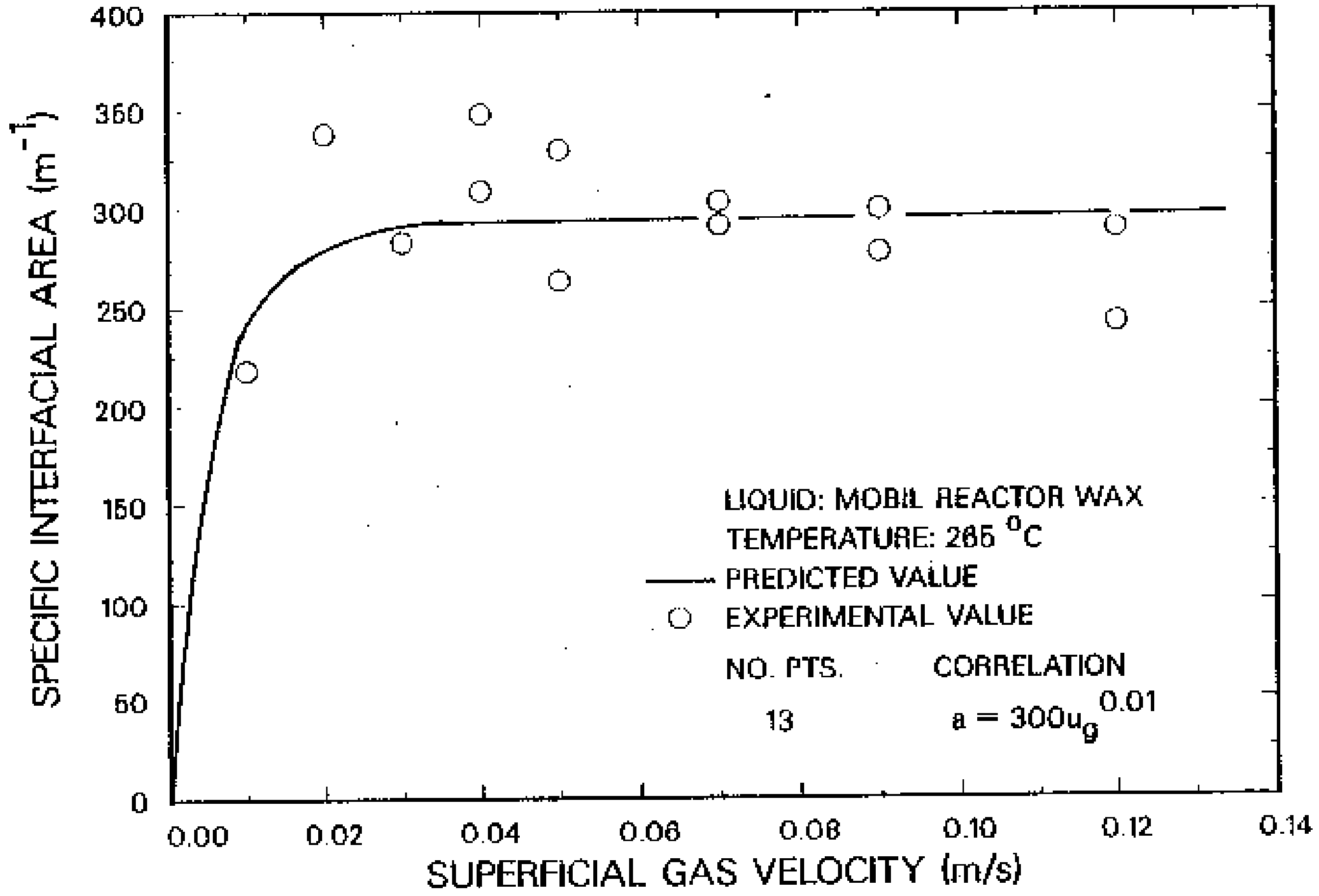

Figure 50. Comparison between experimental specific gas-liquid interfacial area and predictions for Mobil reactor wax.

The above correlation was developed to predict hold-up values for pure liquids and aqueous solutions of alcohols in column diameters greater than 0.1 m and superficial gas velocities between 0.042 and 0.38 m/s. This correlation has a wider range of application than the former, because it covers churn-turbulent regime and all the other flow regimes mentioned earlier.

3. Akita and Yoshida (1973) correlation:

$$\frac{\epsilon_{go}}{(1-\epsilon_{go})^4} = 0.2 \left(\frac{gD_c{}^2\rho_l}{\sigma_l}\right)^{1/8} \left(\frac{gD_c{}^3\rho_l{}^2}{\mu_l{}^2}\right)^{1/12} \left(\frac{u_g}{\sqrt{gD_c}}\right) \tag{7.9}$$

This correlation was developed from various liquid mixtures with a wide range of physical properties and for column diameters between 0.152 and 0.6 m.

4. Posarac and Tekic (1987) correlation:

$$\epsilon_{go} = \frac{1}{2+\frac{0.35}{u_g}\left(\frac{\rho_l}{1000}\frac{\sigma_l}{0.072}\right)^{1/3}}(1-C_N)^{0.167} \tag{7.10}$$

This correlation was developed by modifying the original equation by Hughmark, (1967) which generalizes gas hold-up values for various liquids. Introducing C_N (number of carbon atoms in the straight chain, 0 for water) the correlation was used to predict gas hold-ups of aqueous solutions of alcohols.

However, the effect of column diameter and distributor type on gas hold-ups does not appear in any of the above correlations. Using the physical properties of water at 24°C, correlations developed by Akita and Yoshida (1973); and by Posarac and Tekic (1987) tend to agree well with measured hold-ups from runs with distilled water (see Figure 51). Whereas, the correlation by Bach and Pilhofer overestimates the hold-up values and the correlation by Hikita and Kikukawa overestimates the hold-up values at low gas velocities.

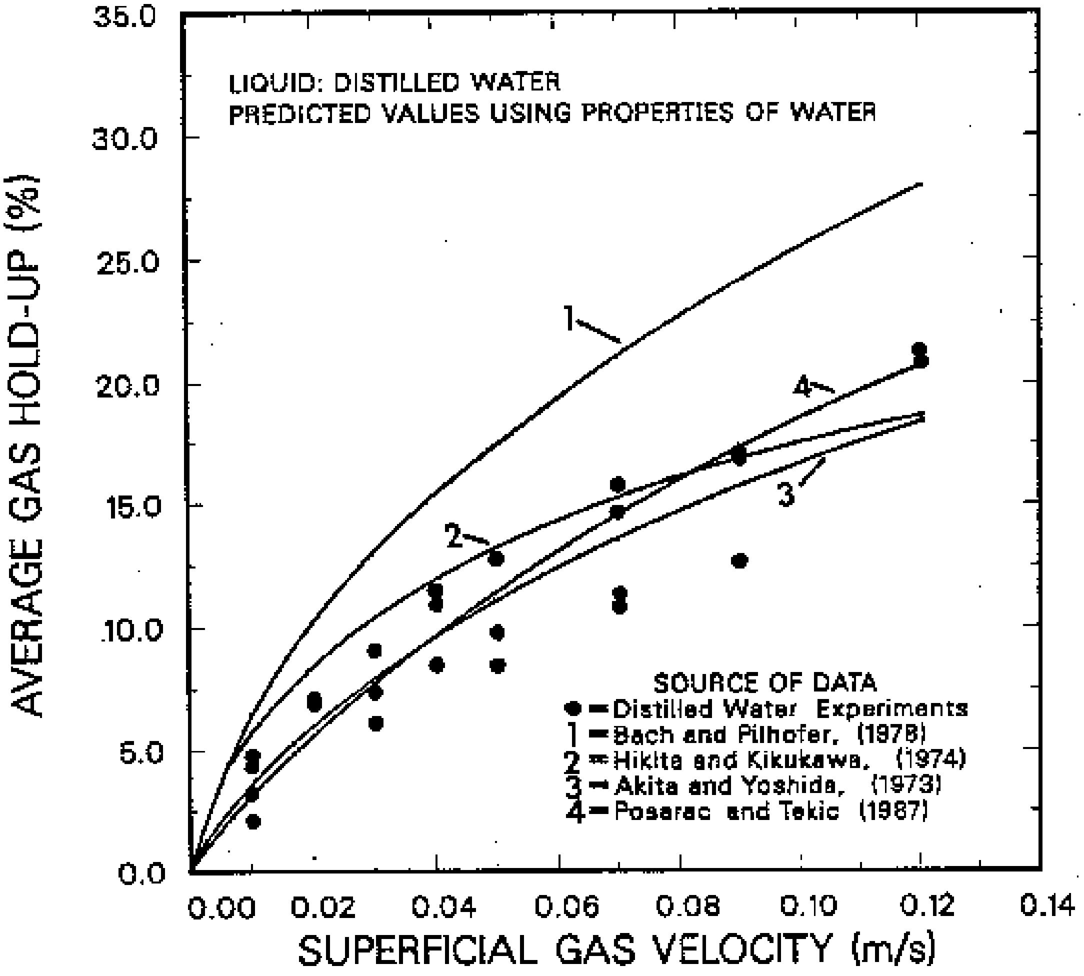

Figure 51. Comparison between experimental hold-ups and hold-ups predicted from literature correlations (experimental data are from all runs with distilled water).

Figure 52 shows the experimental gas hold-ups for n-butanol together with those calculated using physical properties of n-butanol. Correlations developed by Akita and Yoshida (1973) and by Bach and Pilhofer (1978) fit the experimental data better than other correlations (probably because they were developed from hold-up values of organic liquids). The rest of the correlation tend to overestimate the hold-up values.

In summary, the hold-ups for pure liquids obtained in this study were correlated using the existing correlation by Akita and Yoshida. Figure 53 presents the experimental data for distilled water and the predicted values using the correlation by Akita and Yoshida with a ±20% relative deviation from the correlation. 94 % of the data are within the prediction range for distilled water runs and 76 % for n-butanol runs (not shown).

2. Specific Gas-Liquid Interfacial Area

The specific gas-liquid interfacial areas (a_g, m^2/m^3) obtained from the runs with n-butanol (Run B-1 and Run B-2), were correlated using the following correlation by Akita and Yoshida (1974)

$$a_g = \frac{1}{3d_c}\left(\frac{g{d_c}^2\rho_l}{\sigma_l}\right)^{1/2}\left(\frac{g{d_c}^3{\rho_l}^2}{{\mu_l}^2}\right)^{0.1}{\epsilon_{go}}^{1.13} \tag{7.11}$$

The predicted values and the experimental values of interfacial area are compared on the parity plot (see Figure 54). 75 % of the experimental data are within ± 20 % relative deviation. No a_g data from runs with distilled water were available because the video tape for DGD analysis was not good.

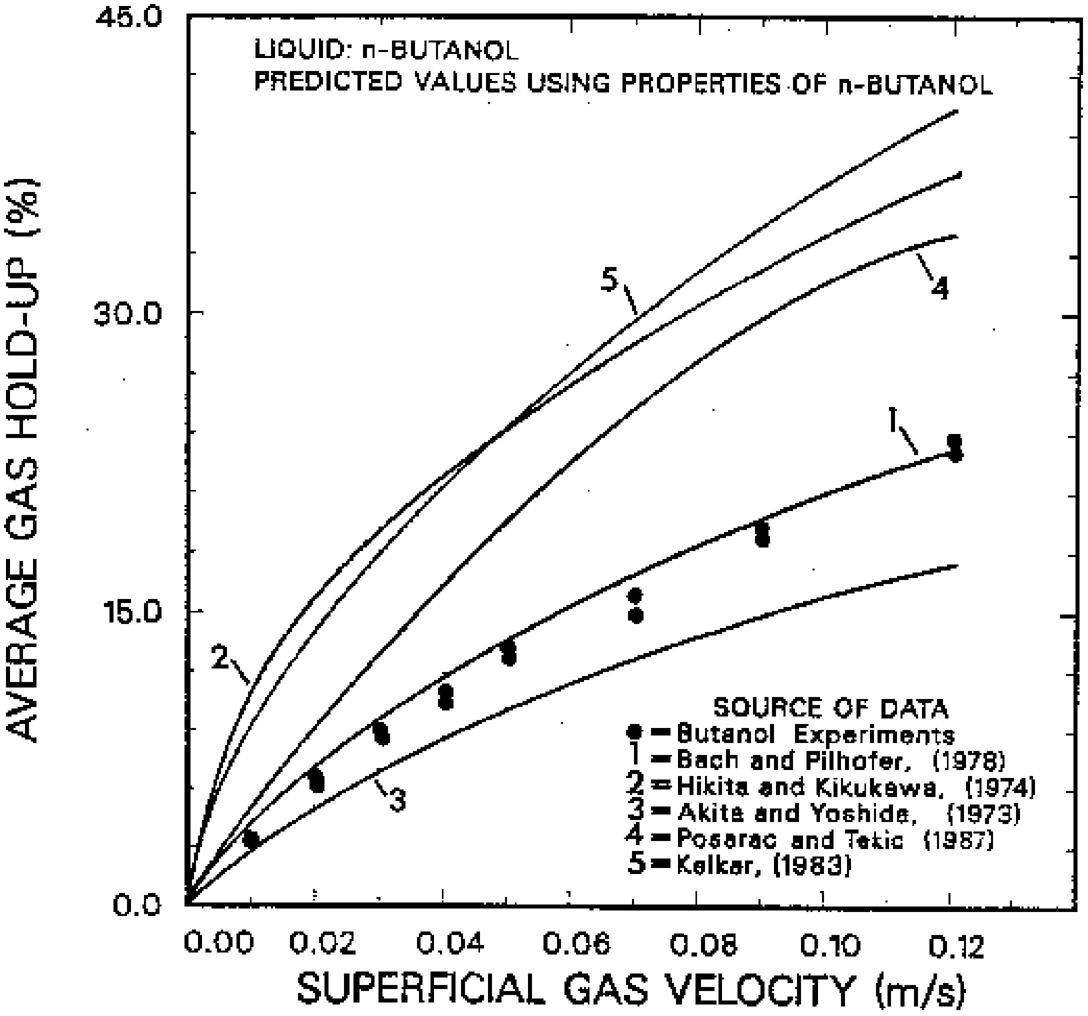

Figure 52. Comparison between experimental hold-ups and hold-ups predicted from literature correlations (experimental data are from all runs with n-butanol).

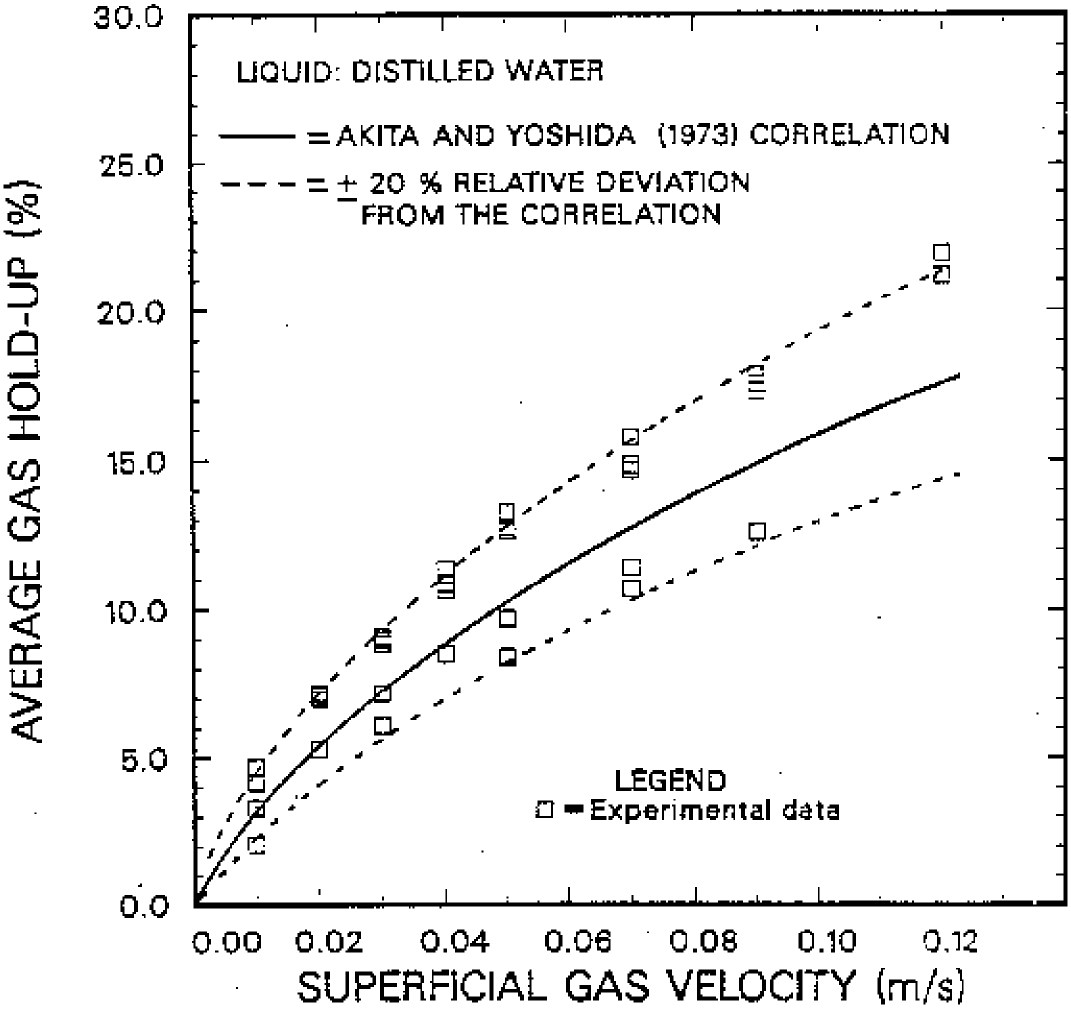

Figure 53. Comparison between experimental hold-ups and hold-ups predicted using Akita and Yoshida correlation within ± 20 % relative deviation (distilled water data).

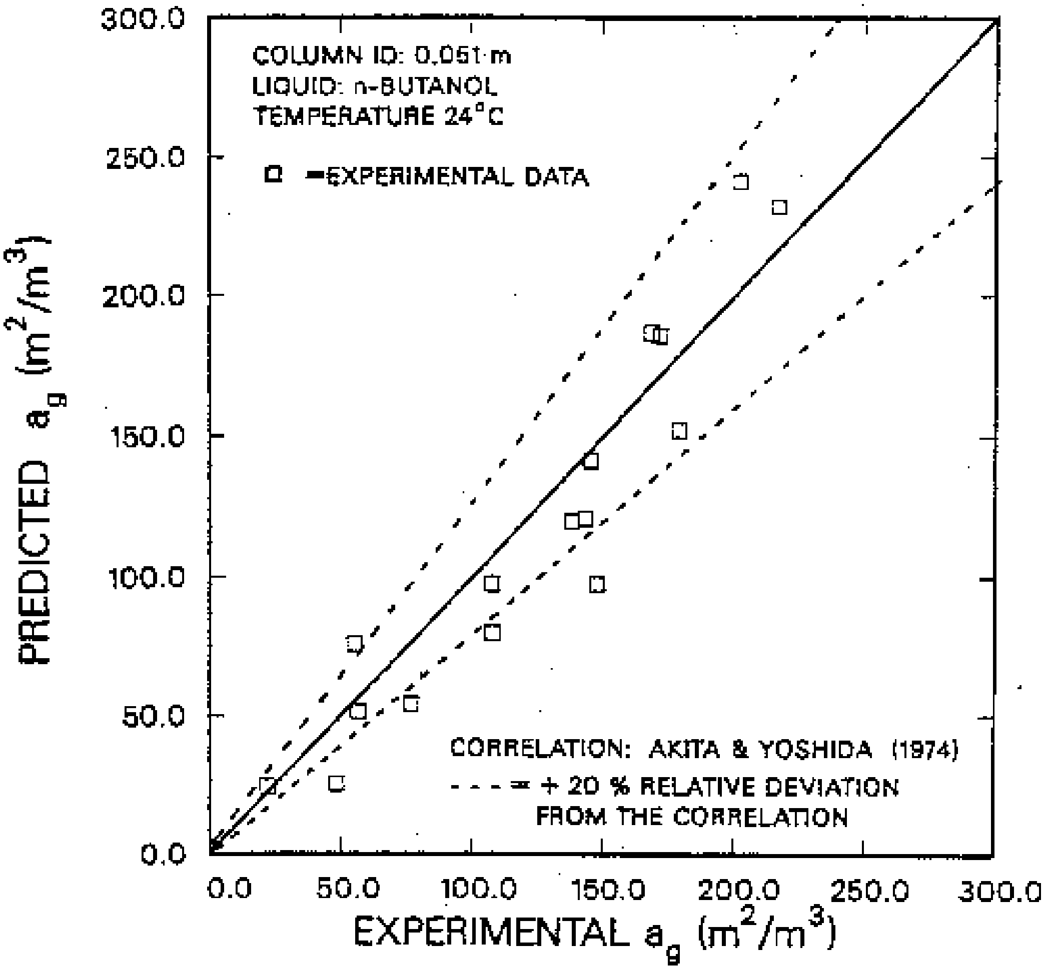

Figure 54. Scatter plot for specific gas-liquid interfacial area for n-butanol in the 0.051 m ID column (Runs B-1 and B-2)

C. Aqueous Solutions of n-Butanol

1. Average Gas Hold-up

The above correlations by Akita and Yoshida, Hikita and Kikukawa, and by Posarac and Tekic are also applicable for predicting gas hold-ups of aqueous solutions of alcohols. Kelkar *et al.* (1983) proposed the following correlation:

$$\epsilon_{go} = \frac{0.96u_g^{0.58}C_N^{0.26}}{1+2.6u_l} \tag{7.12}$$

for prediction of gas hold-ups of aqueous solutions of alcohols. Hold-up data obtained from the 0.051 m ID column using 0.5 wt % butanol with 1.85 mm orifice plate and 40 μm SMP distributors, were predicted better by the correlation developed by Posarac and Tekic (1987). Whereas, the correlation developed by Kelkar *et al.* (1983) overestimates the hold-ups and the correlation developed by Akita and Yoshida underestimates the hold-ups, also the correlation developed by Hikita and Kikukawa (1974). Figure 55 illustrates the predicted hold-ups using Posarac and Tekic correlation within ± 20 % relative deviation. All data from this study are within this range. At high concentration of butanol (1.0 wt %) no single correlation was found to predict the hold-up values in the entire range of gas velocity used in this study (0.01 to 0.12 m/s). It was found that, the correlation developed by Posarac and Tekic predicts the gas hold-up values at low gas velocity (< 0.03 m/s) better than other correlations. Whereas, at high gas velocities, correlation by Kelkar *et al.* (1983) describes the data better than other correlations (see Figure 56).

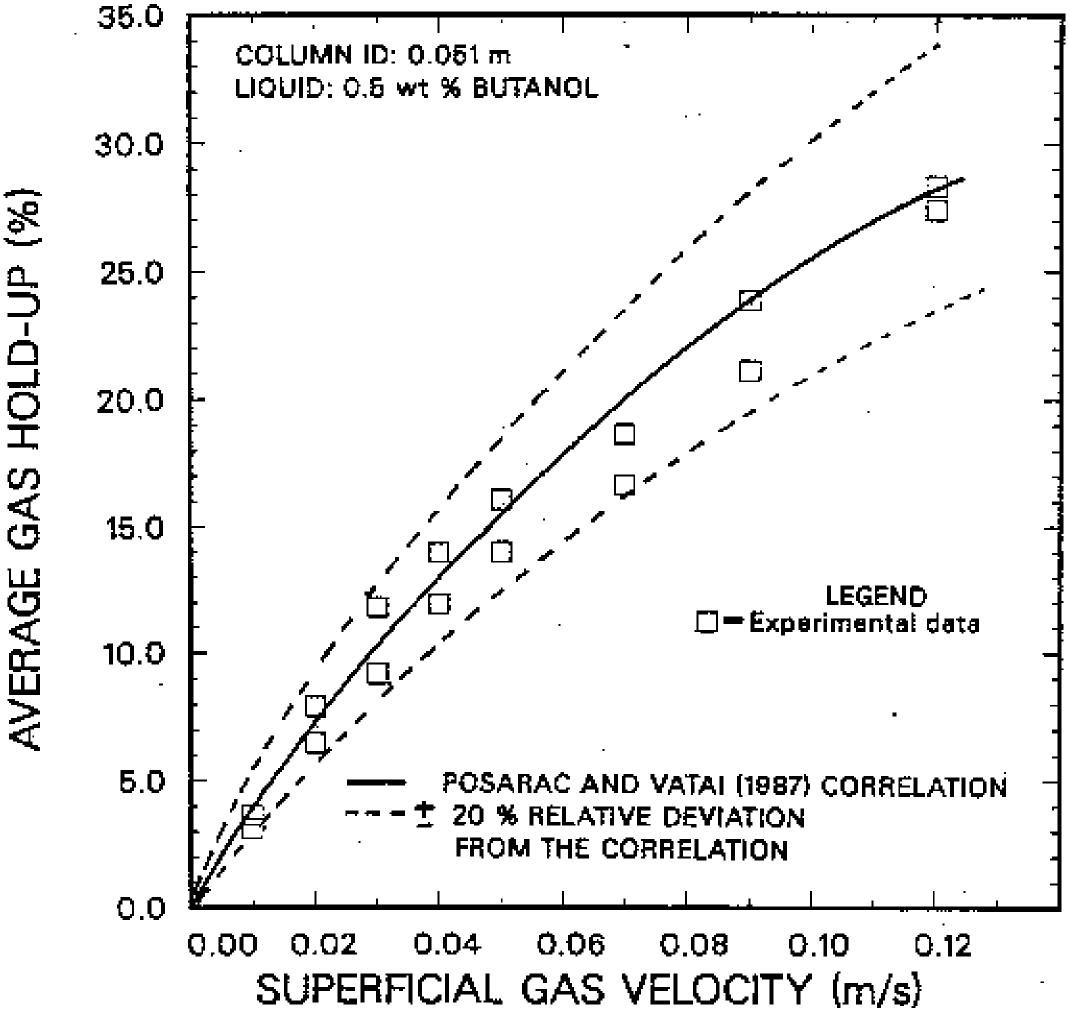

Figure 55. Comparison between experimental hold-ups and hold-ups predicted using the correlation by Posarac and Tekic (1987) within ± 20 % relative deviation (experimental data are from all runs with 0.5 wt % butanol solution).

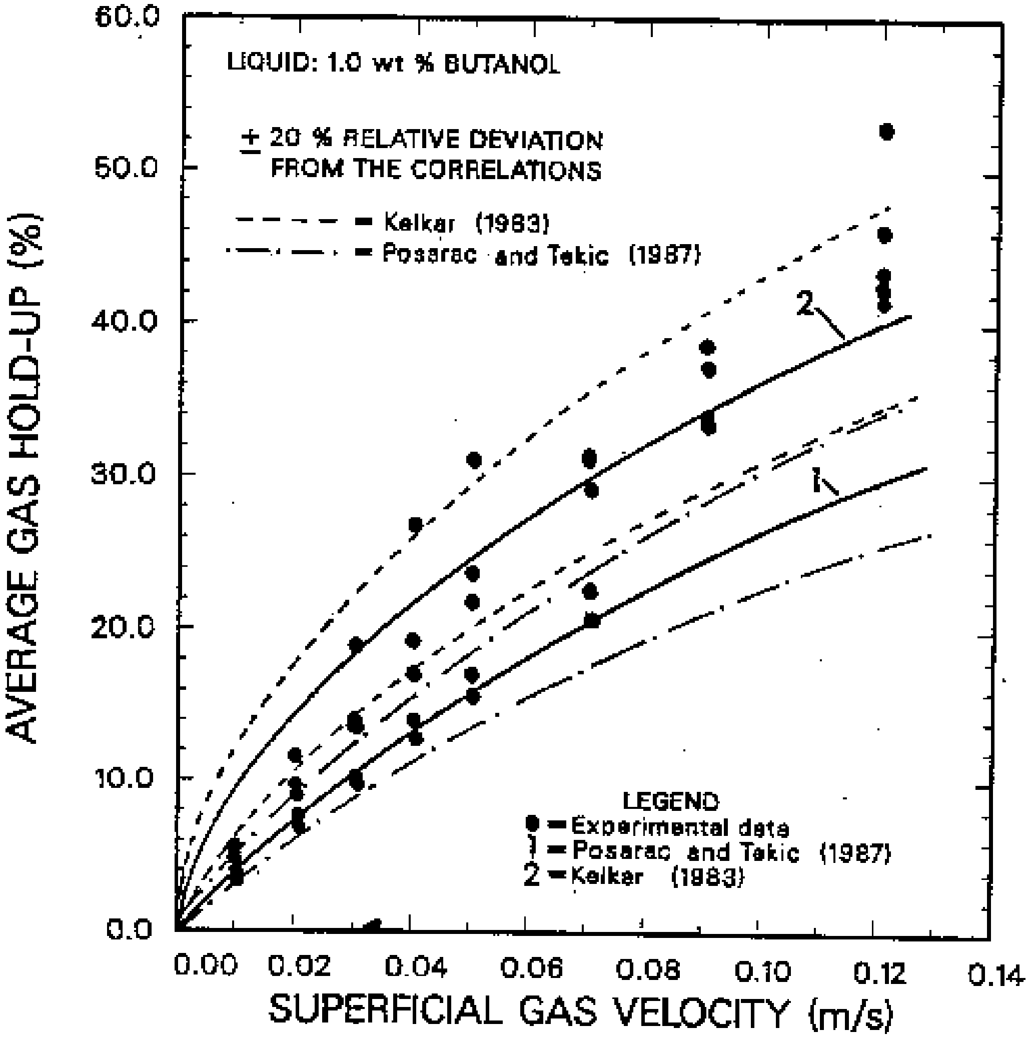

Figure 56. Comparison between experimental hold-ups and hold-ups predicted using correlations by Posarac and Tekic (1987) and by Kelkar (1983) within ± 20 % relative deviation (experimental data are from all runs with 1.0 wt % butanol solution).

2. Specific Gas-Liquid Interfacial Area

The experimental values of specific gas-liquid interfacial area for aqueous solutions of n-butanol (1.0 and 0.5 wt %), were fitted to a correlation similar to that of Akita and Yoshida (1974). Since, the difference in viscosity for the two mixtures is small (0.9 mPa.s for the 0.5 wt % solution compared to 0.912 for the 1.0 wt % solution) and all data were obtained from the 0.051 m ID column. Then the correlation was reduced into the following form;

$$a_g = k_1\left(\frac{g{d_c}^2\rho_l}{\sigma_l}\right)^{k_2}{\epsilon_{go}}^{k_3} \tag{7.13}$$

To obtain the parameters: k_1, k_2, and k_3, the correlation was linearized using log-log and then using the GLM (generalized linear model, package in SAS). The following results were obtained;

Number of data = 27

Mean square error = 0.09

Parameters:

$k_1 = 16.72$

$k_2 = 1.108$

$k_3 = 1.816$

Thus, equation 4.22 becomes;

$$a_g = 16.72\left(\frac{g{d_c}^2\rho_l}{\sigma_l}\right)^{1.108}{\epsilon_{go}}^{1.816} \tag{7.14}$$

The predicted values and the experimental data are compared on the parity plot, Figure 57. About 86 % of the experimental data are within ± 20 % relative deviation, which is a good prediction.

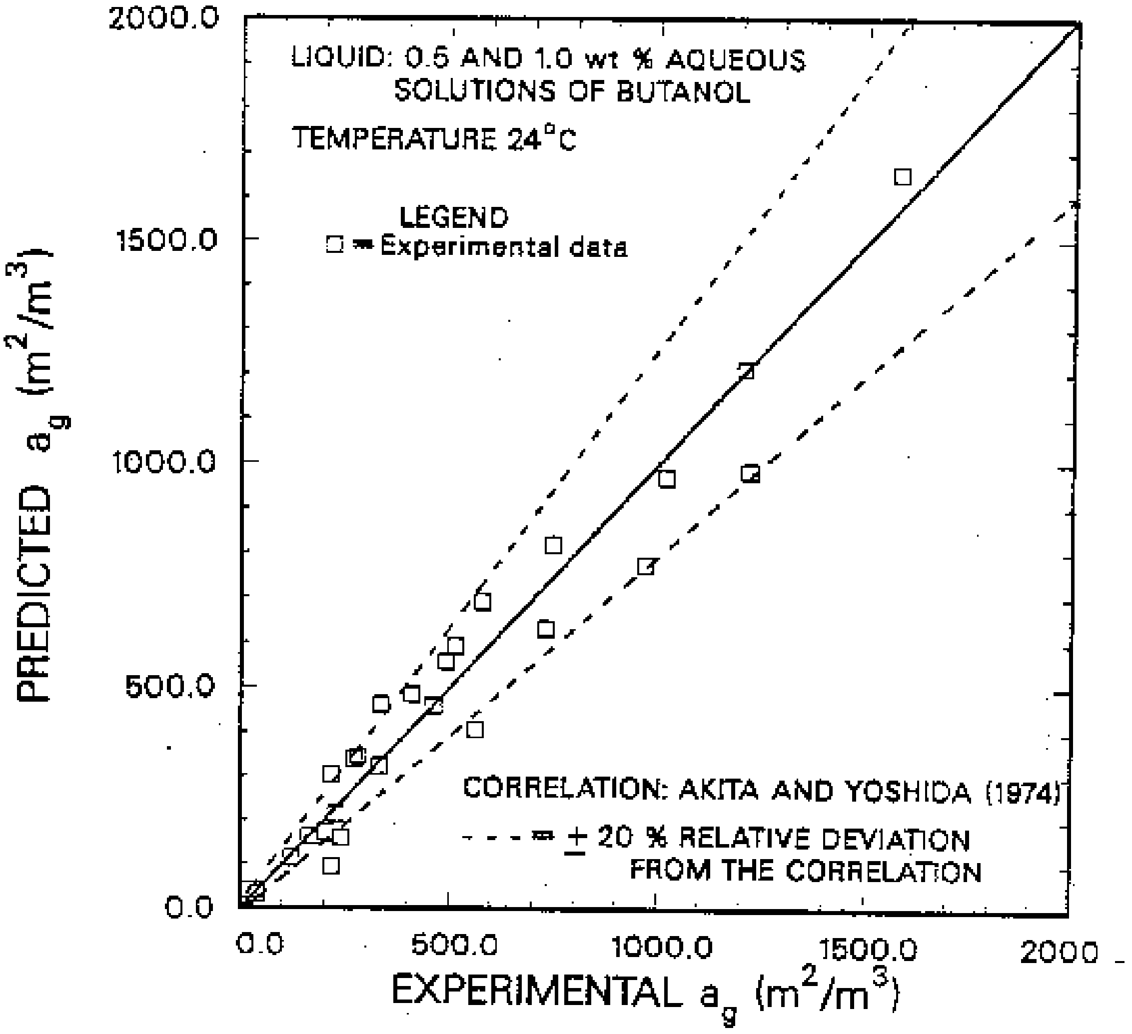

Figure 57. Scatter plot for specific gas-liquid interfacial area for n-butanol solutions in the 0.051 m ID column (Runs B-3, 5, 6, 7, and 8)

D. Aqueous Solutions of n-Butanol With CMC

1. Average Gas Hold-up

The average gas hold-ups for non-Newtonian aqueous solutions using orifice distributors were fitted using the existing correlations from the literature.

1. Vatai and Tekic (1987) correlation:

$$\epsilon_{go} = 0.950 \left(\frac{u_g \mu_l}{\sigma_l}\right)^{0.769} \left(\frac{g \mu_l^4}{\rho_l \sigma_l^3}\right)^{-0.170} \left(\frac{\rho_g}{\rho_l}\right)^{0.062} \left(\frac{\mu_g}{\mu_l}\right)^{0.107} \tag{7.15}$$

2. Haque *et al.* (1986) correlation:

$$\epsilon_{go} = 0.171 u_g^{0.6} \mu_l^{-0.22} d_c^{-0.15} \tag{7.16}$$

Also, equation 7.9 above by Akita and Yoshida (1973) is recommended for the prediction of gas hold-ups for highly viscous non-Newtonian mixtures.

The correlation by Vatai and Tekic (1987) is similar to that by Hikita and Kikukawa (1980), except that the correlation by Vatai and Tekic does take into account the physical properties of the gas used. The correlation developed by Haque *et al.* (1986) is the only correlation in literature which includes the effect of column diameter on gas hold-up for non-Newtonian mixtures. The predicted hold-up values (for the aqueous solution containing 1.0 wt % n-butanol with 0.5 wt % CMC) using the above correlations were plotted against the experimental hold-ups, as shown in Figure 58. In most cases, the predicted hold-ups were lower than the measured hold-ups.

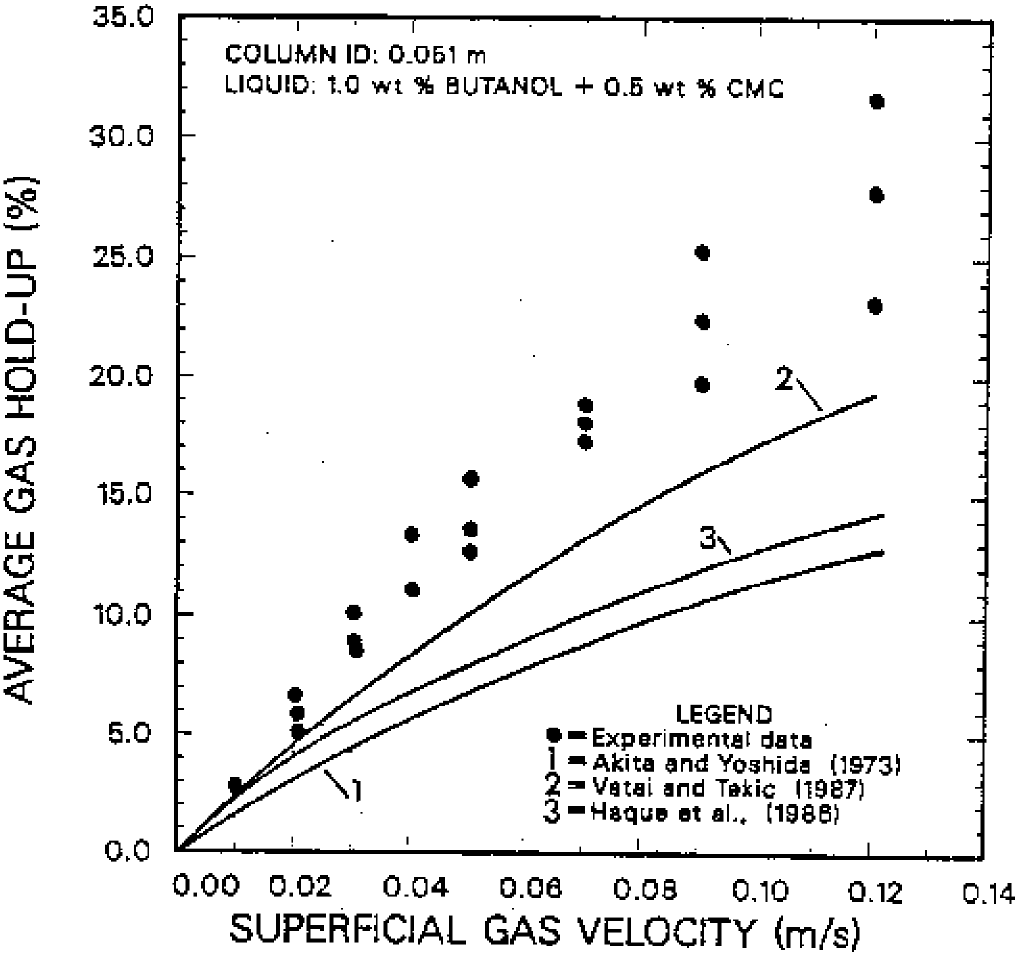

Figure 58. Comparison between experimental hold-ups and predicted hold-ups using literature correlations.

These correlations they partially predict or fail to predict the experimental values at all, because they do not include all parameters which affect the average gas hold-up, such as:

1. Hold-up values increased with increase in gas velocity.
2. Hold-up values decreased with increase in liquid viscosity.
3. For similar mixtures, hold-up values decreased with increase in orifice size of the distributor (in bubbly flow regime).
4. Hold-up values increased as the surface tension of water was decreased.
5. Hold-up values decreased with increase in column diameter for similar liquid mixtures.

In developing a new correlation to fit the experimental data, a dimensionless group Weber number, N_{We}, was introduced to each empirical correlation in order to account for the effect of column diameter and orifice size. Hold-up data obtained from the runs with non-Newtonian mixtures using orifice plates and perforated plates were fit using NLIN (non-linear regression method in SAS) to obtain new parameters. However, the correlation similar to Vatai and Tekic (1987) did not converge after 100 iterations using Gauss-Newton method and Marquardt method. The new developed correlations similar to those of Akita and Yoshida (1973) and Haque *et al.* (1986) had the following parameters:

Correlation 1: Similar to Akita and Yoshida (1973)

$$\frac{\epsilon_{go}}{(1-\epsilon_{go})^4} = k_1 \left(\frac{gD_c{}^2\rho_l}{\sigma_l}\right)^{a_1} \left(\frac{gD_c{}^3\rho_l{}^2}{\mu_l{}^2}\right)^{b_1} \left(\frac{u_g}{\sqrt{gD_c}}\right)^{c_1} \left(\frac{\rho_g u_g{}^2 D_c{}^4}{n^2 d_o{}^3 \sigma_l}\right)^{d_1} \quad (7.17)$$

or in terms of dimensionless groups

$$\frac{\epsilon_{go}}{(1-\epsilon_{go})^4} = k_1 \left(N_{Bo}\right)^{a_1} \left(N_{Ga}\right)^{b_1} \left(N_{Fr}\right)^{c_1} \left(N_{We}\right)^{d_1}$$

Number of data points = 70

Mean square error = 0.073

Parameters:

$k_1 = 0.0317$

$a_1 = -0.0564$

$b_1 = 0.308$

$c_1 = 1.196$

$d_1 = 0.246$

therefore, the correlation is:

$$\frac{\epsilon_{go}}{(1-\epsilon_{go})^4} = 0.0317 \left(N_{Bo}\right)^{-0.0564} \left(N_{Ga}\right)^{0.308} \left(N_{Fr}\right)^{1.196} \left(N_{We}\right)^{0.246} \qquad (7.18)$$

Correlation 2: Similar to Haque *et al.* (1987)

$$\epsilon_{go} = k_2 u_g{}^{a_2} \mu_l{}^{b_2} \left(\frac{\rho_g u_g{}^2 D_c{}^4}{n^2 d_o{}^3 \sigma_l}\right)^{c_2} \qquad (7.19)$$

Number of data points = 70

Mean square error = 0.091

Parameters:

$k_2 = 0.362$

$a_2 = 0.522$

$b_2 = -0.148$

$c_2 = 0.114$

thus, the correlation is:

$$\epsilon_{go} = 0.362 u_g{}^{0.522} \mu_l{}^{-0.148} \left(\frac{\rho_g u_g{}^2 D_c{}^4}{n^2 d_o{}^3 \sigma_l}\right)^{0.114} \qquad (7.20)$$

The correlation 1 fits the experimental data better than correlation 2. Over 89 % of the experimental data are within the ± 30 % relative deviation range for correlation 1 and about 60 % for correlation 2. The parity (scatter) plot for correlation 1 is shown on Figure 59.

Correlation 1 developed above is only applicable for orifice and perforated plate type distributors and not for SMP, because N_{We} is not defined for SMP. Therefore, the gas hold-ups (for non-Newtonian mixtures) obtained using the SMP distributor were correlated using a correlation similar to that described by Godbole *et al.*, 1984

$$\epsilon_{go} = k_1 u_g^{k_2} \mu_l^{k_3} \tag{7.21}$$

Using NLIN procedure to fit the experimental data, the following results were obtained;

Number of data points = 16

Mean square error = 0.35

Parameters:

$k_1 = 1.42$

$k_2 = 1.00$

$k_3 = -0.272$

Thus, equation 7.21 can be written as;

$$\epsilon_{go} = 1.42 u_g^{1.0} \mu_l^{-0.272} \tag{7.22}$$

This correlation predicted over 85 % of the experimental data within ± 20 % relative deviation, see parity (scatter) plot on Figure 60.

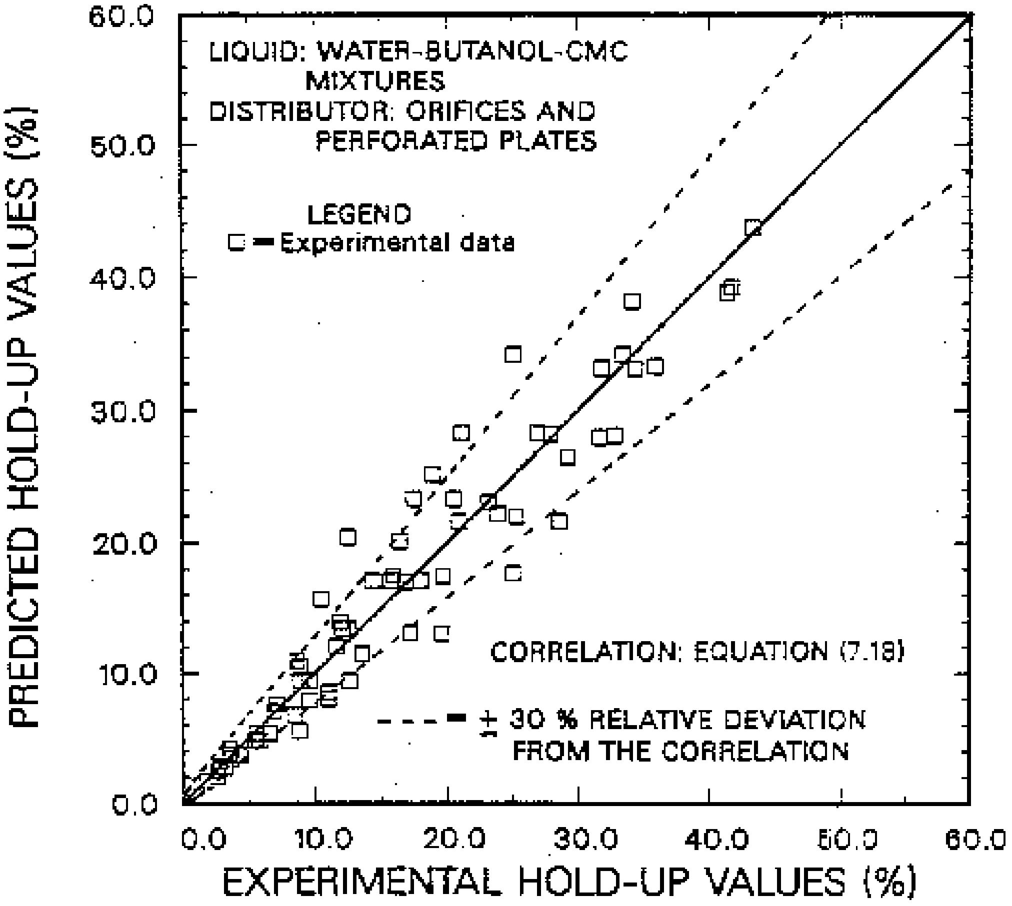

Figure 59. Comparison between experimental hold-ups and predicted hold-ups for mixtures containing water, butanol, and CMC for runs with orifice and perforated plate distributors.

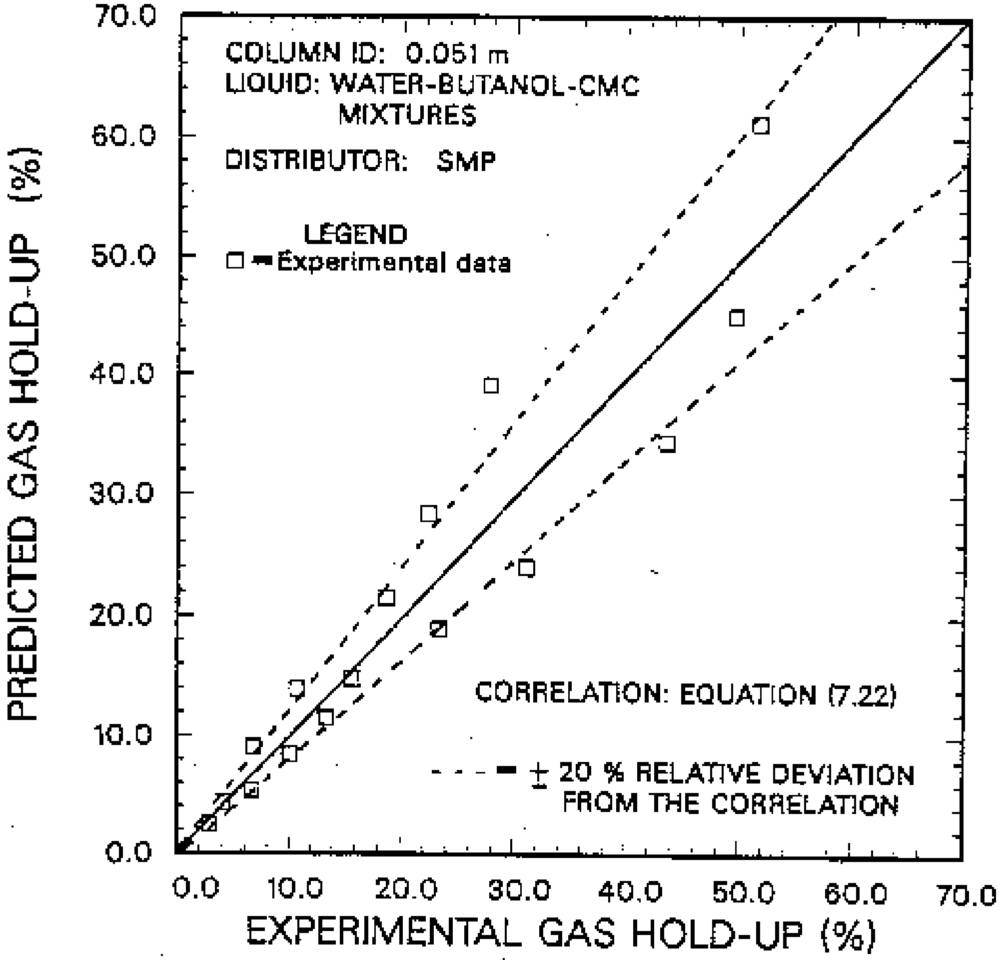

Figure 60. Scatter plot for average gas hold-ups in the 0.051 m ID column using 40 μm SMP distributor for aqueous solutions of n-butanol with CMC (Runs B-9 and B-14)