CHAPTER V

RESULTS AND DISCUSSION

In this work, the Monte-Carlo Technique was used to create random dispersion patterns for single additive systems and binary additive systems. It used mathematical functions to generate pseudo-uniform random numbers and pseudo-normal random numbers, which were used to create specified random dispersion patterns as well as partially and completely ordered materials. The objectives of the computer experiments were to evaluate and quantify additive dispersion states in terms of various quantitative indexes and to identify the suitable indexes that are sensitive to changes in the concentration of particles and in the particle size for single additive systems ,and changes in the concentration ratio, particle size ratio and adhesion probability for binary additive systems, including ordered mixtures. In all simulations the area size was 100 x 100 square.

5.1 Single additive system

In this work, the single additive component system is composed of particles which are monodispersed or have the same particle size. Ideal dispersion of the particles may be either uniform random dispersion, normal random dispersion or a combination of both in the matrix.

5.1.1 Random pattern of additive dispersion

5.1.1.1 Uniform random dispersion

Figure 5.1 shows an example of the uniform random dispersion, in which the concentration of additive particles equals 100 particles/area. The particle diameter is 0.5 unit and the area size is 100 x 100.

5.1.1.2 Normal random dispersion

In this case an example of the normal (Guassian) random dispersion with the concentration of additive equal to 100 particles/area is shown in Figure 5.2. In this figure, it can be seen that the additive particles were randomly dispersed around the center of the sampled area in the fashion of a two-dimensional normal distribution.

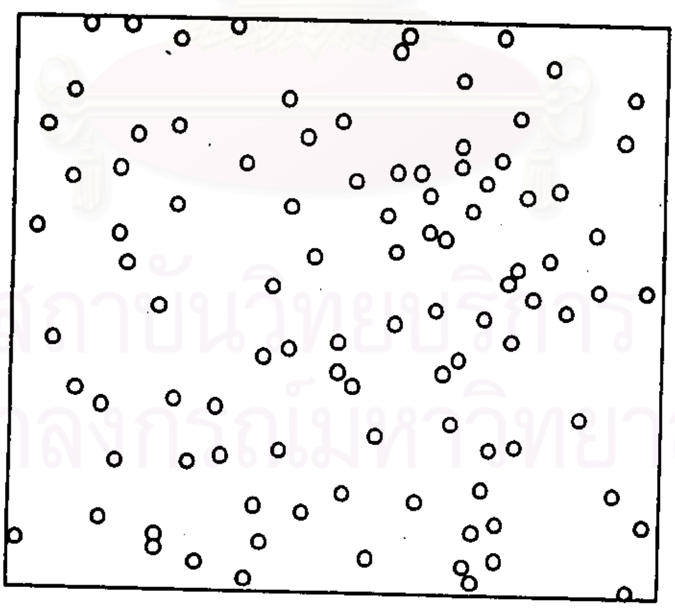

Figure 5.1 Example of uniform random dispersion of additive particles obtained from computer simulation

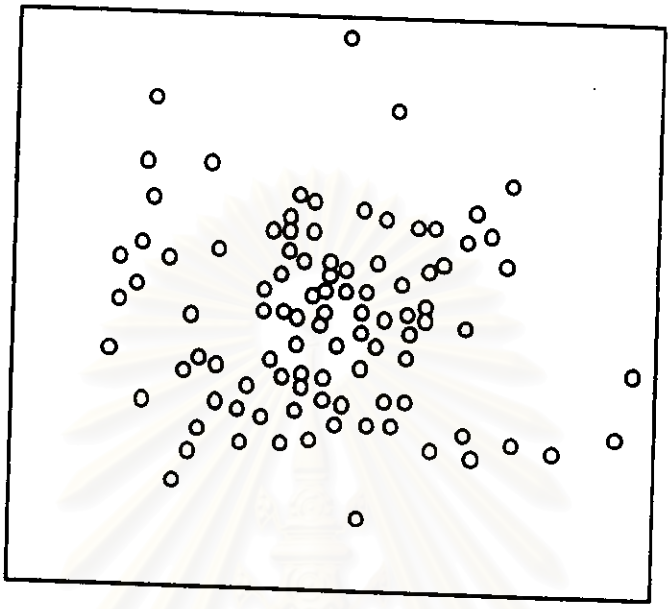

Figure 5.2 Example of normal random dispersion of additive particles obtained from computer simulation

5.1.2 Effect of concentration

The effect of the concentration of additive particles on the quantifying indexes was investigated at 50, 100, 200, 500, 1000, 1500, 2000, 2500, 3000, 5000, and 10000 particles/area, while the particle size of the monodispersed additive was constant at 0.5 unit.

5.1.2.1 Degree of mixedness

The relationship between the concentration and observed degree of mixedness in the case of additive particle size D = 0.5 unit was listed in Table 5.1 and shown in Figure 5.3 .

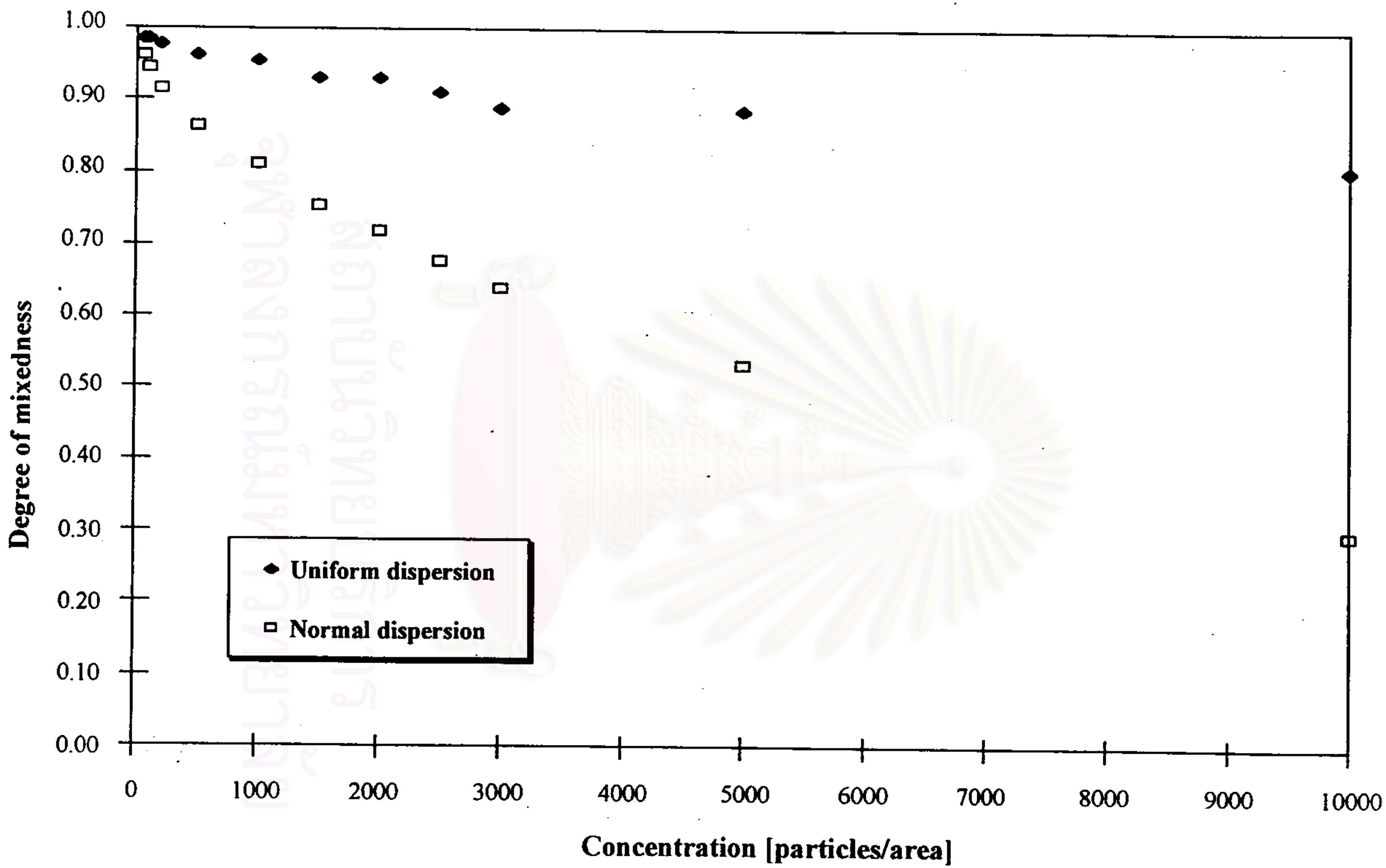

Figure 5.3 Relationship between the concentration and degree of mixedness (D = 0.5 unit).

Table 5.1 The relationship between the concentration and degree of mixedness : additive particle size D = 0.5 unit.

Concentration [number/area]	Degree of mixedness (M)	
	Uniform random dispersion	Normal random dispersion
50	0.9844	0.9628
100	0.9849	0.9459
200	0.9780	0.9168
500	0.9636	0.8630
1000	0.9556	0.8110
1500	0.9305	0.7544
2000	0.9304	0.7189
2500	0.9111	0.6783
3000	0.8874	0.6406
5000	0.8856	0.5345
10000	0.8069	0.2983

From Figure 5.3 , it can be seen that the observed degree of mixedness for both the ideal uniform and normal random dispersions decreased as the concentration increased. Obviously, when the concentration increased, the degree of mixedness for normal random dispersion remarkably decreased faster than for uniform random dispersion.

5.1.2.2 Count-based fractal dimension

Similarly, the relationship between the concentration and observed count-based fractal dimension in the case of additive particle size D = 0.5 unit was listed in Table 5.2 and shown in Figure 5.4.

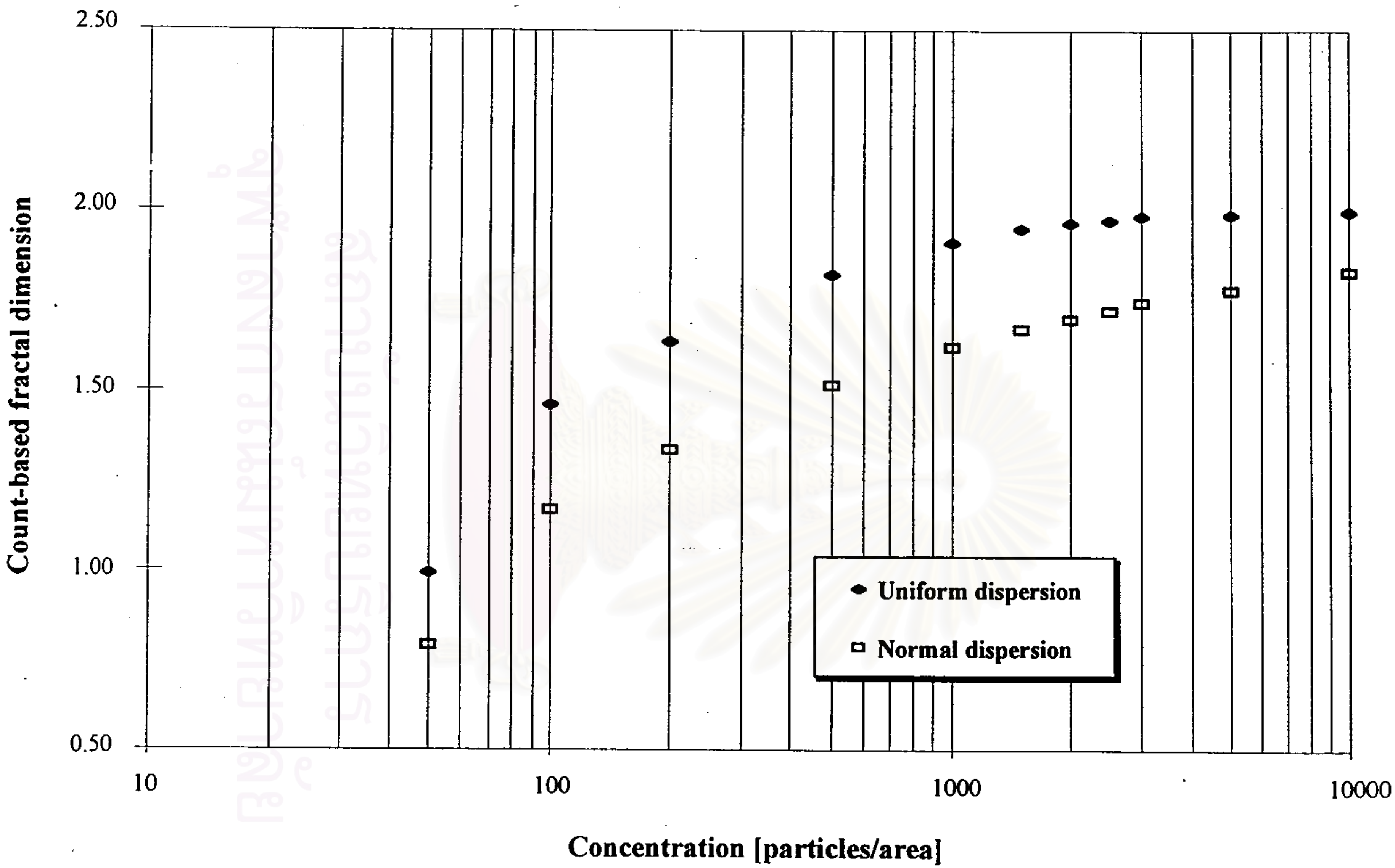

Figure 5.4 Relationship between the concentration and count-based fractal dimension (D = 0.5 unit).

Table 5.2 The relationship between the concentration and count-based fractal dimension : additive particle size D = 0.5 unit.

Concentration [number/area]	Count-based fractal dimension (F_C)	
	Uniform random dispersion	Normal random dispersion
50	0.9930	0.7884
100	1.4597	1.1674
200	1.6340	1.3350
500	1.8210	1.5151
1000	1.9110	1.6193
1500	1.9510	1.6701
2000	1.9660	1.6967
2500	1.9740	1.7219
3000	1.9850	1.7424
5000	1.9900	1.7781
10000	1.9970	1.8279

From the results in Figure 5.4, it can be seen that the count-based fractal dimension for both the uniform and normal dispersions increased rapidly when the concentration first increased. As the concentration further increased, the count-based fractal dimension increased more gradually and approached an asymptote of 2. Furthermore, the count-based fractal dimension for the ideal uniform random dispersion was always greater than for the normal random dispersion. More specifically, the count-based fractal dimension for the uniform random dispersion ranged from 0.99 to almost 2.0, whereas the corresponding values for the normal random dispersion ranged from 0.78 to 1.83 .

To eliminate the influence of concentration, the relationship between the concentration and the normalized count-based fractal dimension for the normal random dispersion (the count-based fractal dimension for normal dispersion was divided by the respective value for uniform dispersion) was listed in Table 5.3 and shown in Figure 5.5.

Table 5.3 The relationship between the concentration and normalized count-based fractal dimension (F_C^*) : additive particle size D = 0.5 unit.

Concentration [number/area]	Normalized count-based fractal dimension (F_C^*)
50	0.7940
100	0.7998
200	0.8170
500	0.8320
1000	0.8473
1500	0.8560
2000	0.8630
2500	0.8723
3000	0.8778
5000	0.8935
10000	0.9153

From Figure 5.5, it can be seen that the normalized count-based fractal dimension increased as the concentration increased.

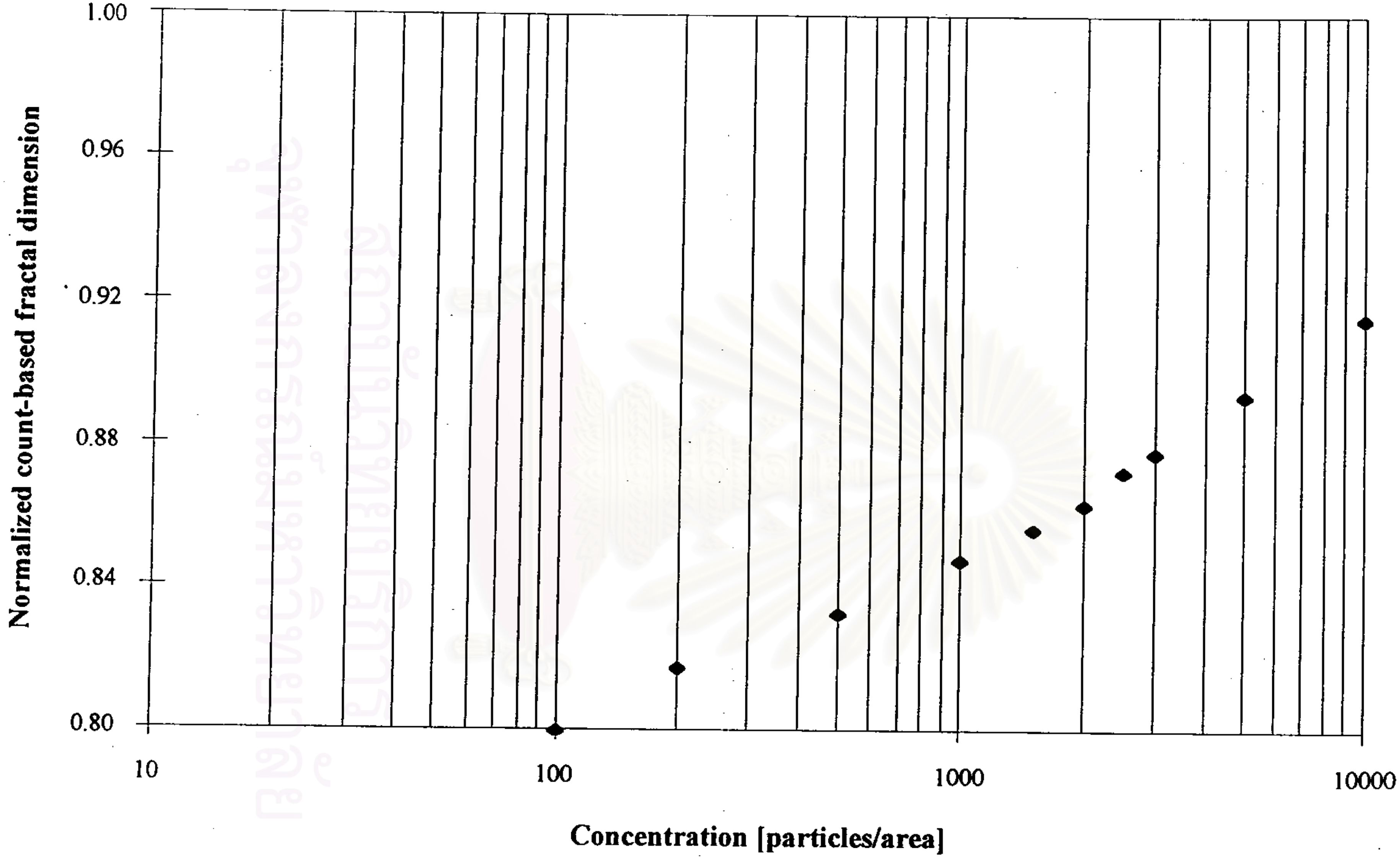

Figure 5.5 Relationship between the concentration and normalized count-based fractal dimension (D = 0.5 unit).

5.1.2.3 Area-based fractal dimension

Table 5.4 and Figure 5.6 show the relationship between the concentration and observed area-based fractal dimension in the case of additive particle size D = 0.5 unit.

Table 5.4 The relationship between the concentration and area-based fractal dimension : additive particle size D = 0.5 unit.

Concentration [number/area]	Area-based fractal dimension (F_A)	
	Uniform random dispersion	Normal random dispersion
50	0.9976	0.9313
100	1.0133	0.8778
200	0.9986	0.7722
500	1.0008	0.5704
1000	0.9943	0.4038
1500	1.0075	0.3036
2000	0.9969	0.2583
2500	0.9972	0.2220
3000	0.9947	0.1898
5000	1.0015	0.1208
10000	0.9973	0.0687

As seen from Figure 5.6 , the area-based fractal dimension for the ideal uniform random dispersion remained essentially constant around unity, while that for the normal random dispersion decreased rapidly with the concentration. Clearly, when too small a number of particles are present in a sample, it is hard to distinguish between good and bad dispersions.

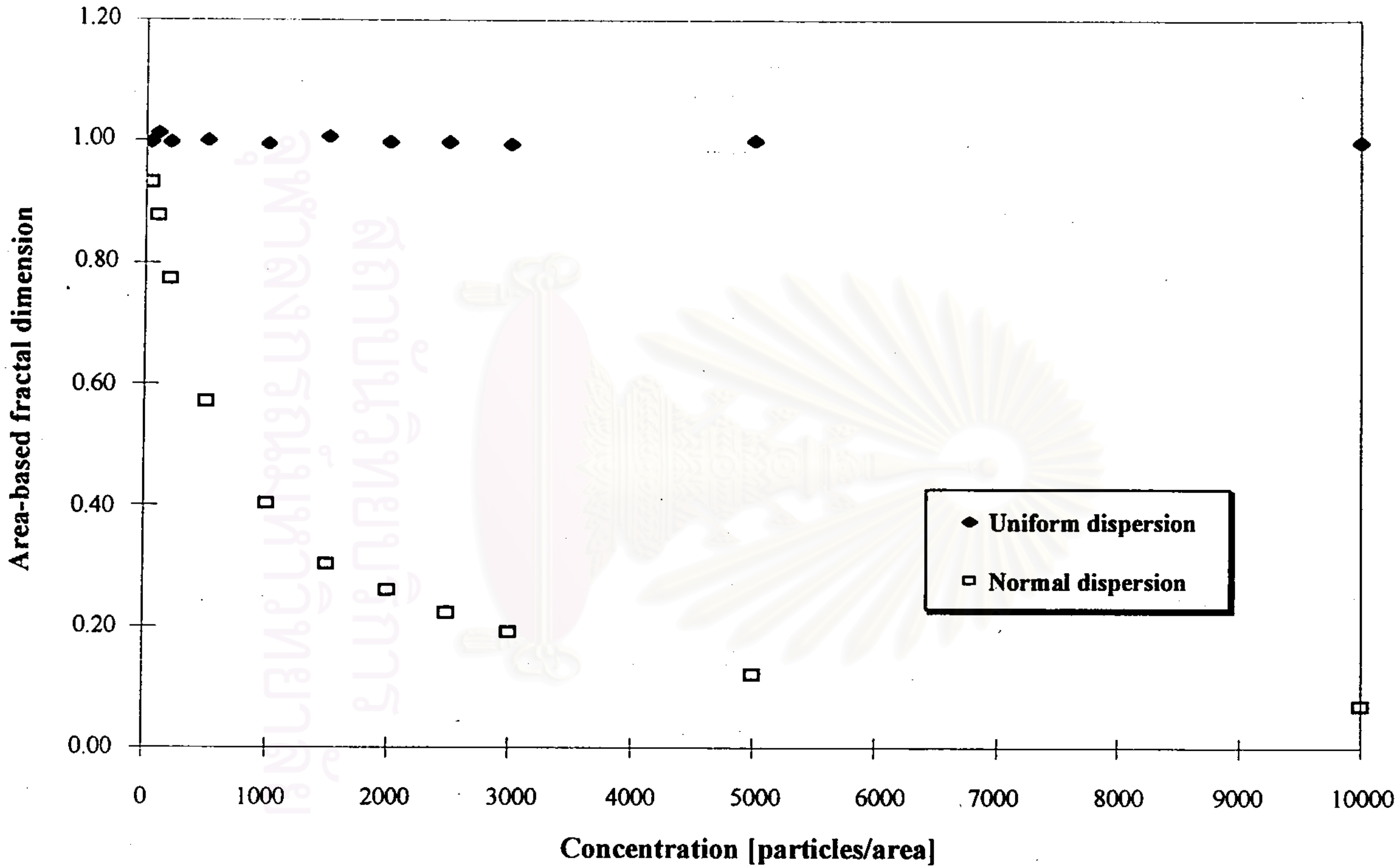

Figure 5.6 Relationship between the concentration and area-based fractal dimension (D = 0.5 unit).

Generally speaking, the area-based fractal dimension is a more accurate and robust measure of dispersibility than the count-based fractal dimension and the degree of mixedness. In the case of ideal uniform random dispersion, the area-based fractal dimension remains essentially unity (between 0.98 and 1.02) regardless of the concentration. In the case of normal random dispersion, the area-based fractal dimension dropped rapidly to 0.06 as the concentration increased. This confirms the common sense that the larger the concentration, the easier the differentiation between the normal random and uniform random dispersions.

5.1.3 Effect of particle size

The particle size of an additive could possibly affect some quantifying indexes. Thus the particle size was varied as 0.5, 0.2, and 0.1 unit, while the concentration was changed from 50 to 10000 as follows.

5.1.3.1 Degree of mixedness

The relationship between the particle size and the observed degree of mixedness was listed in Table 5.5 and shown in Figure 5.7.

From Figure 5.7, it can be seen that the observed degree of mixedness for both the ideal uniform and normal random dispersions at the same concentration decreased as the particle size increased. In the case of normal random dispersion, the degree of mixedness dropped significantly when the particle size is greater than 0.2 unit. In any case the higher the concentration, the easier it is to distinguish between uniform random dispersion and normal random dispersion. On the other hand, the sensitivity of this index decreases remarkably as the particle size decreases from 0.5 to 0.1.

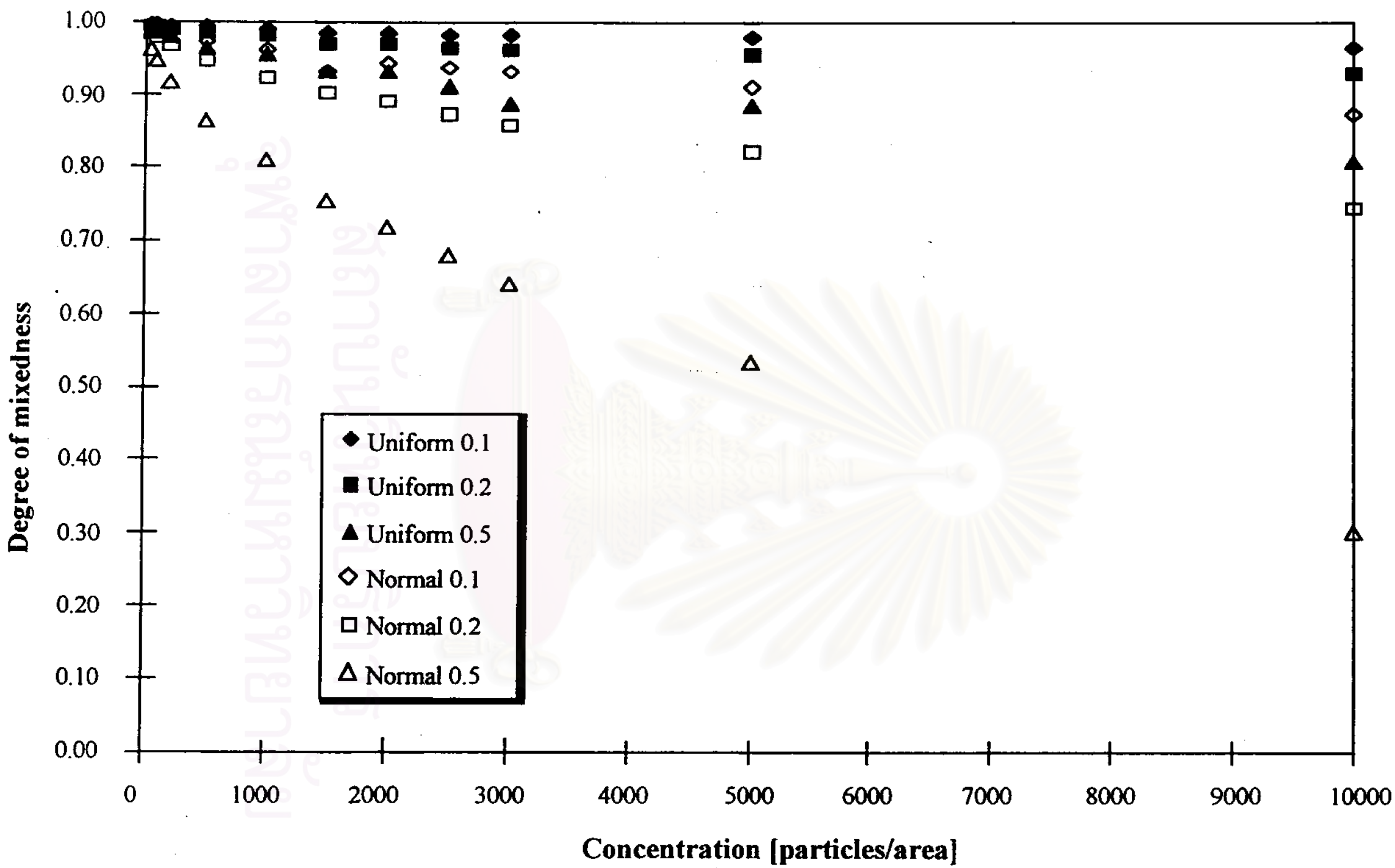

Figure 5.7 Effect of particle size on the relationship between the concentration and degree of mixedness.

Since a general quantitative index for evaluating the dispersion state should not be influenced by the observed concentration or the particle size, the degree of mixedness fails to qualify.

Table 5.5 Effect of particle size on the relationship between the particle size and degree of mixedness.

Concentration	Degree of mixedness					
	Uniform random dispersion			Normal random dispersion		
	particle size (unit)					
[number/area]	0.5	0.2	0.1	0.5	0.2	0.1
50	0.9844	0.9945	0.9967	0.9628	0.9838	0.9923
100	0.9849	0.9942	0.9967	0.9459	0.9794	0.9892
200	0.9780	0.9913	0.9955	0.9168	0.9682	0.9845
500	0.9636	0.9860	0.9932	0.8630	0.9452	0.9733
1000	0.9556	0.9812	0.9909	0.8110	0.9227	0.9615
1500	0.9305	0.9715	0.9858	0.7544	0.9011	0.9310
2000	0.9304	0.9714	0.9856	0.7189	0.8891	0.9435
2500	0.9111	0.9640	0.9821	0.6783	0.8736	0.9374
3000	0.8874	0.9609	0.9814	0.6406	0.8588	0.9308
5000	0.8856	0.9558	0.9780	0.5345	0.8215	0.9112
10000	0.8069	0.9284	0.9646	0.2983	0.7441	0.8724

5.1.3.2 Count-based fractal dimension

Similarly, the relationship between the particle size and the observed count-based fractal dimension was listed in Table 5.6 and shown in Figure 5.8.

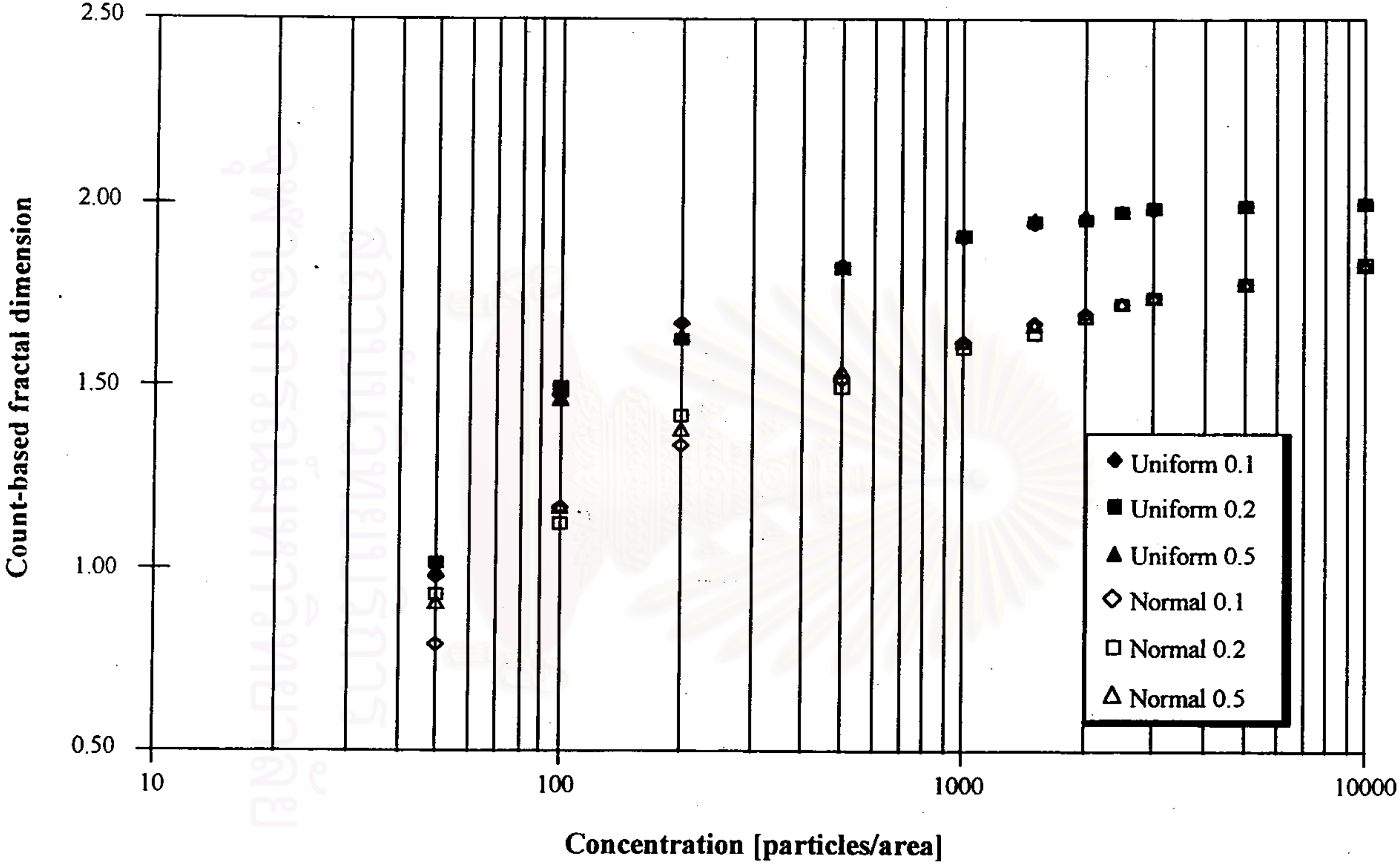

Figure 5.8 Effect of particle size on the relationship between the concentration and count-based fractal dimension.

Table 5.6 Relationship between the particle size and count-based fractal dimension.

Concentration	Count-based fractal dimension (F_C)					
	Uniform random dispersion			Normal random dispersion		
	particle size (unit)					
[number/area]	0.5	0.2	0.1	0.5	0.2	0.1
50	0.9930	1.0115	0.9755	0.7884	0.9286	0.8839
100	1.4597	1.4960	1.4730	1.1674	1.1230	1.1997
200	1.6340	1.6260	1.6720	1.3350	1.4197	1.3588
500	1.8210	1.8234	1.8260	1.5151	1.4922	1.4974
1000	1.9110	1.9108	1.9042	1.6193	1.6047	1.6115
1500	1.9510	1.9480	1.9410	1.6701	1.6414	1.6534
2000	1.9660	1.9537	1.9534	1.6967	1.6856	1.6962
2500	1.9740	1.9736	1.9738	1.7219	1.7235	1.7233
3000	1.9850	1.9847	1.9836	1.7424	1.7431	1.7456
5000	1.9900	1.9896	1.9904	1.7781	1.7782	1.7772
10000	1.9970	1.9967	1.9963	1.8279	1.8310	1.8278

From Table 5.6 and Figure 5.8, it can be seen that the observed count-based fractal dimension at the same concentration for either type of ideal dispersions was only slightly affected by the particle size difference. At very high concentrations (more than 5000 particles/area), the observed count-based fractal dimension for the ideal uniform and normal random dispersions remained essentially constant around 2.0 and 1.83, respectively, regardless of the particle size. One conclusion is that, as a quantitative index, the count-based fractal dimension is fairly sensitive to the difference in the two ideal dispersions.

5.1.3.3 Area-based fractal dimension

Table 5.7and Figure 5.9 show the relationship between the particle size and the observed area-based fractal dimension.

Table 5.7 The relationship between the particle size and area-based fractal dimension.

Concentration	Area-based fractal dimension (F_A)					
	Uniform random dispersion			Normal random dispersion		
	particle size (unit)					
[number/area]	0.5	0.2	0.1	0.5	0.2	0.1
50	0.9976	1.0289	0.9797	0.9313	0.9373	0.9130
100	1.0133	1.0088	1.0128	0.8778	0.8988	0.8825
200	0.9986	0.9850	0.9951	0.7722	0.7734	0.7814
500	1.0008	1.0040	1.0213	0.5702	0.5818	0.5687
1000	0.9943	1.0033	0.9759	0.4038	0.4060	0.4103
1500	1.0075	0.9892	1.0086	0.3036	0.3019	0.3027
2000	0.9969	0.9870	0.9845	0.2583	0.2610	0.2547
2500	0.9972	0.9755	1.0033	0.2220	0.2189	0.2254
3000	0.9947	0.9977	0.9852	0.1898	0.1907	0.1890
5000	1.0015	0.9946	0.9968	0.1208	0.1236	0.1199
10000	0.9973	1.0115	0.9890	0.0687	0.0719	0.0679

At the same concentration, Table 5.7 and Figure 5.9 reveal that the area-based fractal dimension for both the ideal uniform and normal random dispersions was hardly affected by the particle size. One important feature is that the area-based fractal dimension is highly sensitive to the difference between good (uniform) and bad (normal) dispersions. The higher the concentration, the more sensitive the area-based fractal dimension.

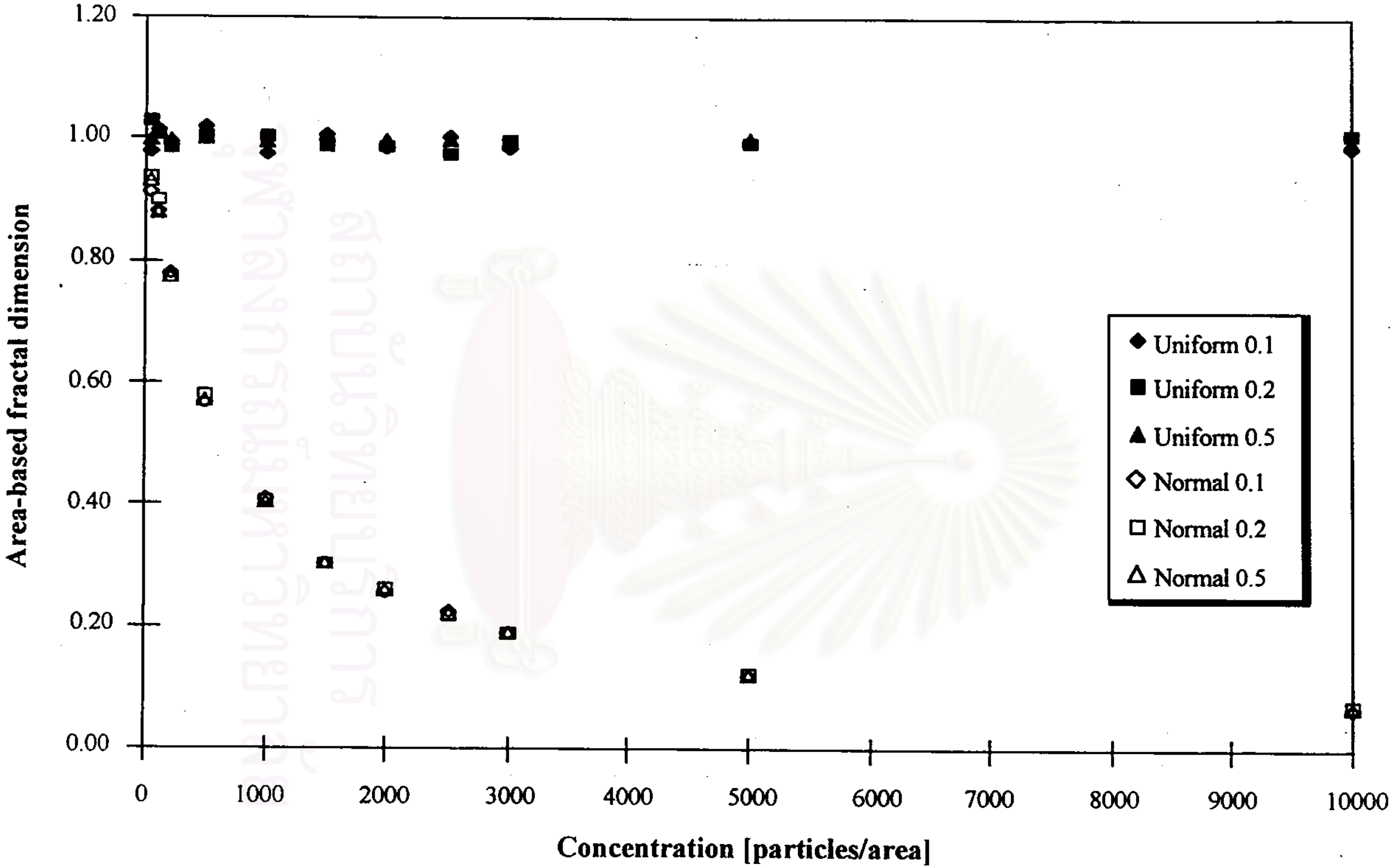

Figure 5.9 Effect of particle size on the relationship between the concentration and area-based fractal dimension.

5.1.4 Effect of nonideal dispersion

Consider a nonideal dispersion in which a portion of the particles (population) follows the ideal uniform random dispersion and the rest follows the ideal normal random dispersion. For convenience, the former will be called A particles and the latter B particles, even though in reality they are exactly the same here. In other words, the system is still single component.

The purpose here is to see what happens to the count-based and area-based fractal dimensions when the ratio of A to B particles is varied to yield a nonideal dispersion, a hybrid mixture of two ideal dispersions.

A so-called "normal-uniform ratio" (N-U ratio) is used here to indicate the degree of nonideality of the dispersion. The N-U or B-A ratios used in the following investigation are :

0:100(uniform), 25:75, 50:50, 75:25, 100:0 (normal)

← most uniform least uniform →

For simplicity, only the percentage of B particles will be specified from now on.

5.1.4.1 Count-based fractal dimension

The relationship between the total concentration and the observed count-based fractal dimension in the case of additive particle size D = 0.5 unit was listed in Table 5.8 and depicted in Figure 5.10.

Figure 5.10 reveals that for every fixed N-U the count-based fractal dimension increased, as the total concentration increased. Especially, at low concentration, the count-base fractal dimension increased rapidly. This is because the absolute number of A particles which were dispersed uniformly increased.

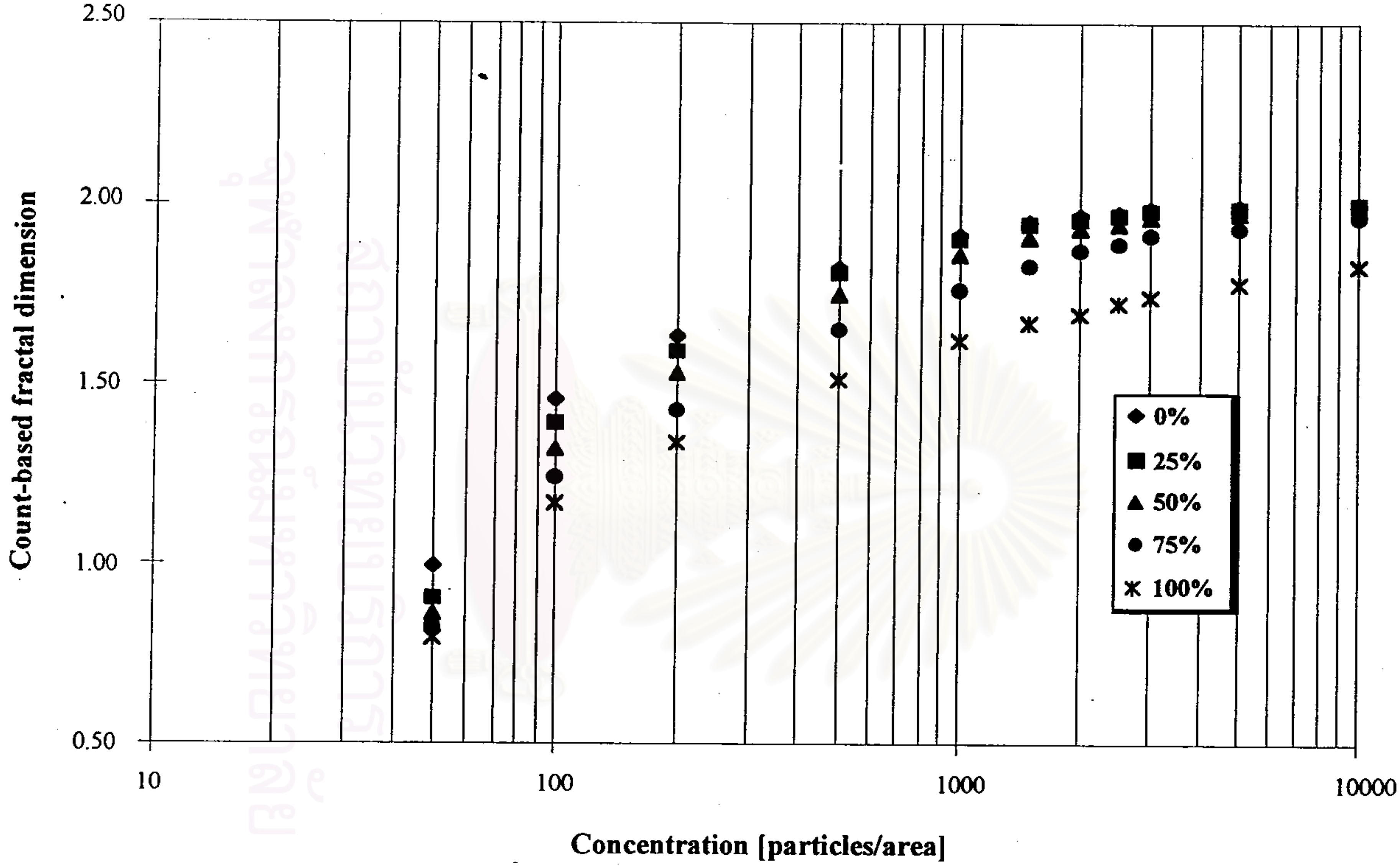

Figure 5.10 Relationship between the total concentration and count-based fractal dimension (D = 0.5 unit) at each N-U ratio.

On the other hand, at a fixed concentration the differences in the count-based fractal dimension among different N-U ratios are less distinct at 0% to 50%.

Table 5.8 The relationship between the total concentration and the count-based fractal dimension at each N-U ratio (additive particle size D = 0.5 unit).

Total concentration [particles/area]	Count-based fractal dimension				
	N-U ratio				
	0%	25%	50%	75%	100%
50	0.9930	0.8977	0.8560	0.8202	0.7884
100	1.4597	1.3896	1.3210	1.2364	1.1674
200	1.6340	1.5899	1.5332	1.4298	1.3350
500	1.8210	1.8068	1.7501	1.6487	1.5151
1000	1.9110	1.9015	1.8593	1.7632	1.6193
1500	1.9510	1.9432	1.9081	1.8261	1.6701
2000	1.9660	1.9542	1.9286	1.8677	1.6967
2500	1.9740	1.9666	1.9411	1.8870	1.7219
3000	1.9850	1.9808	1.9591	1.9128	1.7424
5000	1.9900	1.9860	1.9710	1.9315	1.7781
10000	1.9970	1.9943	1.9865	1.9600	1.8279

5.1.4.2 Area-based fractal dimension

The relationship between the total concentration and the observed area-based fractal dimension in the case of additive particle size D = 0.5 unit was listed in Table 5.9 and shown in Figure 5.11.

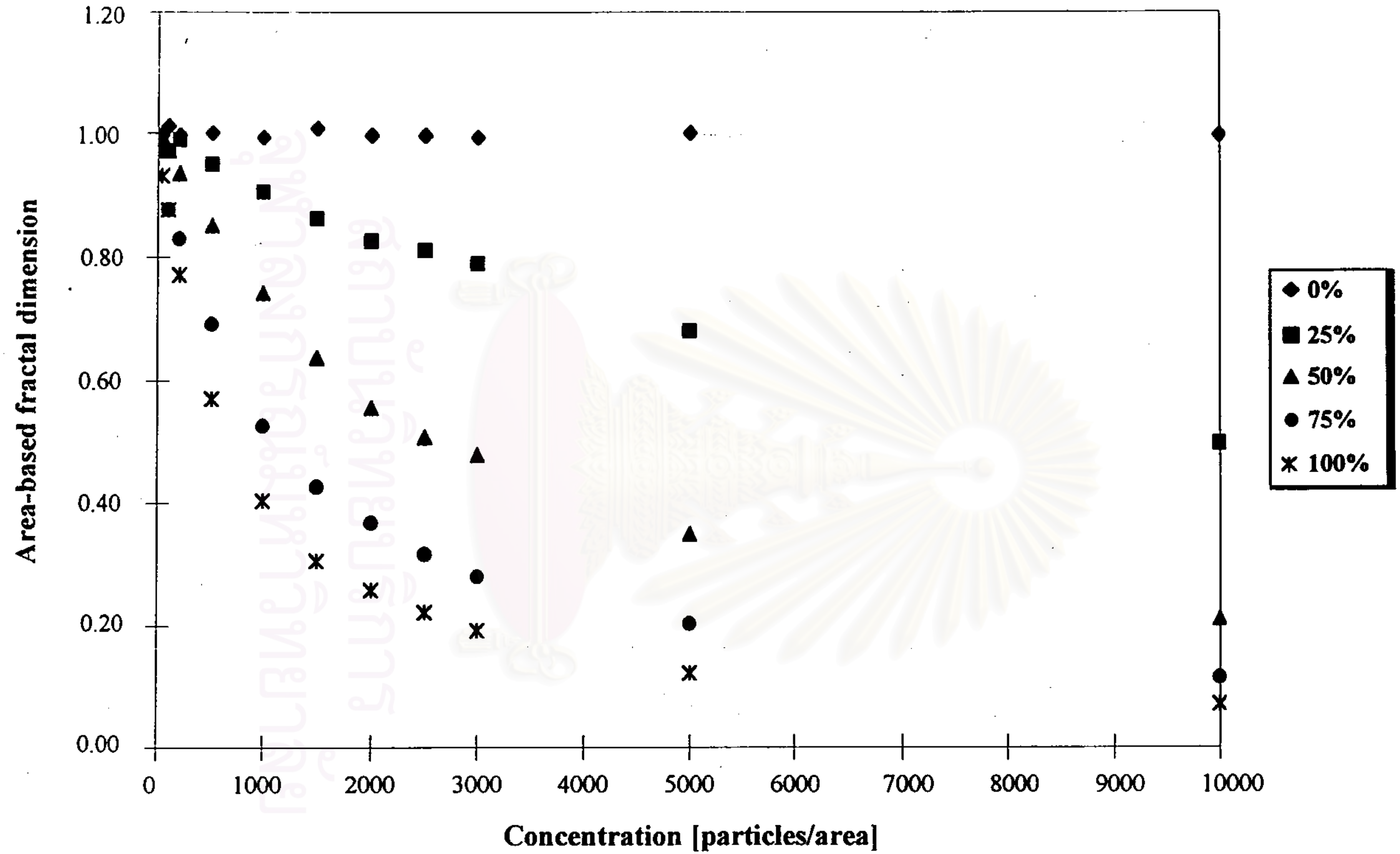

Figure 5.11 Relationship between the total concentration and area-based fractal dimension (D = 0.5 unit) at each N-U ratio.

Figure 5.11 shows that the area-based fractal dimension for every fixed N-U ratio decreased steeply, as the total concentration increased except at B 0% (ideal uniform). This is because the absolute number of B particles which follow the normal random dispersion increased. Thus it may be concluded that the area-based fractal dimension is a sensitive index of the nonideality of a dispersion. The higher the total concentration, the more sensitive the area-based fractal dimension.

Table 5.9 The relationship between the total concentration and the area-based fractal dimension at each N-U ratio (additive particle size D = 0.5 unit).

Total concentration [particles/area]	Area-based fractal dimension				
	N-U ratio				
	0%	25%	50%	75%	100%
50	0.9976	0.9756	0.9963	0.9710	0.9313
100	1.0133	0.9741	0.9710	0.8769	0.8778
200	0.9986	0.9924	0.9352	0.8285	0.7722
500	1.0008	0.9493	0.8526	0.6903	0.5704
1000	0.9943	0.9049	0.7405	0.5233	0.4038
1500	1.0075	0.8633	0.6345	0.4250	0.3036
2000	0.9969	0.8268	0.5540	0.3654	0.2583
2500	0.9972	0.8113	0.5067	0.3140	0.2220
3000	0.9947	0.7907	0.4754	0.2800	0.1898
5000	1.0015	0.6777	0.3475	0.2000	0.1208
10000	0.9973	0.4970	0.2091	0.1128	0.0687

5.2 Binary additive systems

The investigated binary additive systems consist of monodisperse A particles and B particles. The size of A particles is 0.5 unit and the concentration of A particles is always 500 particles/area, whereas the size of B particles is either 0.01, 0.02, 0.05 or 0.1 unit. The dimension of the sample area is 100 x 100 square. The concentration of B particles is either 1, 2, 5 or 10 times the concentration of A particles (500, 1000, 2500, 5000 B particles/area). First, A particles (core particles) are randomly dispersed in the matrix sample area. Next, B particles are generated one by one and are either randomly dispersed in the matrix or made to adhere onto some A particles according to the adhesion probability. Dispersion of A particles may be either uniform or normal random dispersion, and likewise B particles may be of either uniform or normal dispersion. Figures 5.12 to 5.14 show some examples of the simulated dispersion of the binary additive system.

It is important to note that if attention is focused on A particles alone (concentration of A = 500 particles/area), all the results and conclusions obtained for the single component system will be applicable. Therefore, all subsequent analyses and discussions will deal with B particles alone or with A plus B particles together (i.e. without differentiation between A and B).

It should be noted that two major differences exist between the nonideal single component system and the binary component system. First, A and B are of equal size in the former system. Second, B particles do not adhere onto any A particle in the former system.

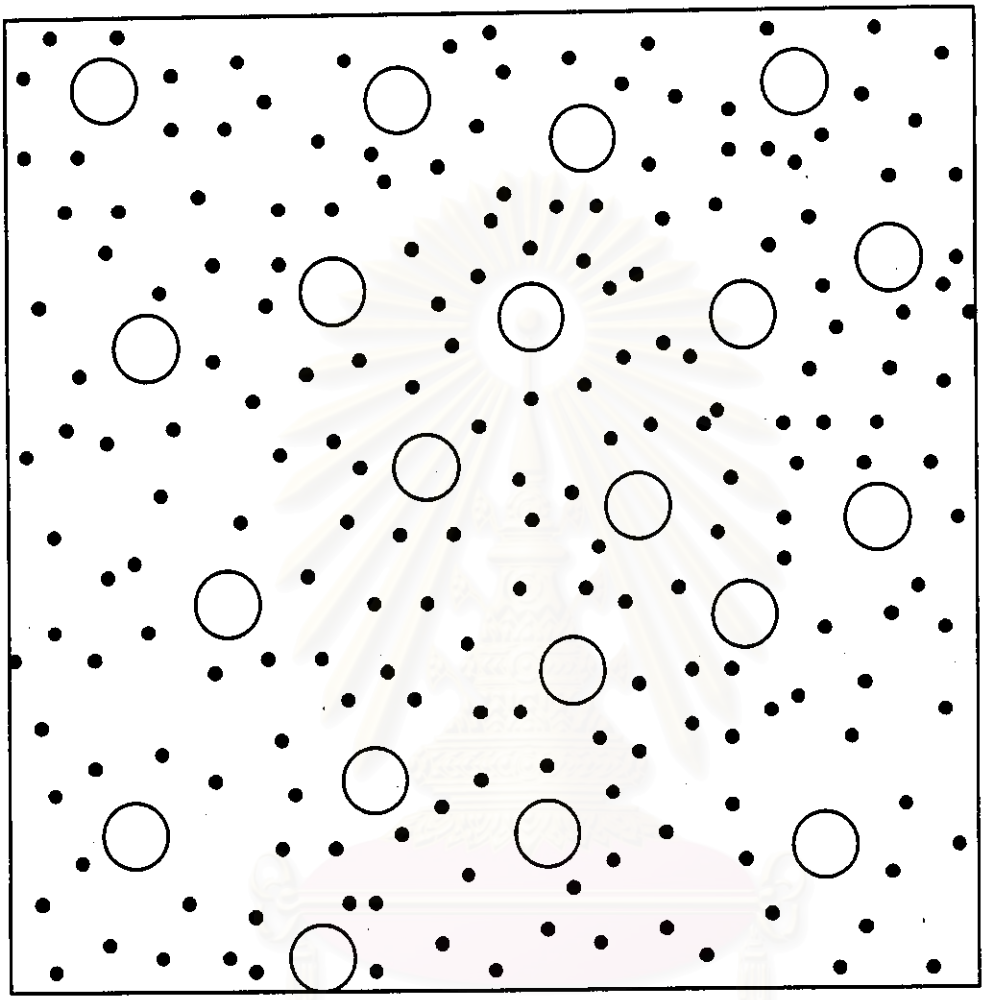

Figure 5.12 Example of dispersion of binary additives at the following conditions :

adhesion probablility : 0 %
particle size of A : 0.5 unit
particle size of B : 0.1 unit
concentration of A : 20 [particles/area]
concentration of B : 200 [particles/area]
concentration ratio (B:A) : 10 : 1

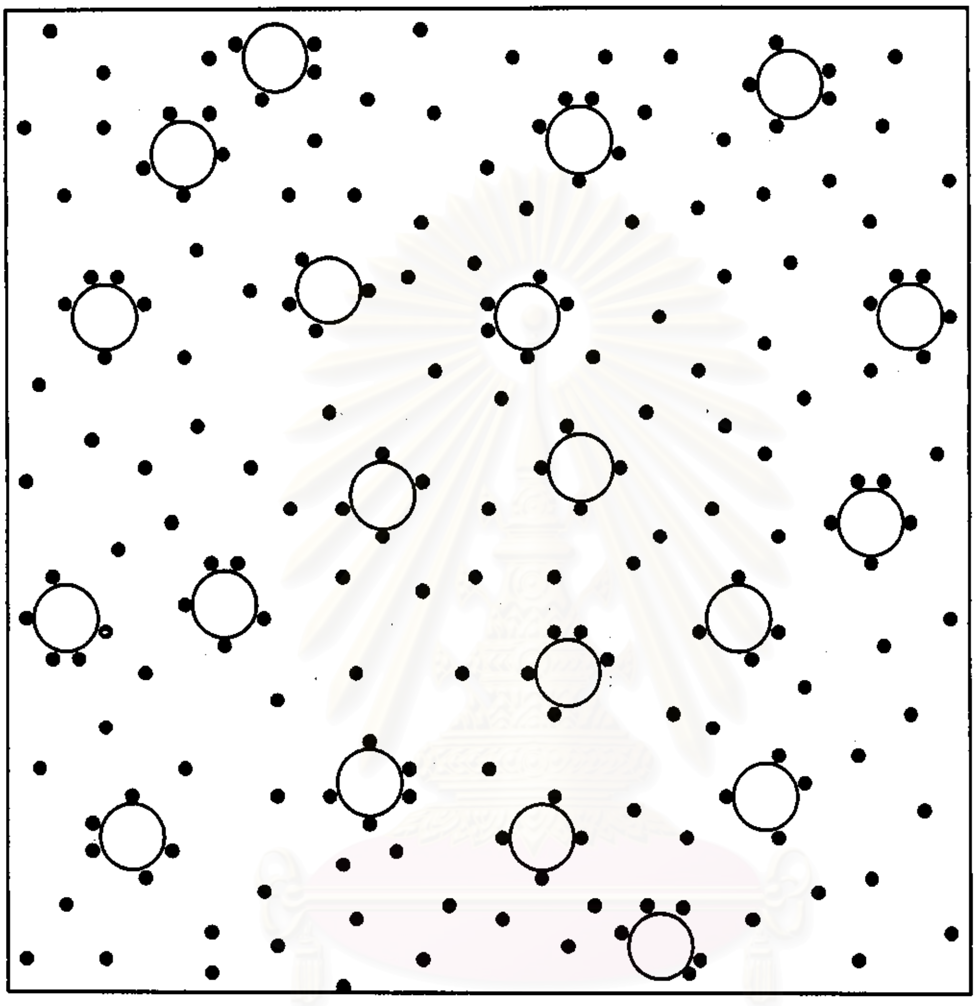

Figure 5.13 Example of dispersion of binary additives at the following conditions :

adhesion probablility : 50 %
particle size of A : 0.5 unit
particle size of B : 0.1 unit
concentration of A : 20 [particles/area]
concentration of B : 200 [particles/area]
concentration ratio : 10 : 1

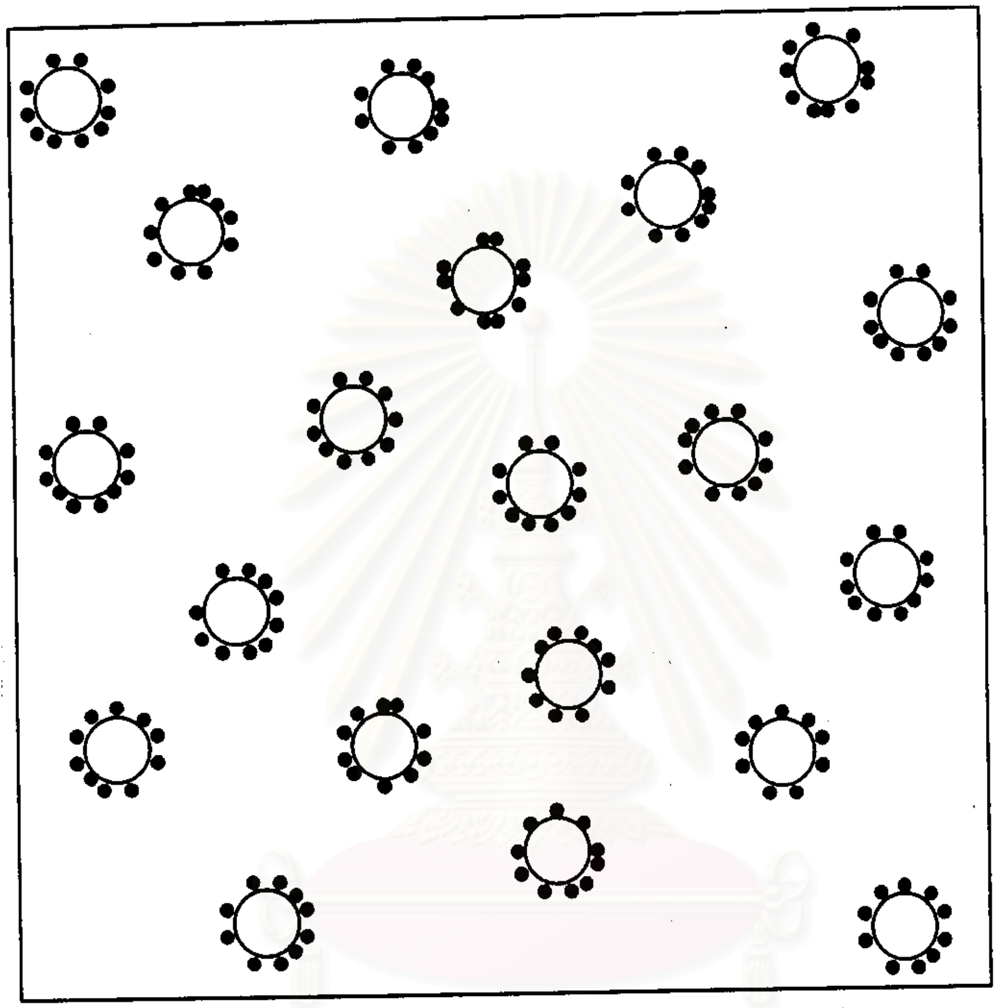

Figure 5.14 Example of dispersion of binary additives at the following conditions :

adhesion probablility : 100 %
particle size of A : 0.5 unit
particle size of B : 0.1 unit
concentration of A : 20 [particles/area]
concentration of B : 200 [particles/area]
concentration ratio : 10 : 1

5.2.1 Effect of adhesion probability

In the simulation of an ideal case of some partially ordered binary mixture, the value of the probability that a new B particle is to adhere onto one of the A particles is specified.

5.2.1.1 Degree of mixedness

To quantify the degree of dispersion of additive particles in the matrix material, the degree of mixedness is sometimes used. It has been found in the case of single component system that this index is influenced by both the concentration and particle size of the component of interest. In this section, the relationship between the adhesion probability and degree of mixedness is investigated.

5.2.1.1.1 Uniform - uniform dispersion.

In this case, both A and B particles were dispersed uniformly in the matrix and some of the B particles adhered onto the A particle according to the specified adhesion probability. The results are plotted in Figures 5.15 to 5.18.

As seen from Figures 5.15 to 5.18, the degree of mixedness tended to decrease as the concentration ratio of B to A increased or as the number of B particles expected to adhere onto the A particles increased. The reason is that when B particles were forced to adhere onto A particles, they lost the freedom of unconstrained dispersion in the matrix. However, the observed differences in the degree of mixedness become hardly discernable as the relative size of B become smaller and smaller.

5.2.1.1.2 Uniform - normal dispersion

Figures 5.19 to 5.22 reveal that the degree of mixedness decreased as the concentration ratio increased. However, an increase in the adhesion probability caused the degree of mixedness to increase. This is because A particles followed uniform dispersion, thus any B particles adhering onto A became uniformly dispersed. In contrast, it was found that the degree of mixedness at 100% adhesion was less than at 80% adhesion. This may be because, as the percentage of adhesion approached 100%, the number of the remaining B particles in the matrix became small, so they appeared to be uniformly dispersed even if they followed the normal dispersion. The result is that the apparent total number of uniformly dispersed particles seemed to increase.

5.2.1.1.3 Normal - uniform dispersion

The results obtained from computer simulations for normal - uniform dispersion and shown as the relationship between the degree of mixedness and adhesion probability were plotted in Figures 5.23 to 5.26. It can be seen that the degree of mixedness of B particles decreased as the adhesion probability increased. The reason for this case was mentioned in 5.2.1.1.1.

5.2.1.1.4 Normal - normal dispersion

From Figures 5.27 to 5.30, it can be seen that the degree of mixedness decreased when there was an increase in the adhesion probability. The reason of this case also was discussed in 5.2.1.1.1.

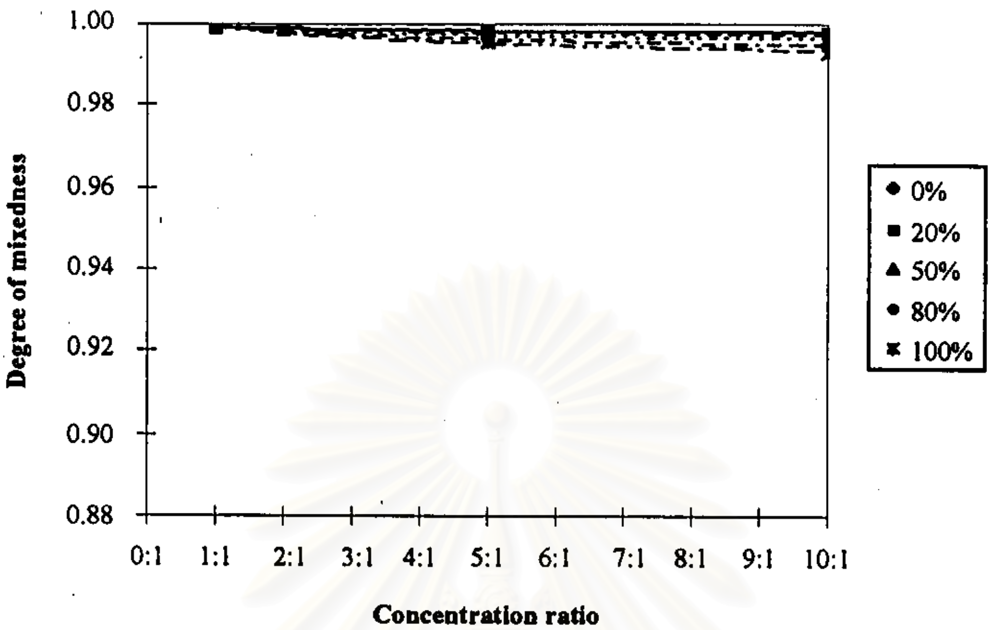

Figure 5.15 Relationship between concentration ratio and degree of mixedness of B particles in the case of uniform - uniform dispersion and particle size ratio = 0.02:1.

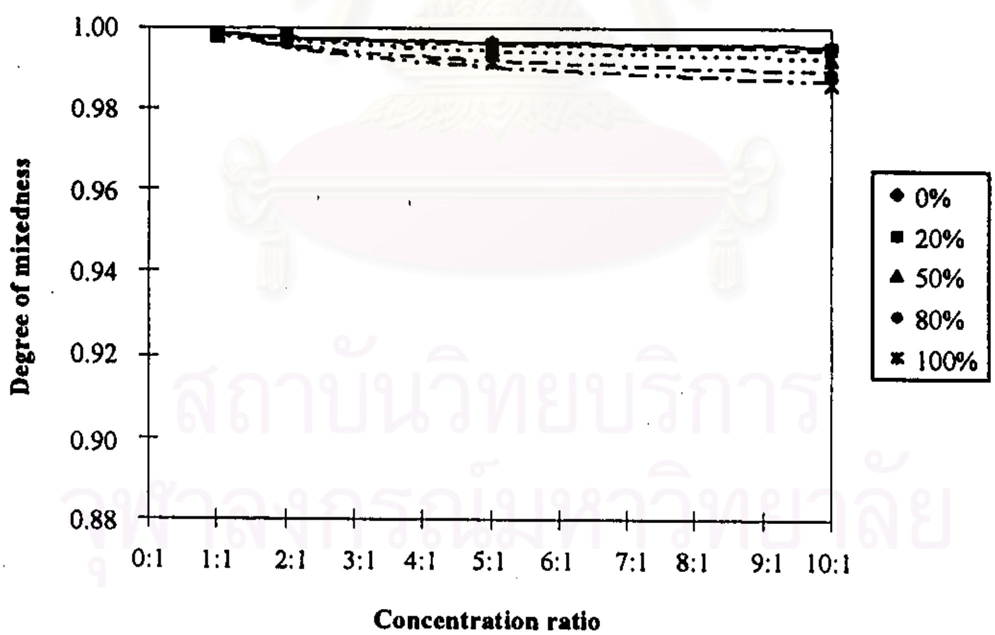

Figure 5.16 Relationship between concentration ratio and degree of mixedness of B particles in the case of uniform - uniform dispersion and particle size ratio = 0.04:1.

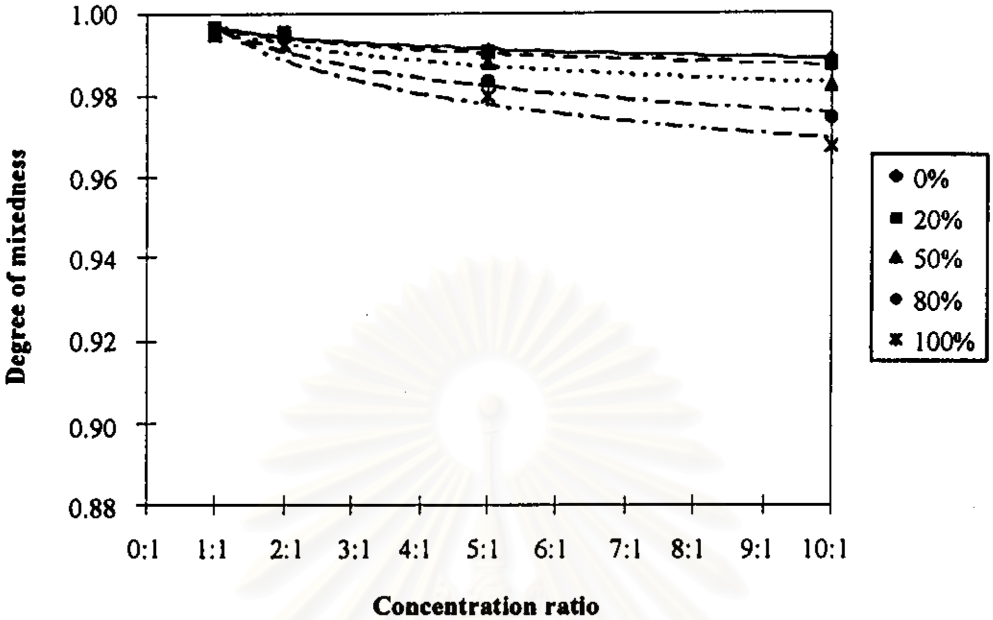

Figure 5.17 Relationship between concentration ratio and degree of mixedness of B particles in the case of uniform - uniform dispersion and particle size ratio = 0.10:1.

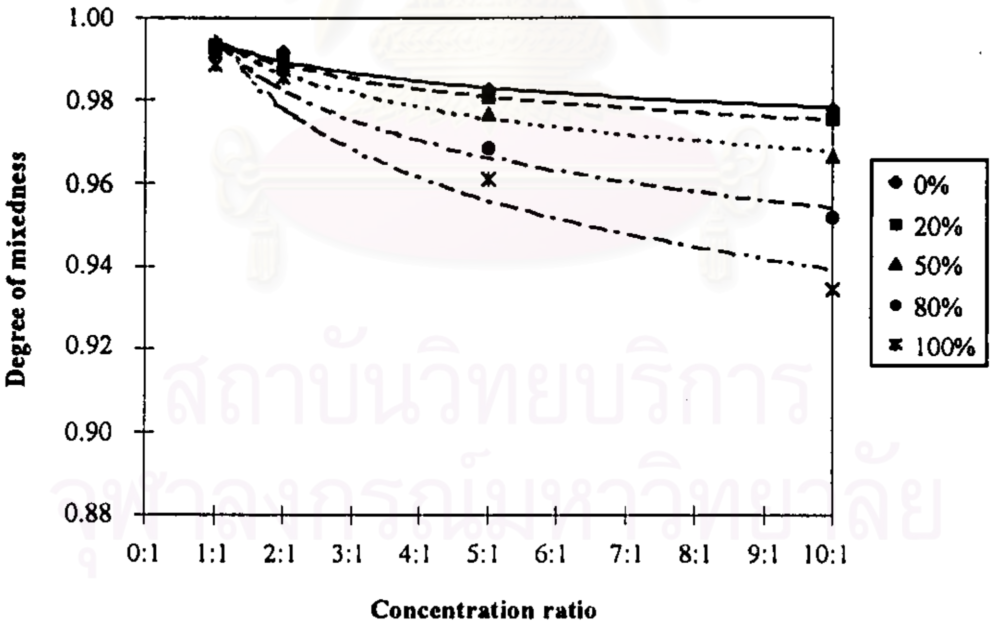

Figure 5.18 Relationship between concentration ratio and degree of mixedness of B particles in the case of uniform - uniform dispersion and particle size ratio = 0.20:1.

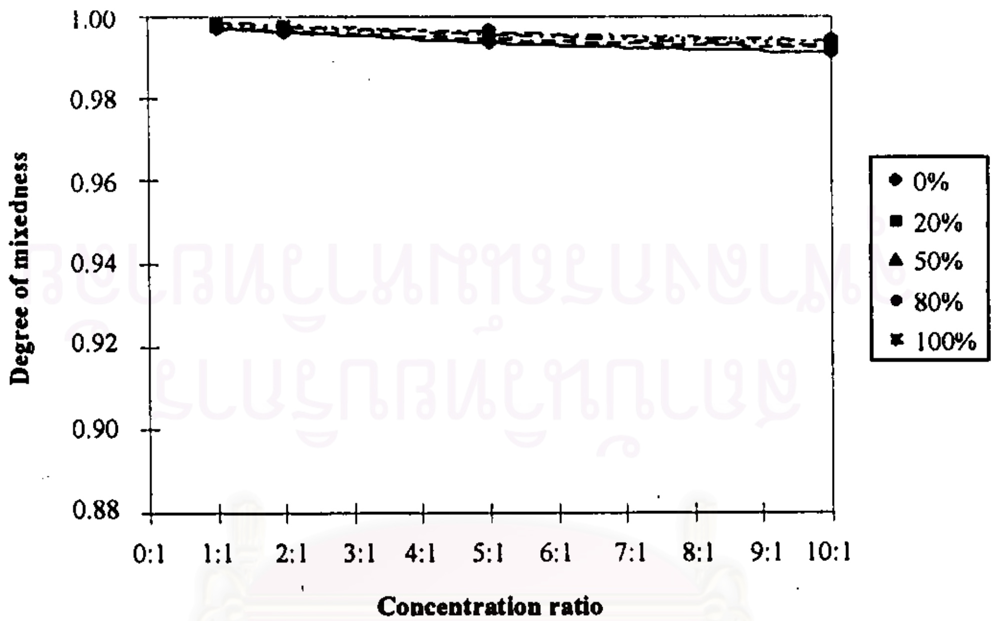

Figure 5.19 Relationship between concentration ratio and degree of mixedness of B particles in the case of uniform - normal dispersion and particle size ratio = 0.02:1.

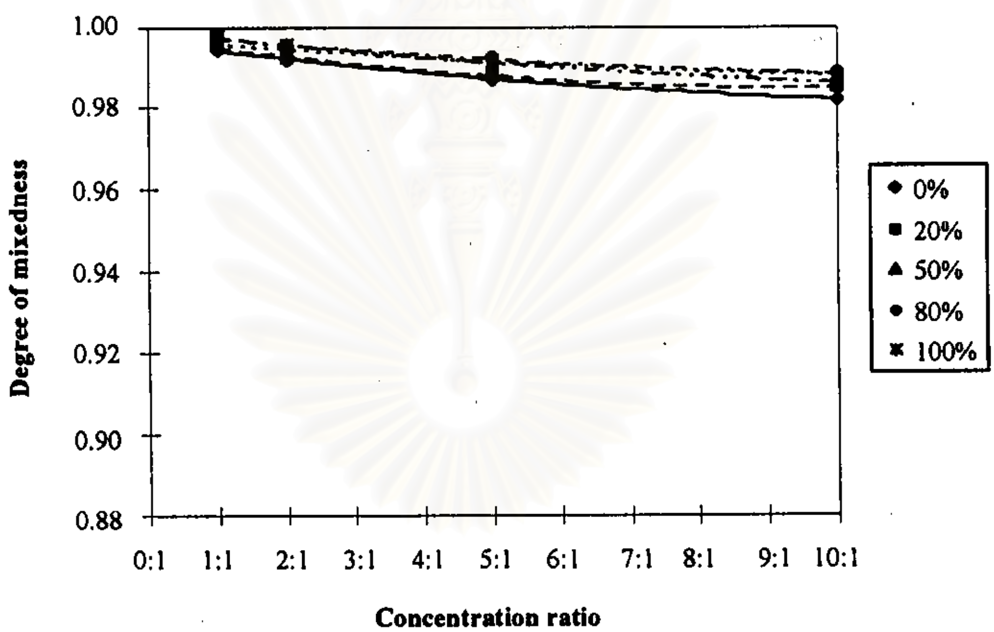

Figure 5.20 Relationship between concentration ratio and degree of mixedness of B particles in the case of uniform - normal dispersion and particle size ratio = 0.04:1.

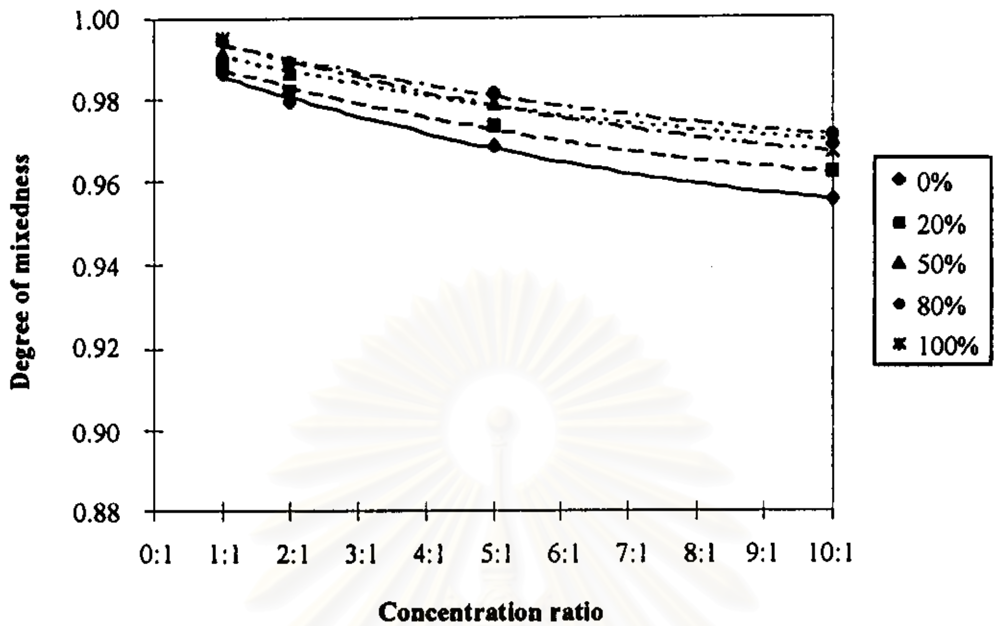

Figure 5.21 Relationship between concentration ratio and degree of mixedness of B particles in the case of uniform - normal dispersion and particle size ratio = 0.10:1.

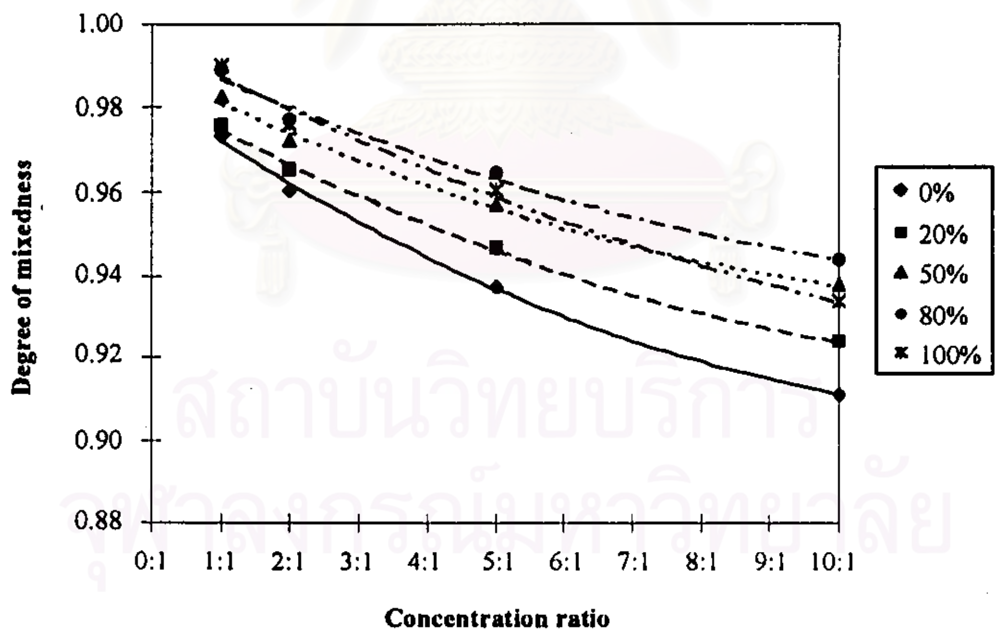

Figure 5.22 Relationship between concentration ratio and degree of mixedness of B particles in the case of uniform - normal dispersion and particle size ratio = 0.20:1.

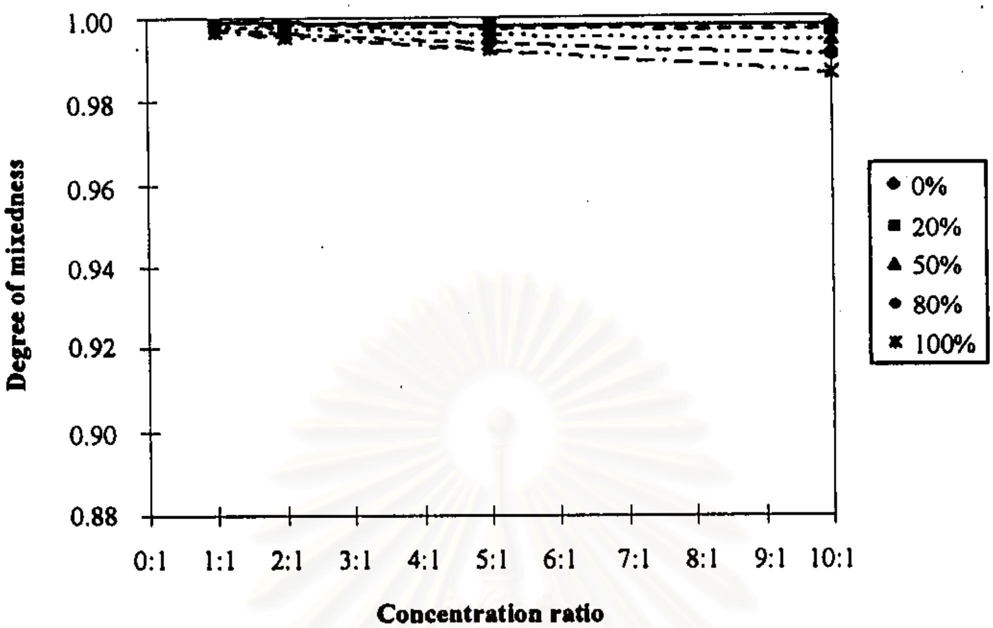

Figure 5.23 Relationship between concentration ratio and degree of mixedness of B particles in the case of normal - uniform dispersion and particle size ratio = 0.02:1.

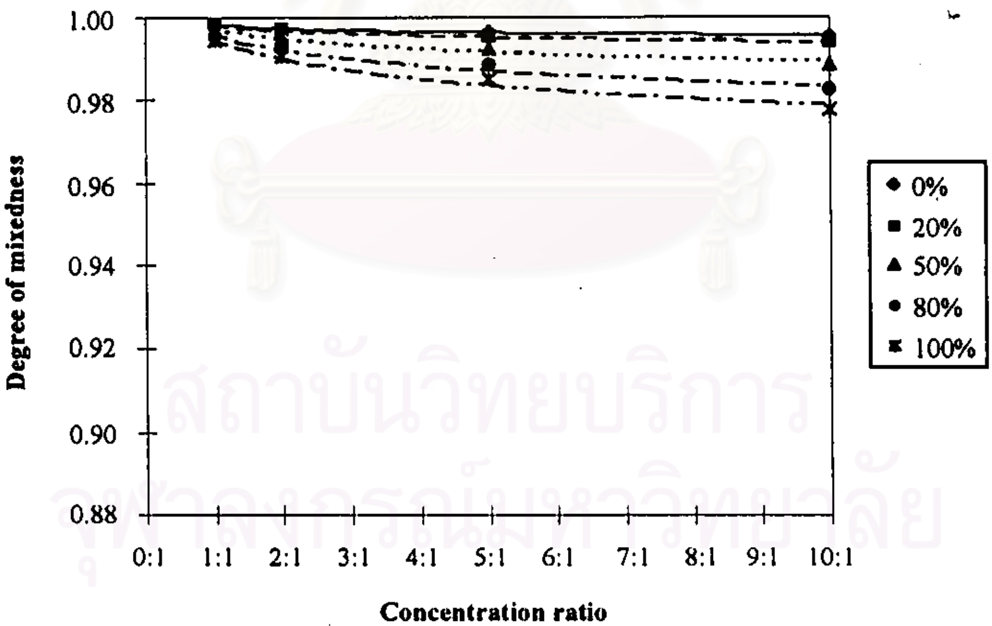

Figure 5.24 Relationship between concentration ratio and degree of mixedness of B particles in the case of normal - uniform dispersion and particle size ratio = 0.04:1.

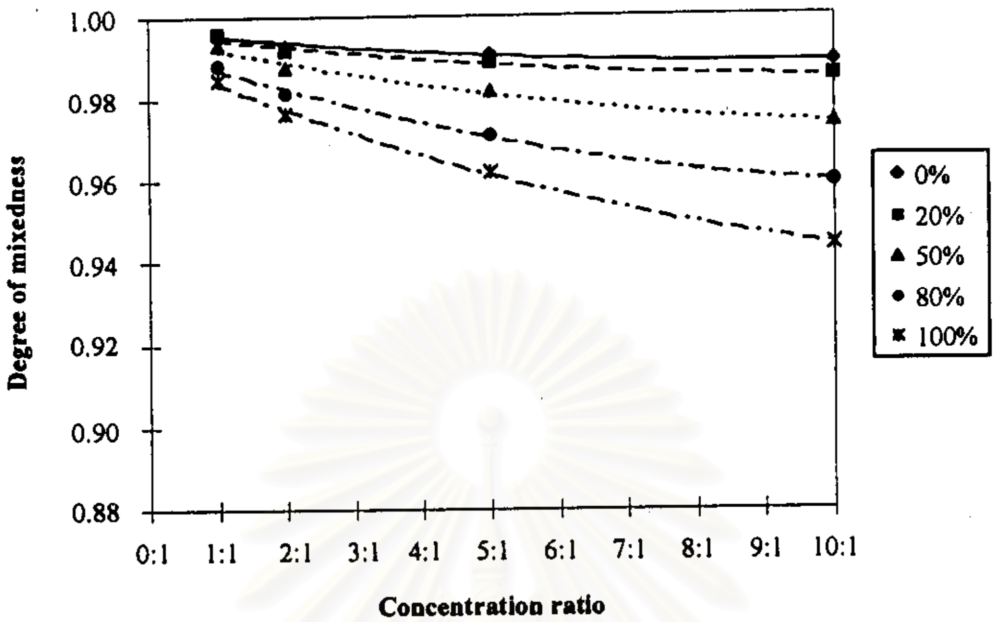

Figure 5.25 Relationship between concentration ratio and degree of mixedness of B particles in the case of normal - uniform dispersion and particle size ratio = 0.10:1.

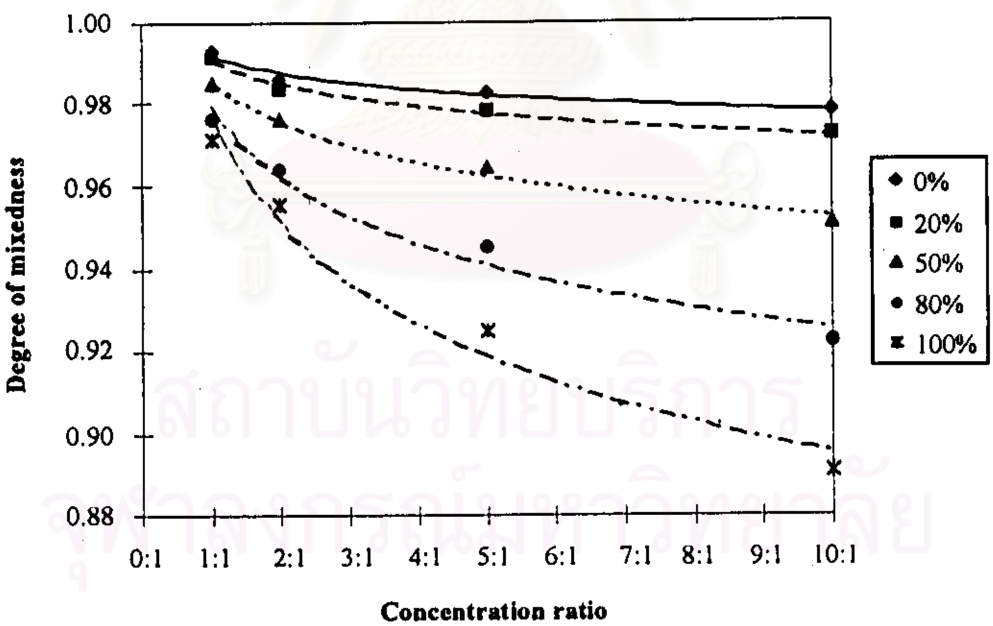

Figure 5.26 Relationship between concentration ratio and degree of mixedness of B particles in the case of normal - uniform dispersion and particle size ratio = 0.20:1.

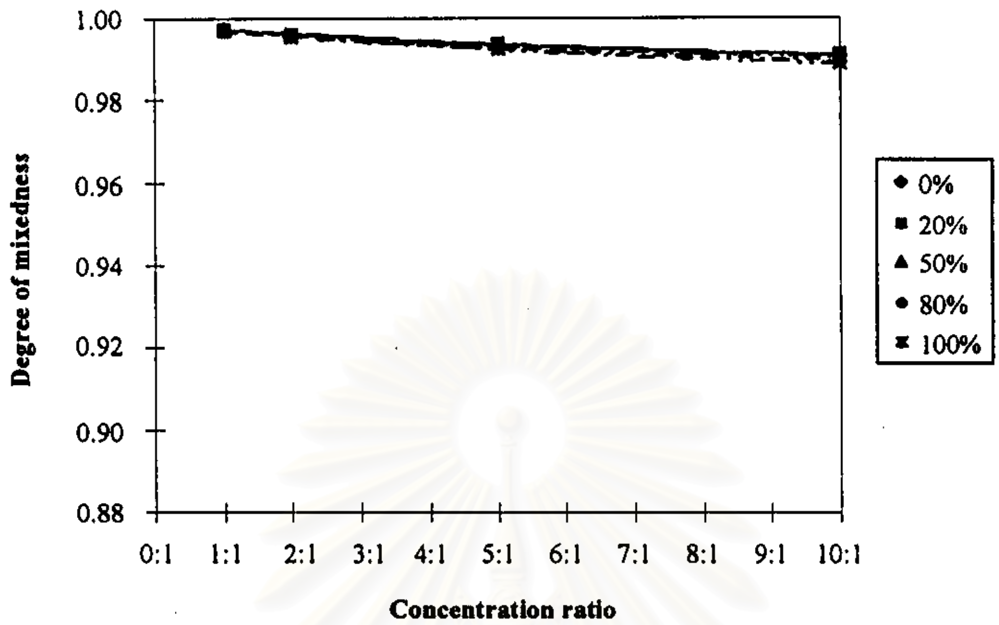

Figure 5.27 Relationship between concentration ratio and degree of mixedness of B particles in the case of normal - normal dispersion and particle size ratio = 0.02:1.

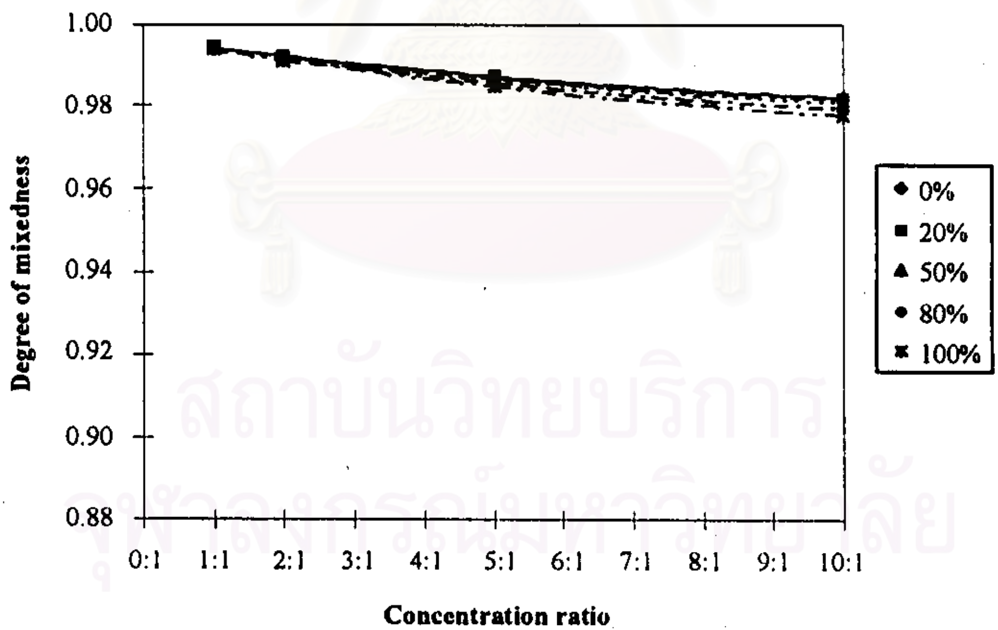

Figure 5.28 Relationship between concentration ratio and degree of mixedness of B particles in the case of normal - normal dispersion and particle size ratio = 0.04:1.

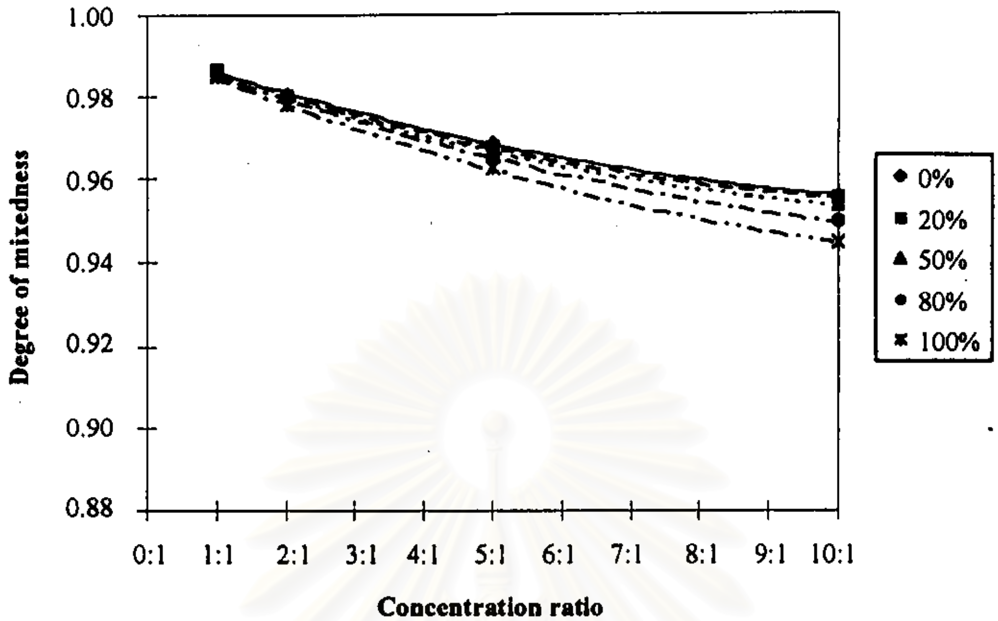

Figure 5.29 Relationship between concentration ratio and degree of mixedness of B particles in the case of normal - normal dispersion and particle size ratio = 0.10:1.

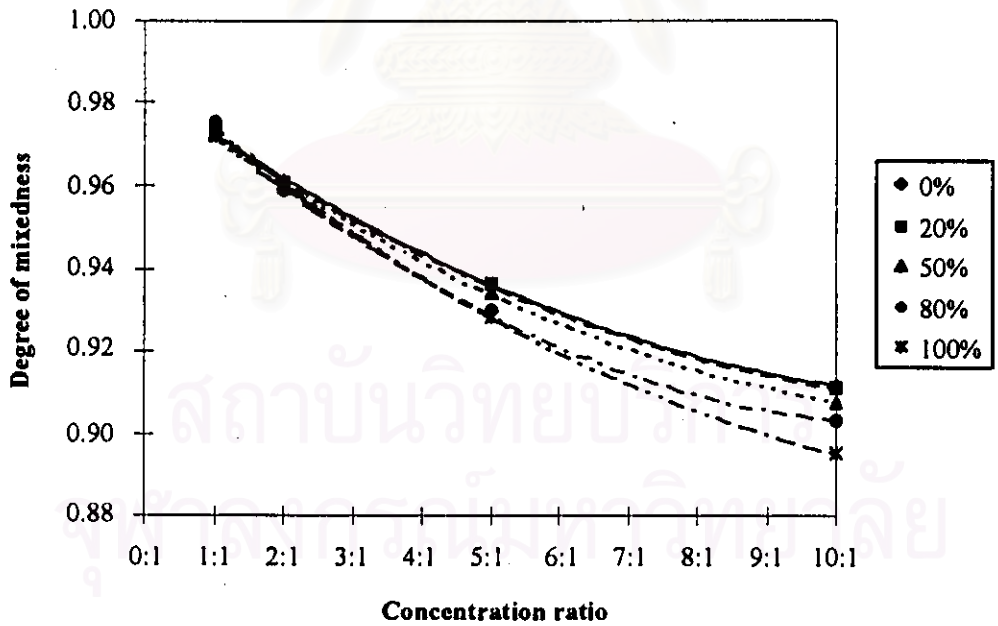

Figure 5.30 Relationship between concentration ratio and degree of mixedness of B particles in the case of normal - normal dispersion and particle size ratio = 0.20:1.

Generally speaking, in each of the above four cases the degree of mixedness is not a good index to differentiate between the various adhesion probabilities. Its usefulness becomes even less when the relative size of B particles decreases. As pointed out in the single component system, the degree of mixedness is not a good index for the degree of dispersion because it is too much influenced by the size of the particles of interest.

5.2.1.2 Count-based fractal dimension

In this work, the observed count-based fractal dimension obtained from computer simulation for each binary additive system was normalized by the corresponding count-based fractal dimension of the ideal uniform dispersion that was obtained previously in the single additive system at the same concentration as the B particles.

Relationship between adhesion probability of B particles and the normalized count-based fractal dimension based on B particles only and on A plus B particles are investigated below.

5.2.1.2.1 Uniform - uniform dispersion

Figures 5.31 to 5.34 show that the normalized count-based fractal dimension of only B decreased, as the adhesion probability increased. This may be because B particles were obliged to adhere onto fewer A particles, which results in clusters of B around A particles.

The same reason may be used to explain the effect of the adhesion probability on the normalized count-based fractal dimension of A plus B particles which was depicted in Figures 5.35 to 5.38. Unlike the degree of mixedness, the count-based fractal dimension is little influenced by the size of B particles.

5.2.1.2.2 Uniform - normal dispersion

Uniform dispersion of A particles should cause an increase in the normalized count-based fractal dimension when the adhesion probability rose. This is because the number of normally dispersed B particles in the matrix was reduced as some of them were forced to adhere onto the uniformly dispersed A particles. Thus the normalized count-based fractal dimension rises when the adhesion probability increases. Such results were depicted in Figures 5.39 to 5.42. At very small concentration ratio and with smaller B particle size, the normalized count-based fractal dimension for 80% adhesion was slightly greater than for 100% adhesion. The reason was given in 5.2.1.1.2.

Figures 5.43 to 5.46 show the effect of the adhesion probability on the normalized count-based fractal dimension of A plus B particles. It is found that the effect is rather confusing because A and B were of different dispersion types and different concentrations. Furthermore, the count of A particles and B particles was the same, although the particle size of A was much larger than B.

5.2.1.2.3 Normal - uniform dispersion

The results of how the normalized count-based fractal dimension of B particles was affected by the adhesion probability was shown in Figures 5.47 to 5.50. It can be seen that the normalized count-based fractal dimension of the B particles decreased, as more and more B particles were controlled to adhere onto A particles. This is because the dispersion of A particles was normal dispersion.

The effect of the adhesion probability on the normalized count-based fractal dimension of A plus B particles was depicted in Figures 5.51 to 5.54. The reason of this results was already mentioned in 5.2.1.2.1.

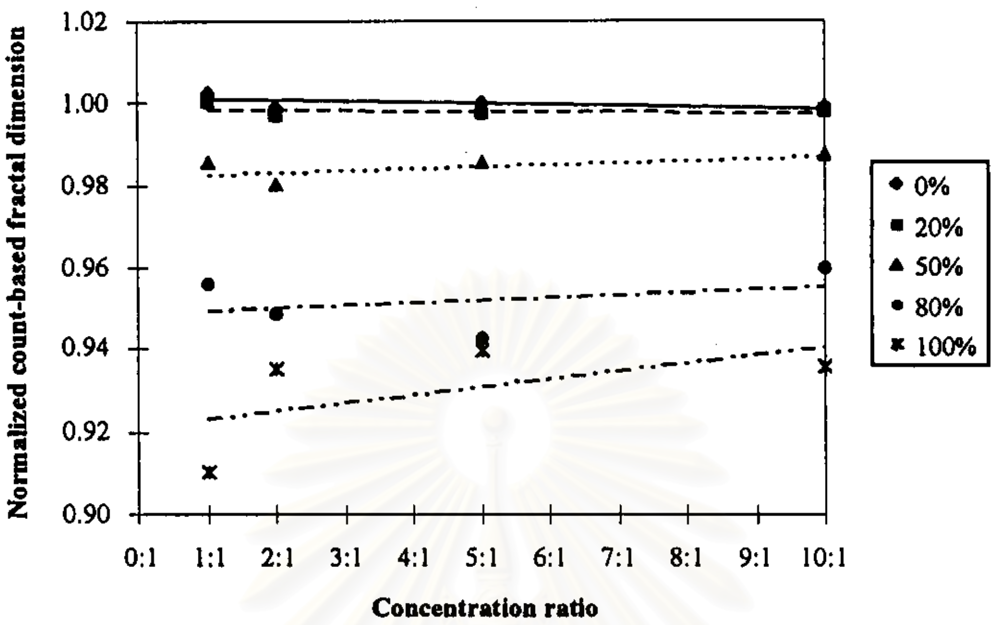

Figure 5.31 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of uniform - uniform dispersion and particle size ratio = 0.02:1.

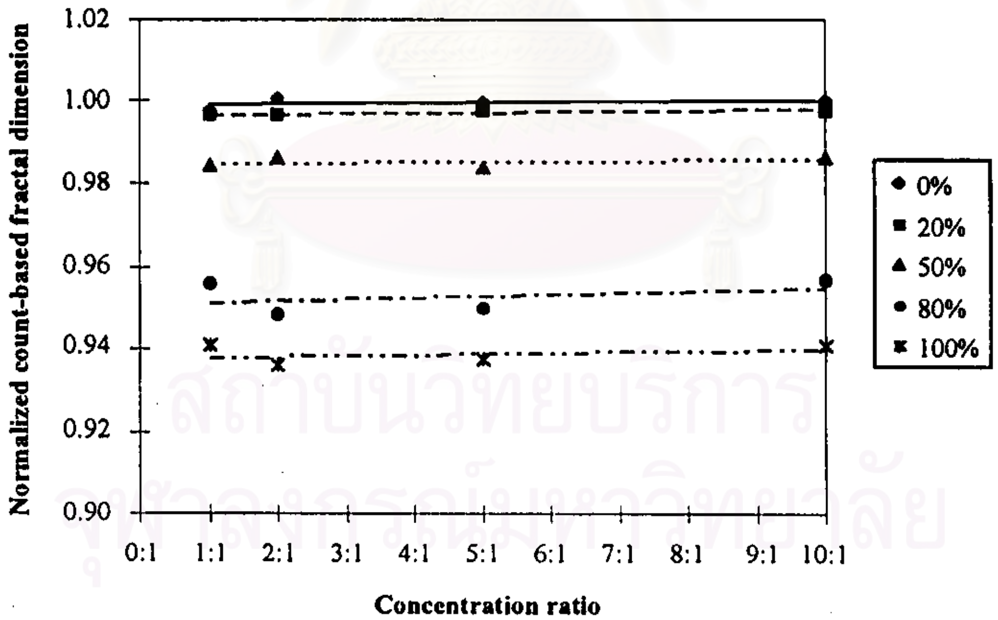

Figure 5.32 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of uniform - uniform dispersion and particle size ratio = 0.04:1.

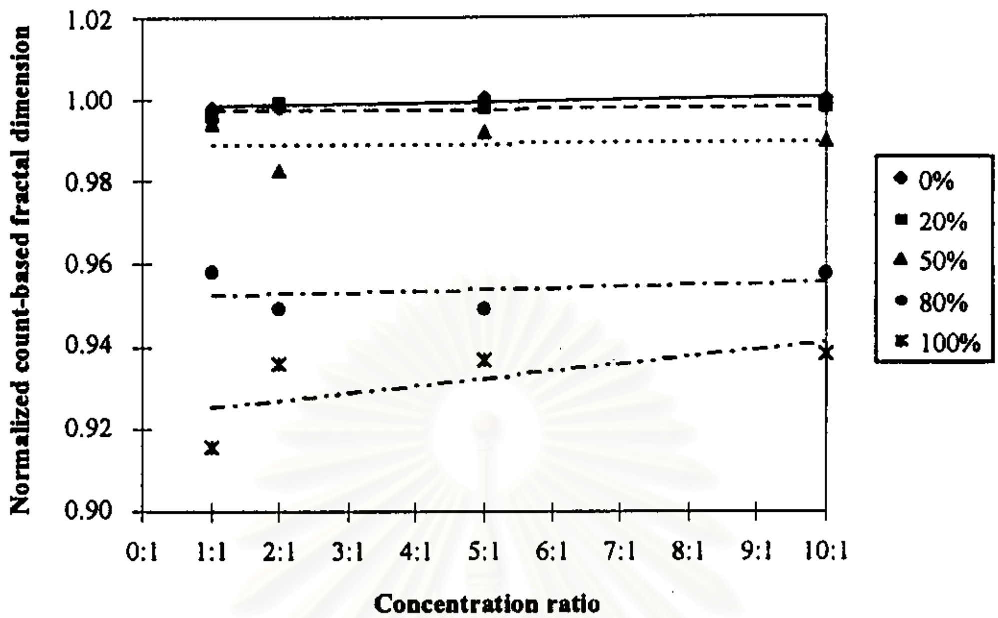

Figure 5.33 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of uniform - uniform dispersion and particle size ratio = 0.10:1.

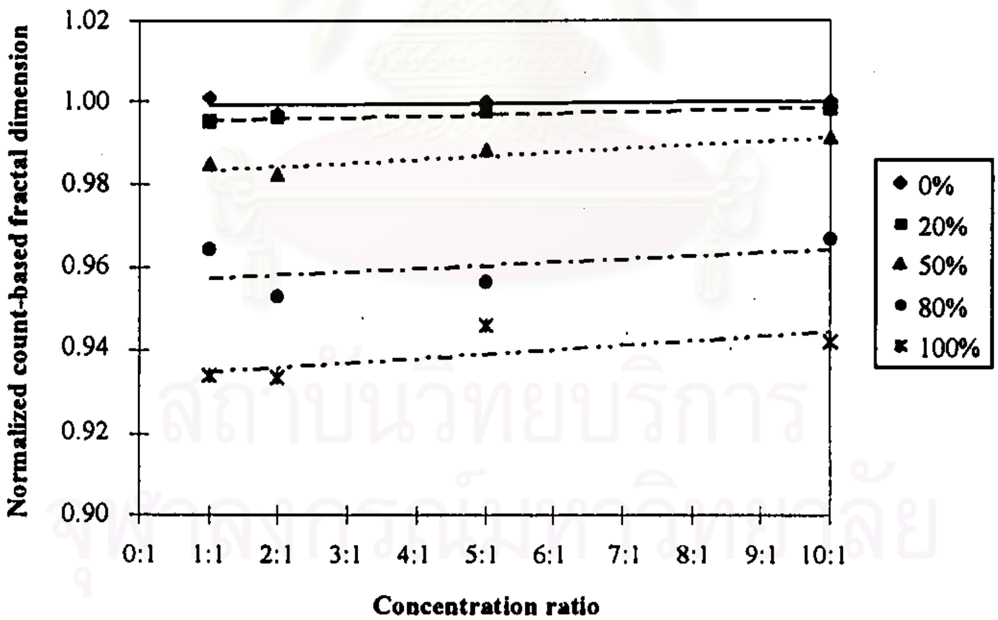

Figure 5.34 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of uniform - uniform dispersion and particle size ratio = 0.20:1.

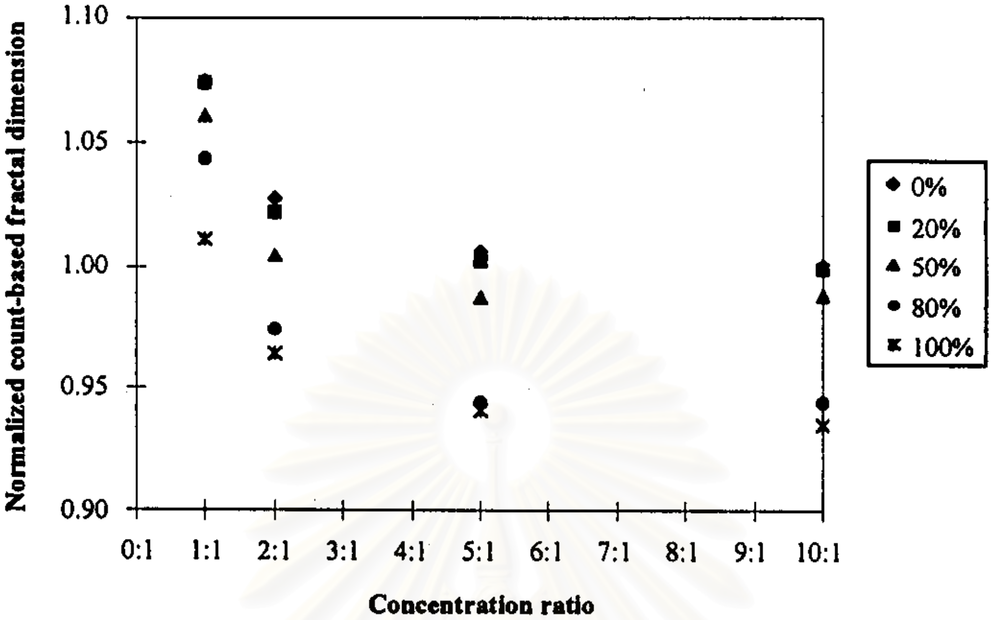

Figure 5.35 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of uniform - uniform dispersion and particle size ratio = 0.02:1.

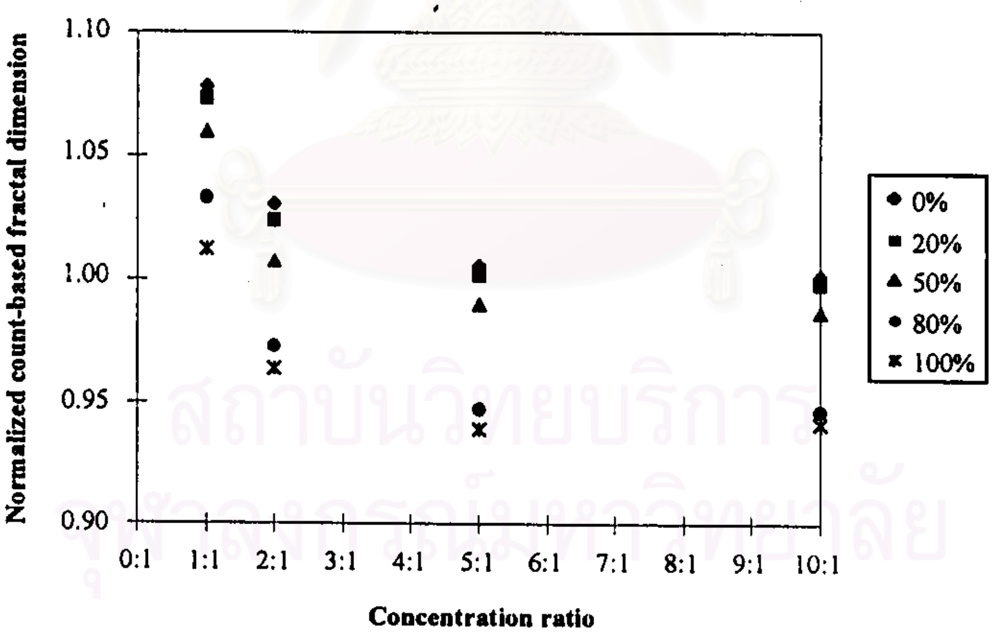

Figure 5.36 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of uniform - uniform dispersion and particle size ratio = 0.04:1.

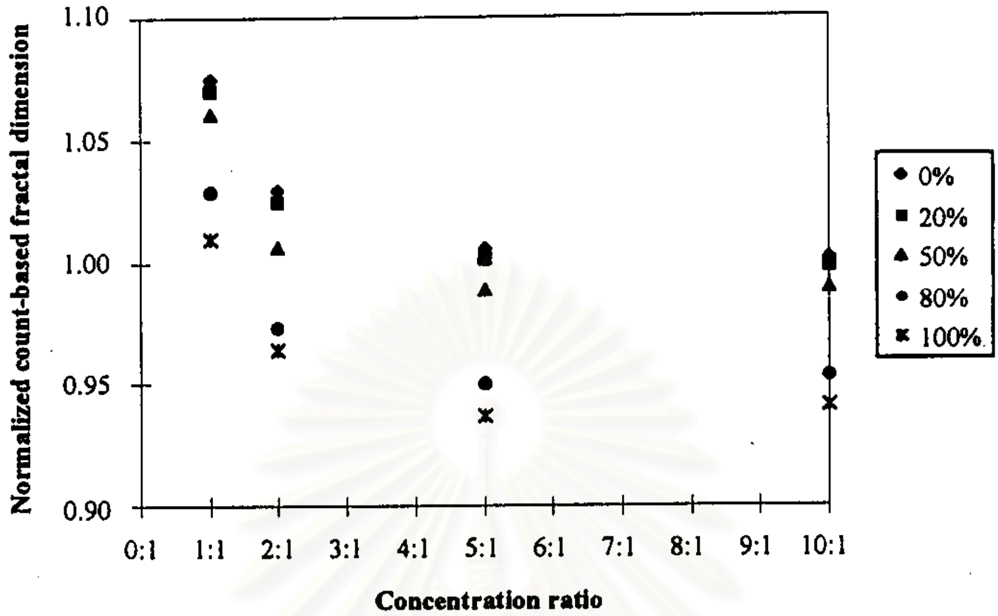

Figure 5.37 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of uniform - uniform dispersion and particle size ratio = 0.10:1.

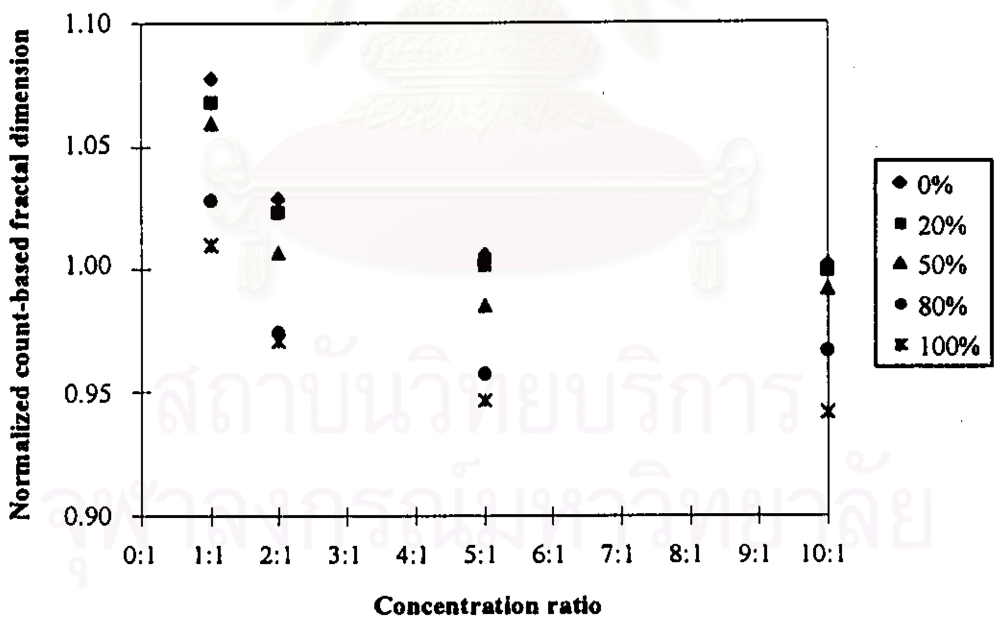

Figure 5.38 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of uniform - uniform dispersion and particle size ratio = 0.20:1.

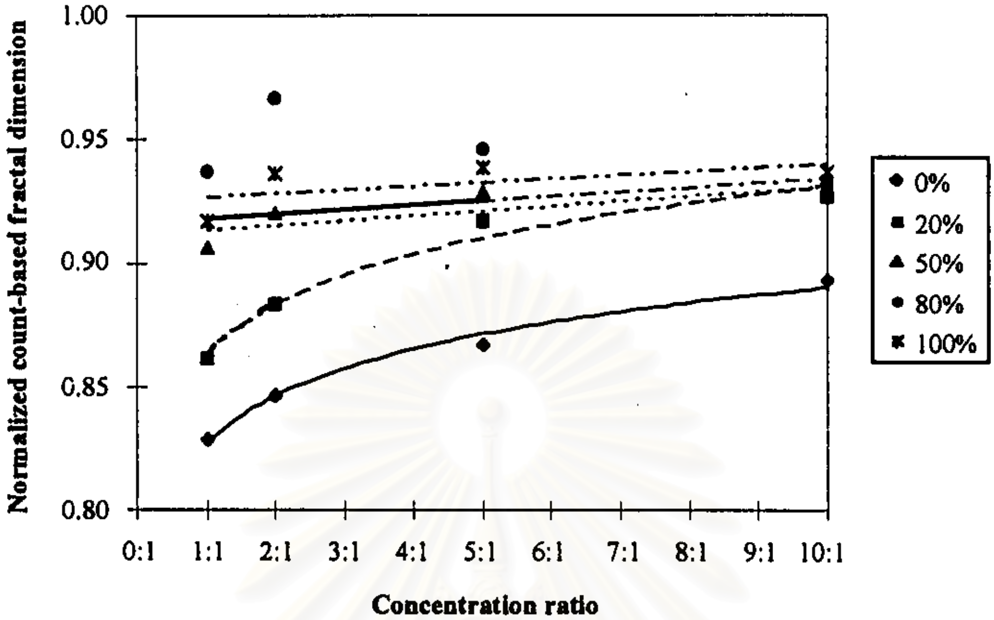

Figure 5.39 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of uniform - normal dispersion and particle size ratio = 0.02:1.

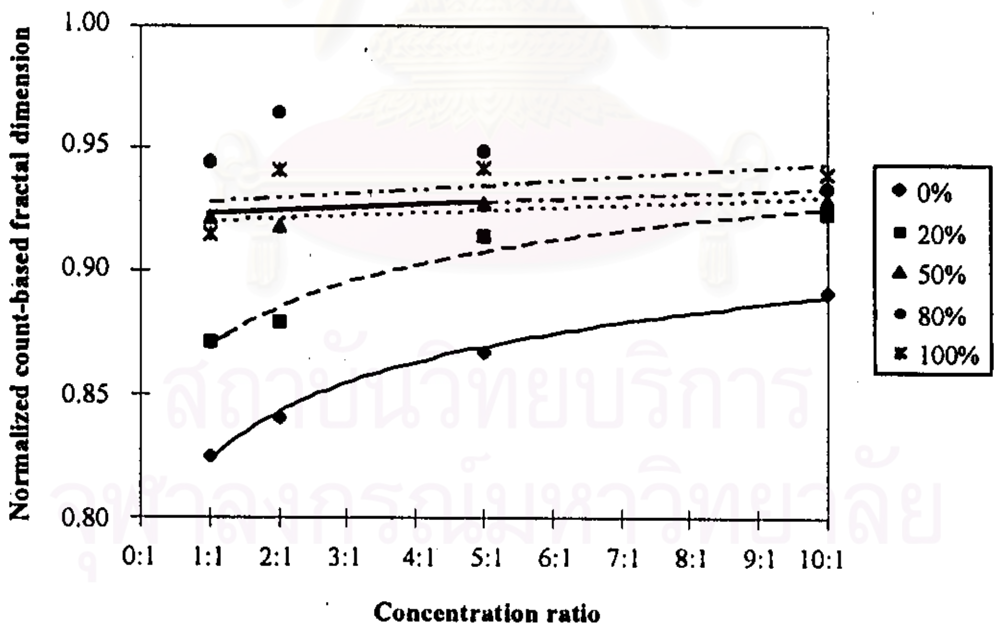

Figure 5.40 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of uniform - normal dispersion and particle size ratio = 0.04:1.

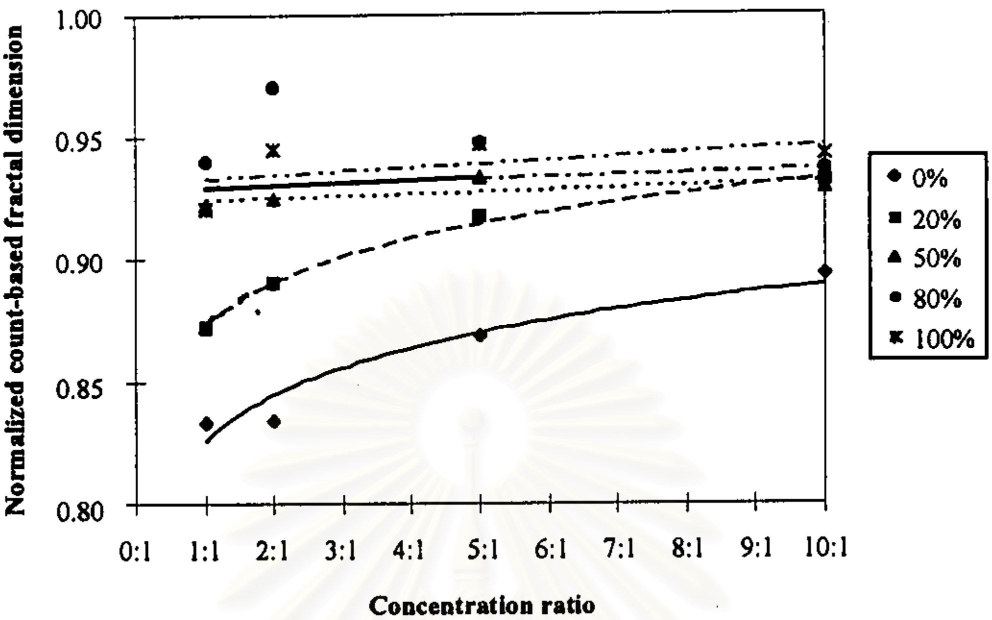

Figure 5.41 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of uniform - normal dispersion and particle size ratio = 0.10:1.

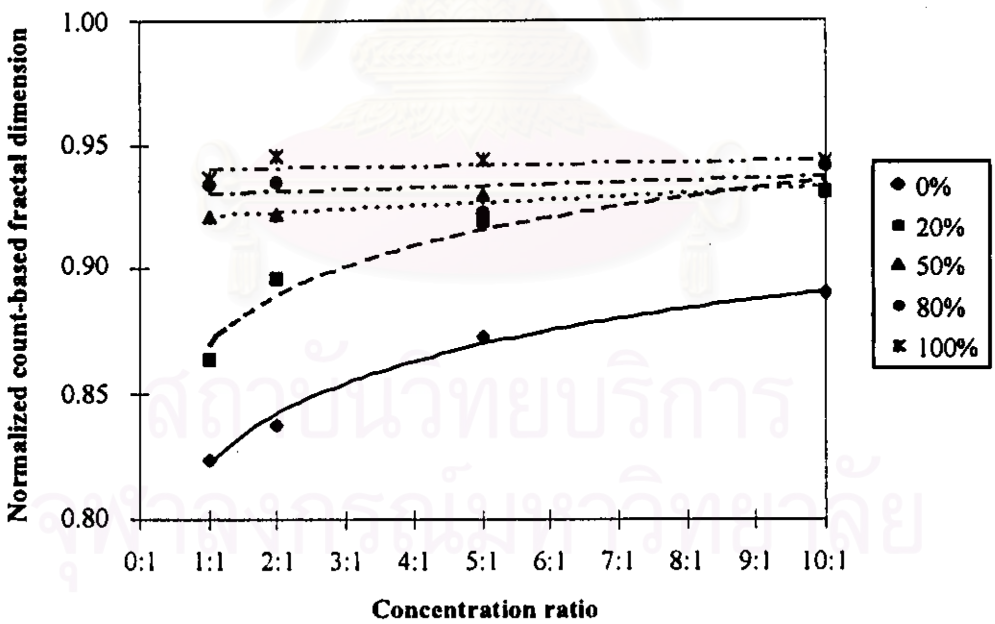

Figure 5.42 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of uniform - normal dispersion and particle size ratio = 0.20:1.

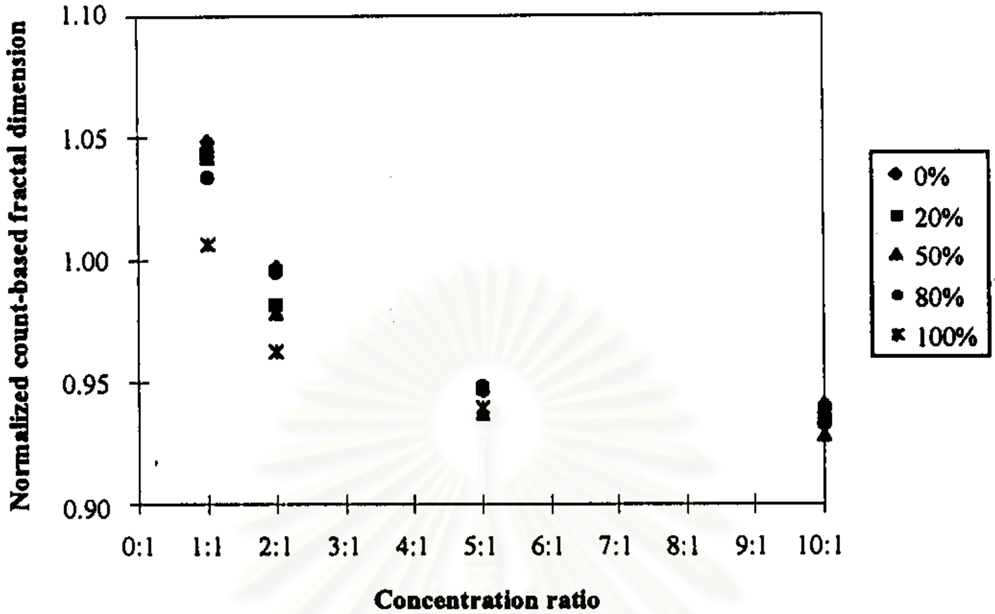

Figure 5.43 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of uniform - normal dispersion and particle size ratio = 0.02:1.

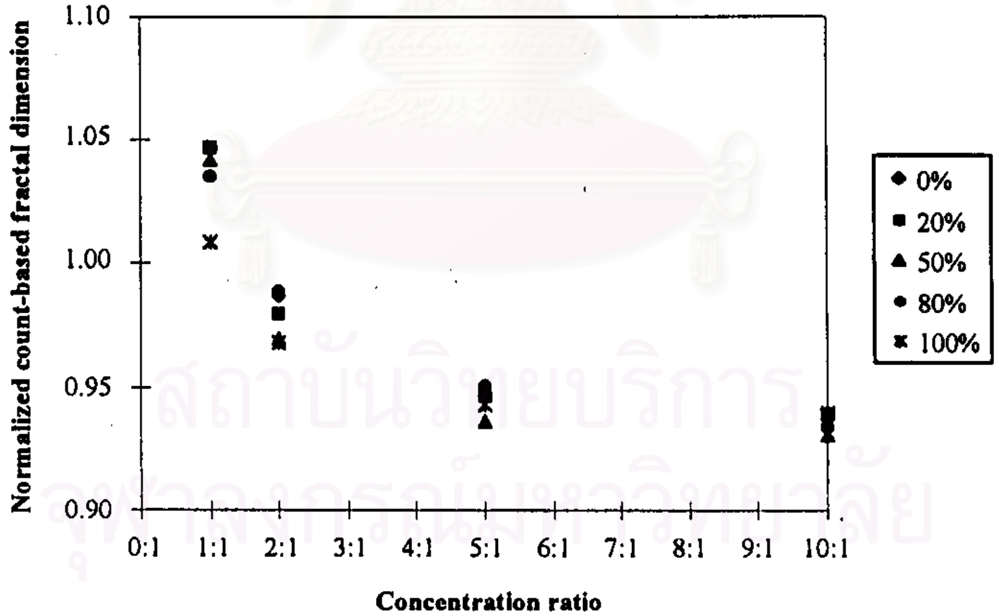

Figure 5.44 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of uniform - normal dispersion and particle size ratio = 0.04:1.

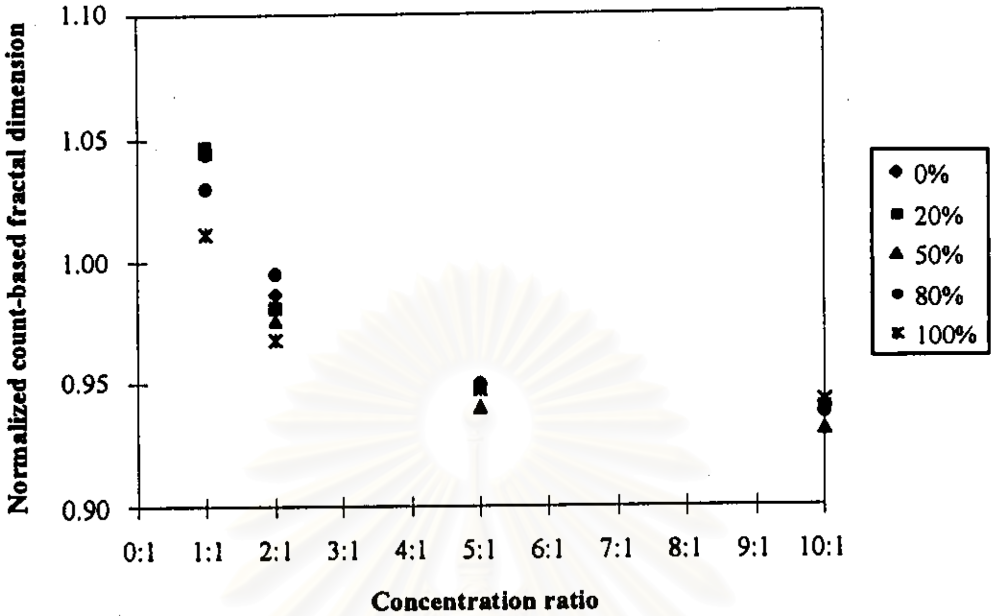

Figure 5.45 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of uniform - normal dispersion and particle size ratio = 0.10:1.

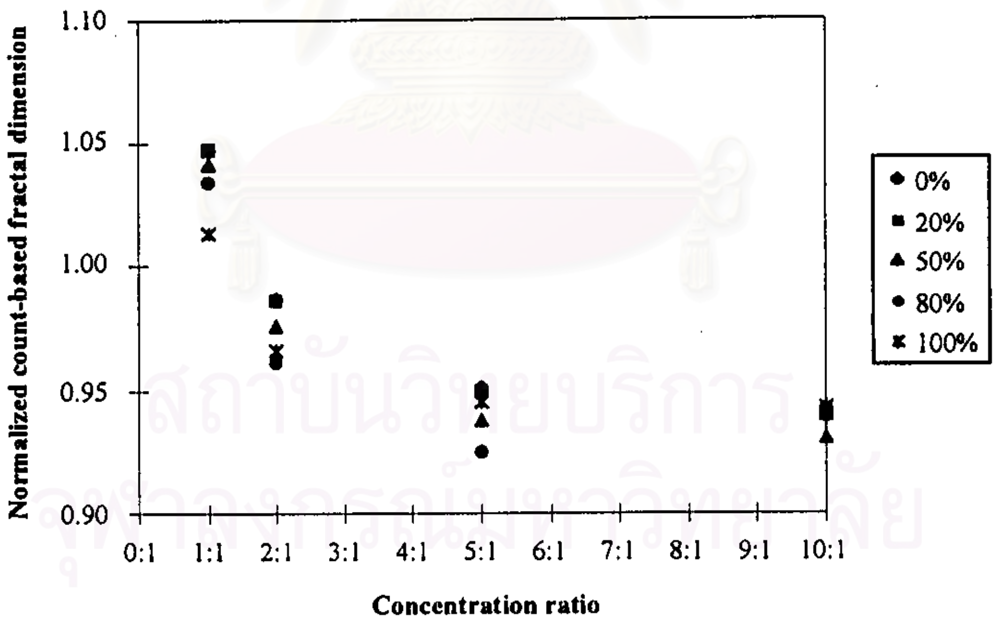

Figure 5.46 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of uniform - normal dispersion and particle size ratio = 0.20:1.

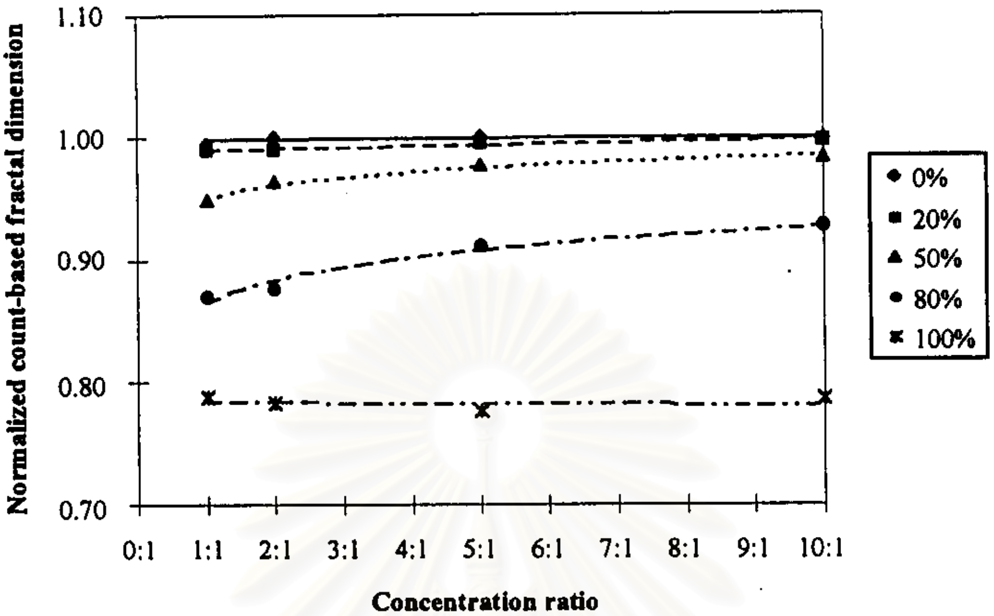

Figure 5.47 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of normal - uniform dispersion and particle size ratio = 0.02:1.

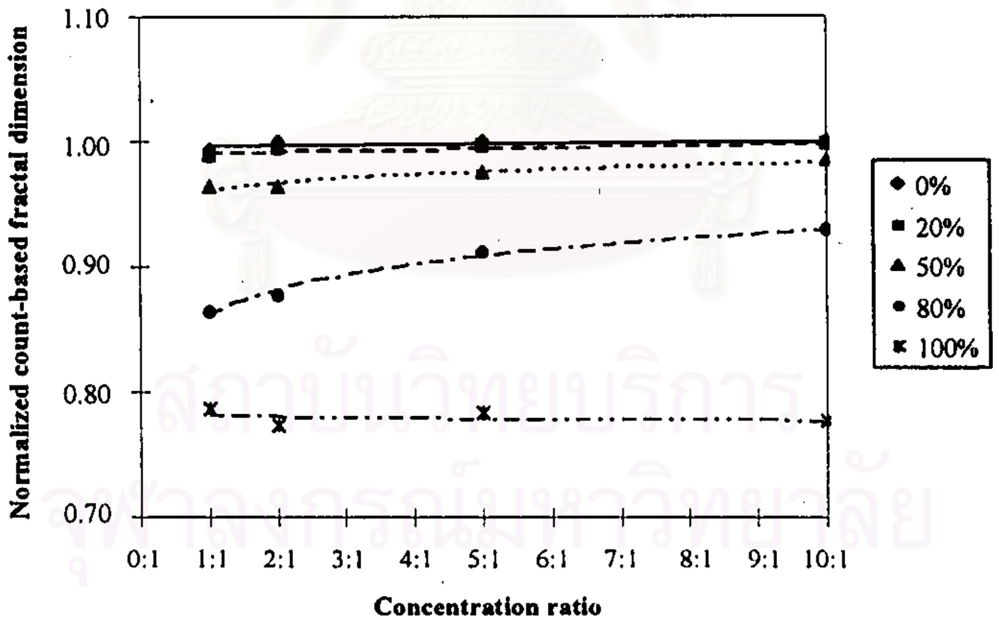

Figure 5.48 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of normal - uniform dispersion and particle size ratio = 0.04:1.

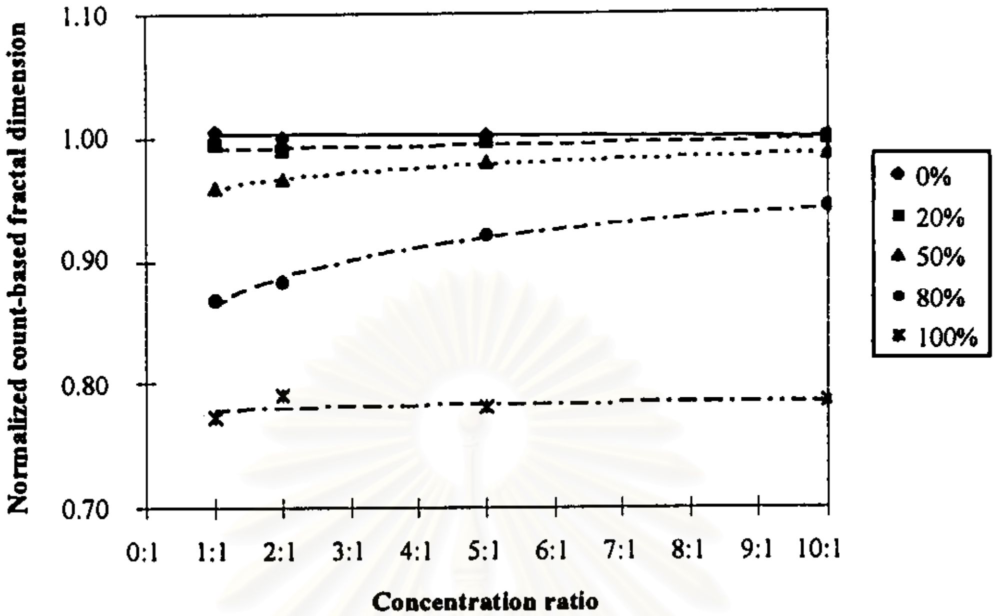

Figure 5.49 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of normal - uniform dispersion and particle size ratio = 0.10:1.

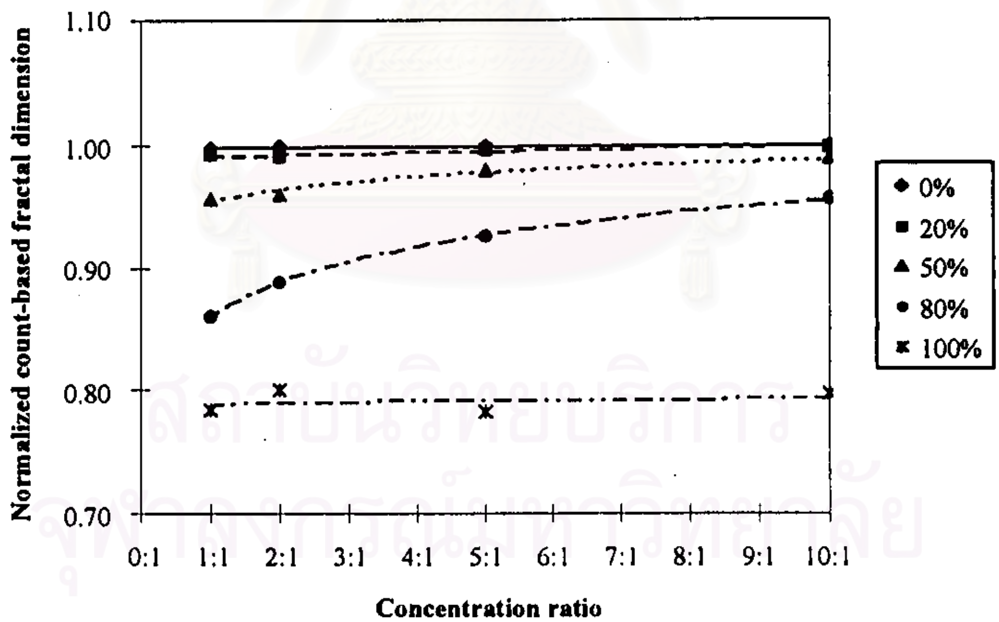

Figure 5.50 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of normal - uniform dispersion and particle size ratio = 0.20:1.

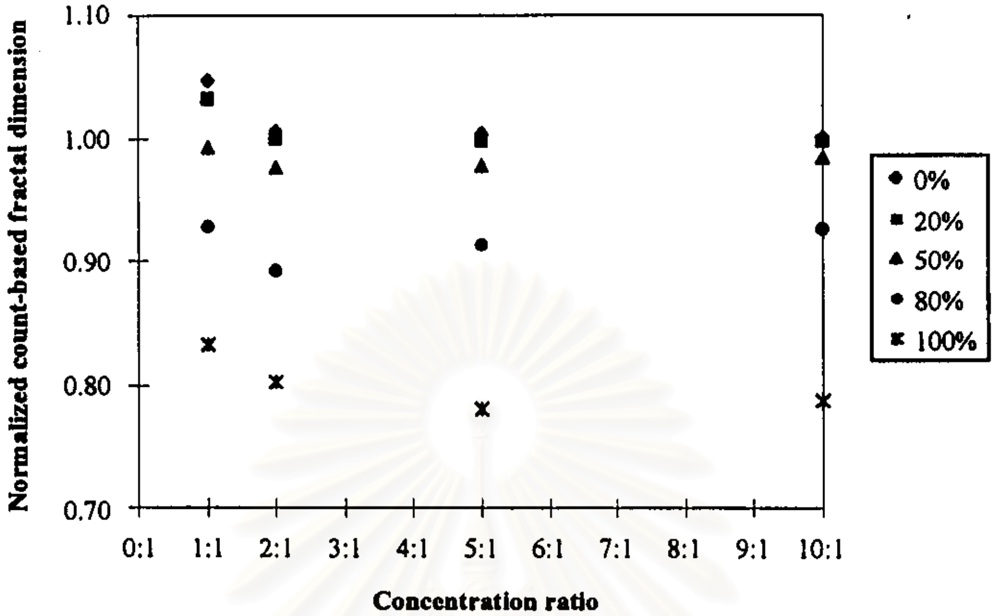

Figure 5.51 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of normal - uniform dispersion and particle size ratio = 0.02:1.

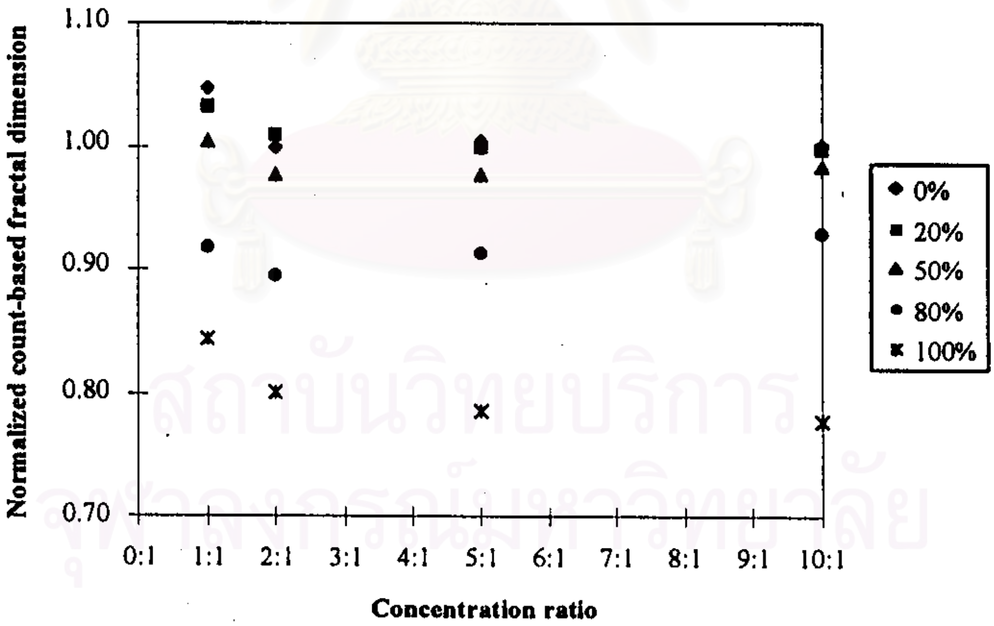

Figure 5.52 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of normal - uniform dispersion and particle size ratio = 0.04:1.

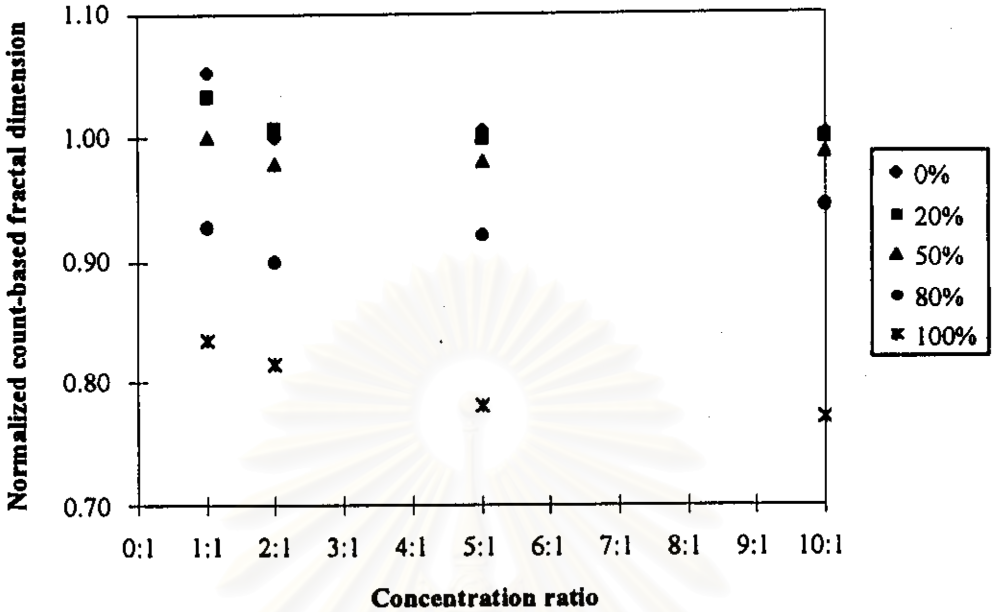

Figure 5.53 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of normal - uniform dispersion and particle size ratio = 0.10:1.

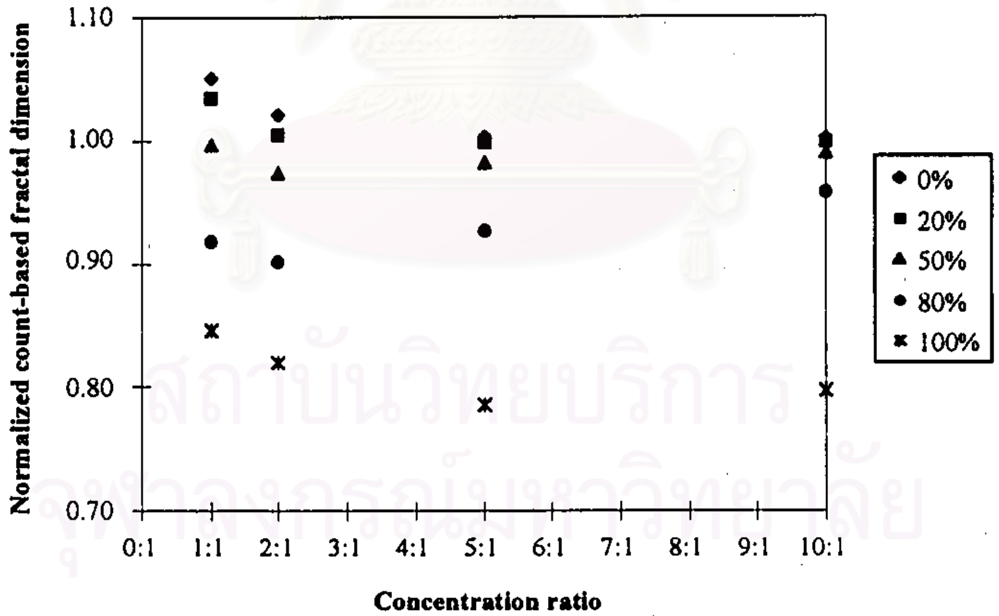

Figure 5.54 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of normal - uniform dispersion and particle size ratio = 0.20:1.

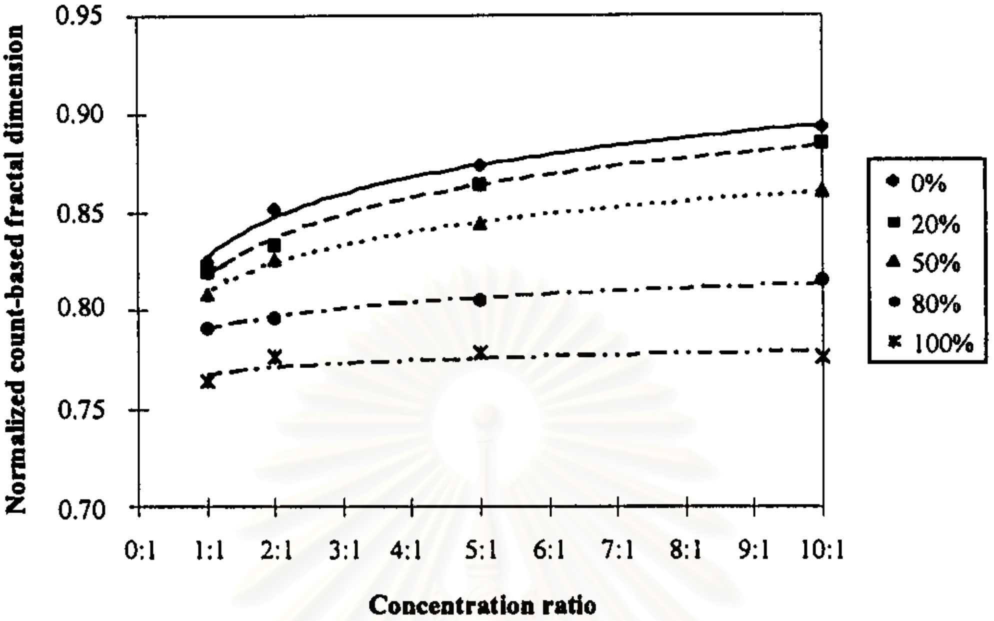

Figure 5.55 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of normal - normal dispersion and particle size ratio = 0.02:1.

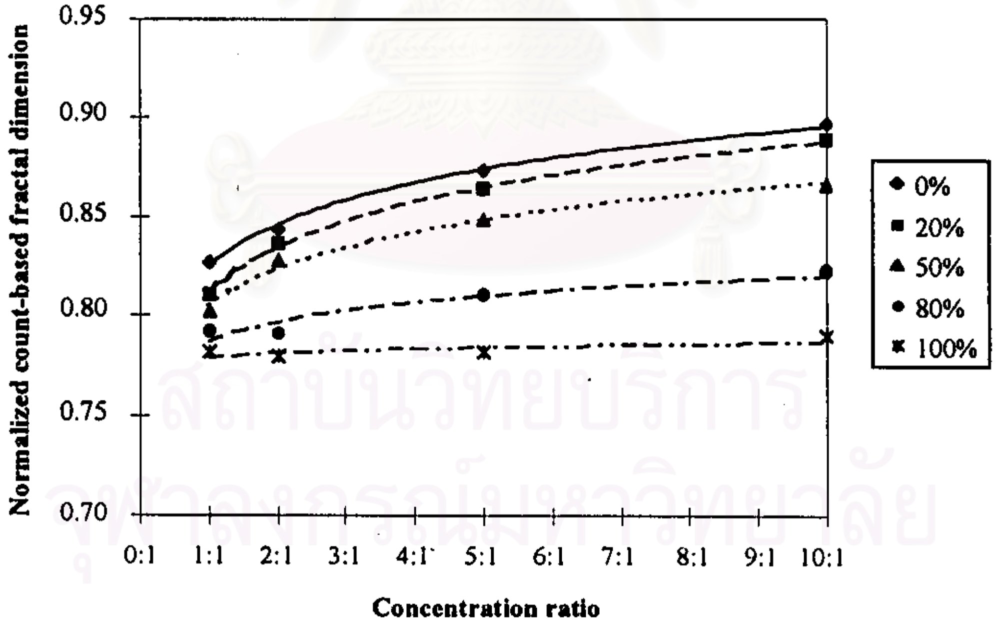

Figure 5.56 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of normal - normal dispersion and particle size ratio = 0.04:1.

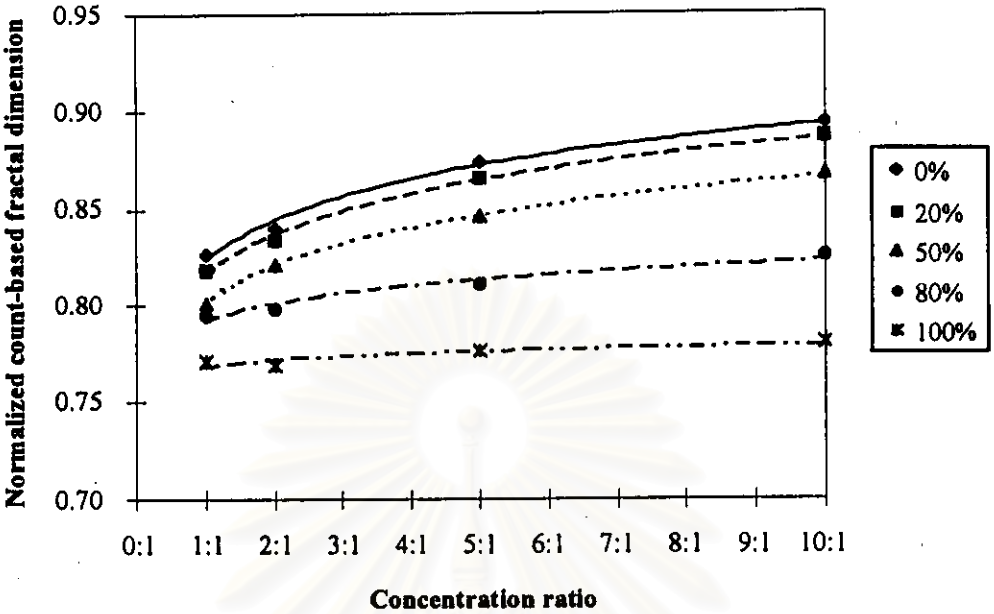

Figure 5.57 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of normal - normal dispersion and particle size ratio = 0.10:1.

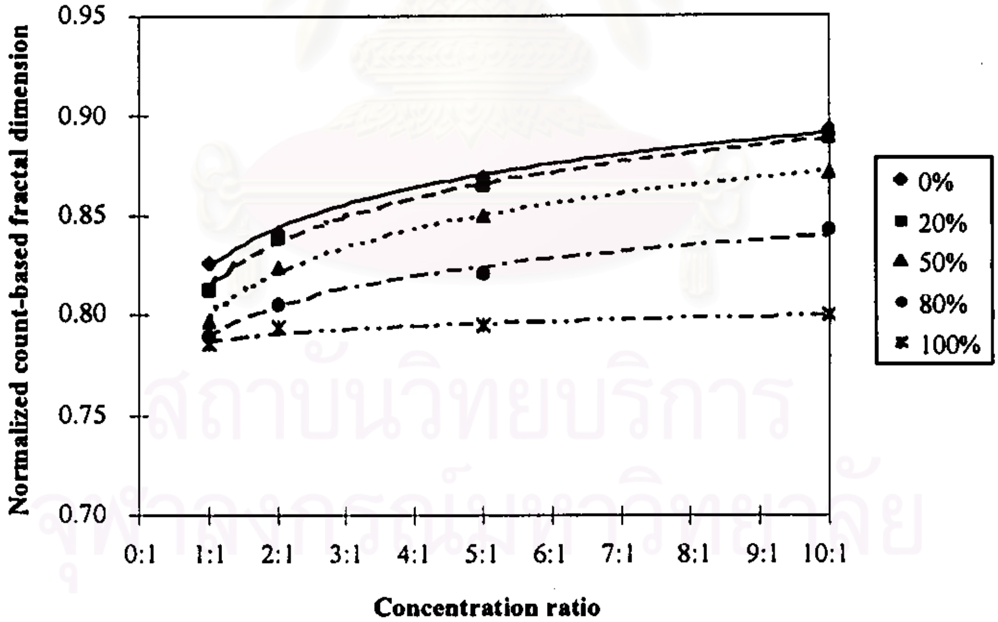

Figure 5.58 Relationship between concentration ratio and normalized count-based fractal dimension of B particles in the case of normal - normal dispersion and particle size ratio = 0.20:1.

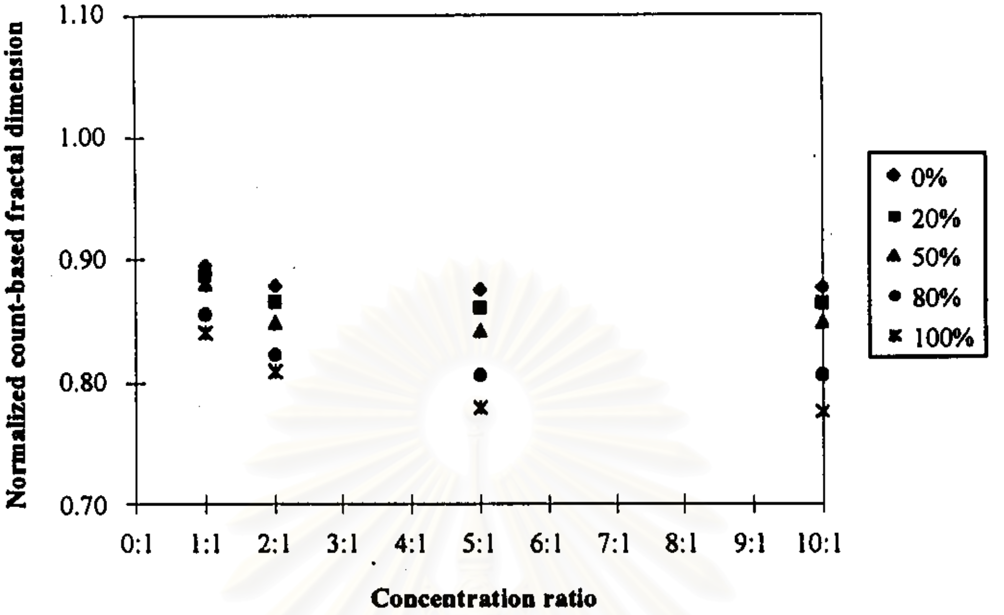

Figure 5.59 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of normal - normal dispersion and particle size ratio = 0.02:1.

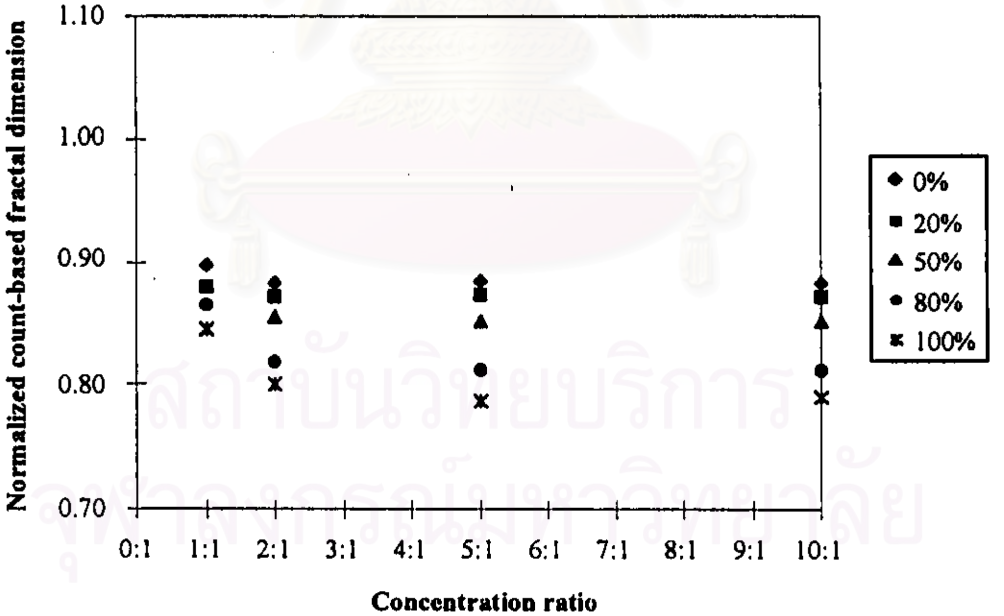

Figure 5.60 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of normal - normal dispersion and particle size ratio = 0.04:1.

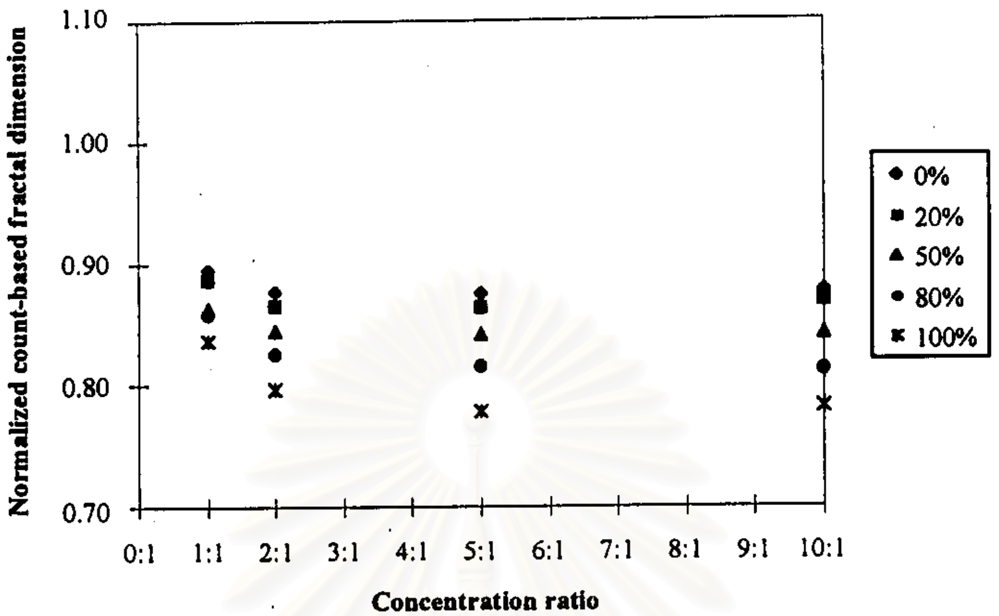

Figure 5.61 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of normal - normal dispersion and particle size ratio = 0.10:1.

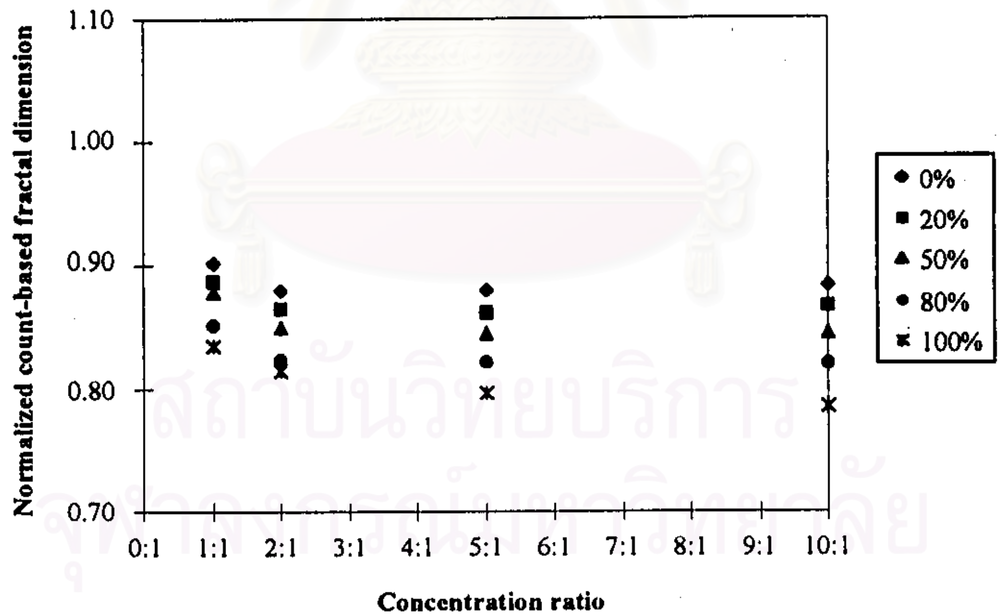

Figure 5.62 Relationship between concentration ratio and normalized count-based fractal dimension of A plus B particles in the case of normal - normal dispersion and particle size ratio = 0.20:1.

5.2.1.2.4 Normal - normal dispersion

The results of the effect of the adhesion probability on the normalized count-based fractal dimension of B particles were depicted in Figures 5.55 to 5.58 and the reason is similar to that given in 5.2.1.2.3.

Figures 5.59 to 5.62 show the effect of the adhesion probability on the normalized count-based fractal dimension of A plus B particles. The same reason given in 5.2.1.2.3 is again applicable.

5.2.1.3 Area-based fractal dimension

In this work, the observed area-based fractal dimension obtained from the analysis of computer simulation for the binary additive system was normalized by the corresponding area-based fractal dimension for the ideal uniform dispersion in the single additive system. However, since the latter remains essentially constant around 1.0, the value of the normalized area-based fractal dimension is unchanged.

Relationship between the adhesion probability and the normalized area-based fractal dimension for B particles only and A plus B particles is investigated and discussed as follows.

5.2.1.3.1 Uniform - uniform dispersion

From Figures 5.63 to 5.66, it can be seen that the normalized area-based fractal dimension of B particles decreased, as the adhesion probability rose. This is because more and more B particles were forced to adhere onto the A particles and lost their own freedom to disperse in the matrix. In this case, the fractal dimension of B was slightly influenced by the size of B particles.

Similarly, Figures 5.67 to 5.70 show that the normalized area-based fractal dimension of A plus B particles also diminished when the adhesion probability rose. Upon comparison, the normalized area-based fractal dimension of A plus B particles was somewhat larger than that of only B particles because each of the A particles occupies a much larger area than a B particle. The A : B area ratios were 2500:1, 625:1, 100:1 and 25:1 when the B : A particle size ratios were 0.02:1, 0.04:1, 0.1:1 and 0.2:1, respectively.

5.2.1.3.2 Uniform - normal dispersion

The effect of the adhesion probability on the normalized area-based fractal dimension of B particles for this case is shown in Figures 5.71 to 5.74. As seen from these Figures, when the adhesion probability rose, more and more B particles were forced to adhere onto the A particles which were uniformly dispersed. Thus the normalized area-based fractal dimension of B particles was enhanced.

From Figures 5.75 to 5.78, it can be seen that the normalized area-based fractal dimension of A plus B particles remained constant around 1.0. So it is hard to discern the effect of adhesion probability, except for large particle size and high concentration of B particles. It is because each A particle occupies a much larger area than a B particle. More specifically, the total area of B particles is large enough to discern the effect of the adhesion probability when the size of B particles was 0.1 unit and the concentration ratio was above 10 : 1.

5.2.1.3.3 Normal - uniform dispersion

Figures 5.79 to 5.82 show that the normalized area-based fractal dimension of B particles declined, as more and more B particles adhered onto the A particles. The reason is the same as that mentioned in 5.2.1.3.1.

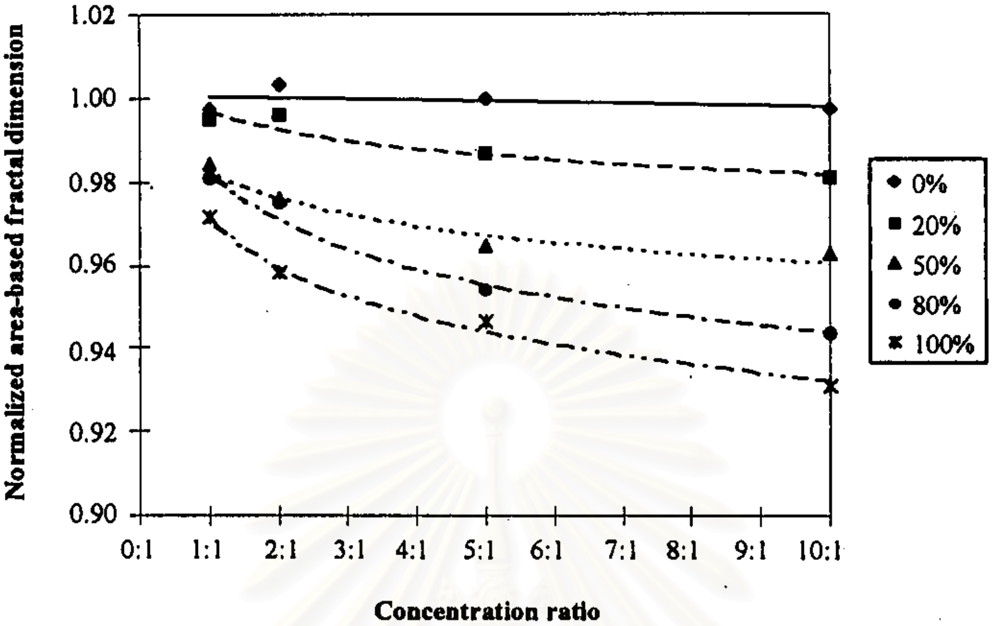

Figure 5.63 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of uniform - uniform dispersion and particle size ratio = 0.02:1.

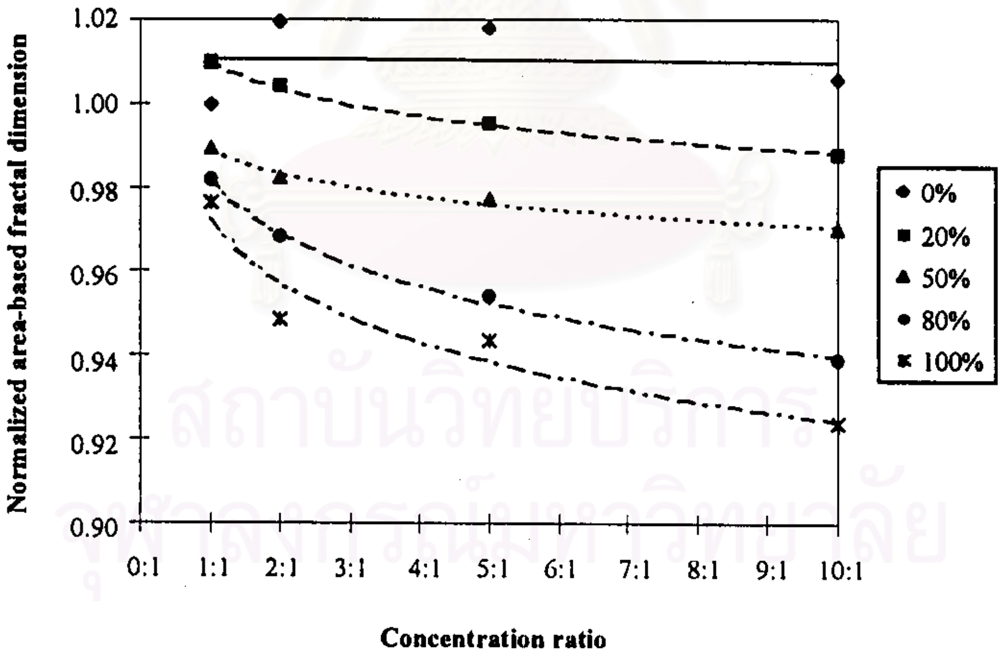

Figure 5.64 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of uniform - uniform dispersion and particle size ratio = 0.04:1.

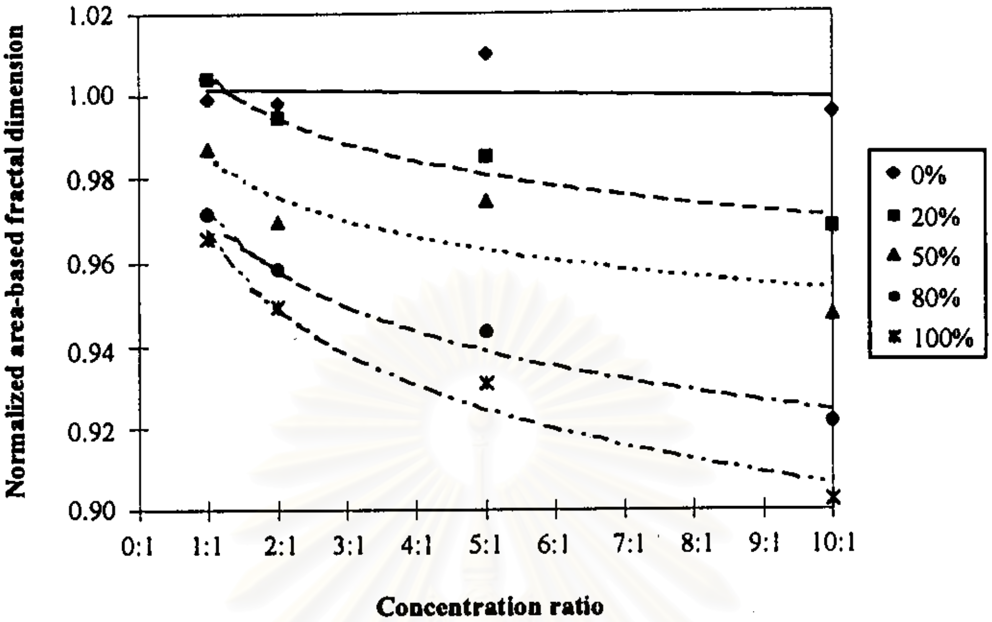

Figure 5.65 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of uniform - uniform dispersion and particle size ratio = 0.10:1.

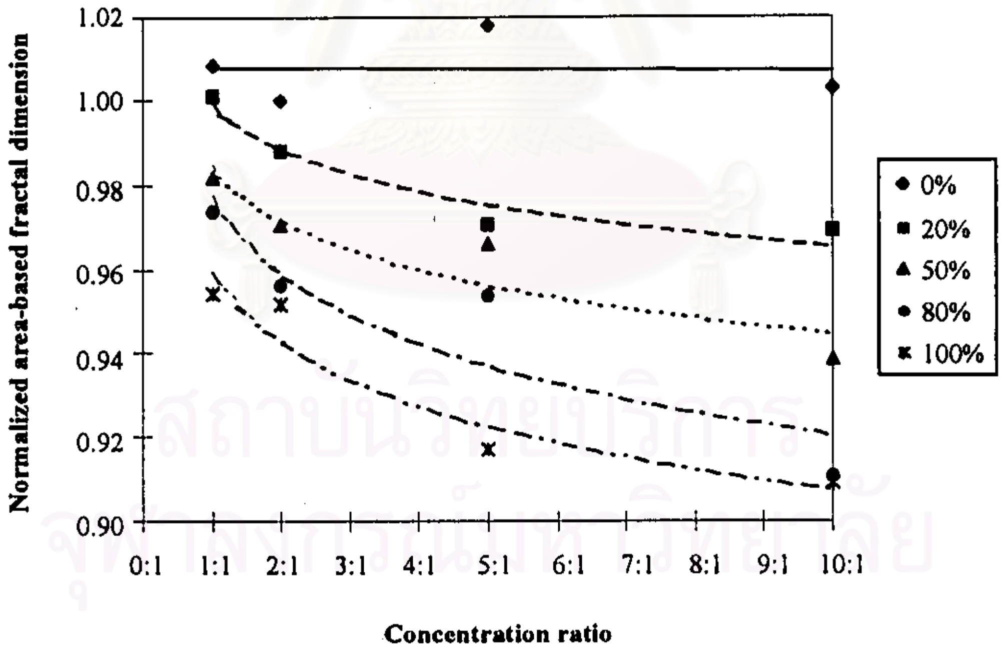

Figure 5.66 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of uniform - uniform dispersion and particle size ratio = 0.20:1.

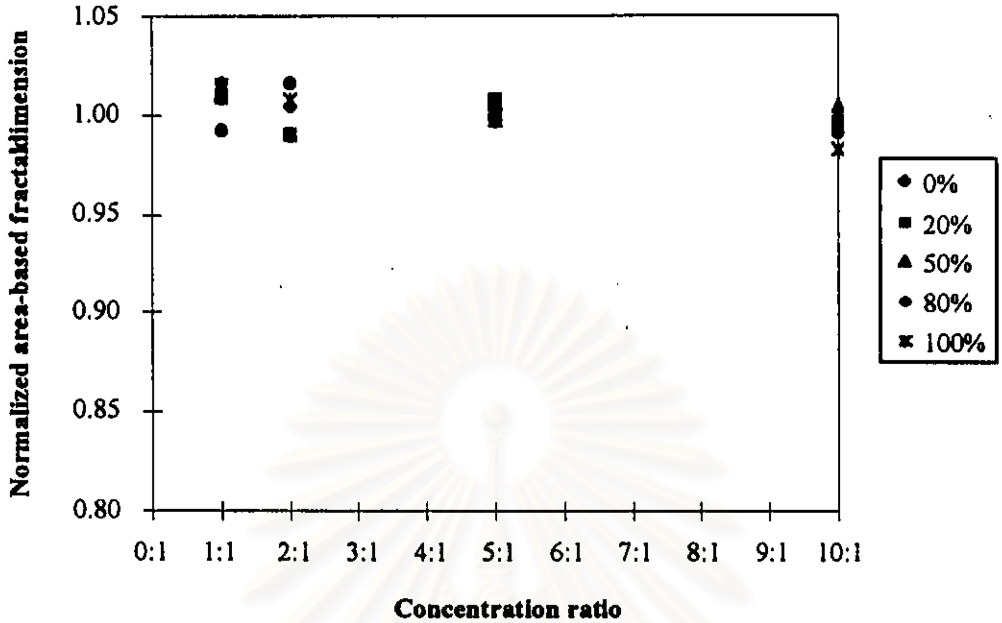

Figure 5.67 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of uniform - uniform dispersion and particle size ratio = 0.02:1.

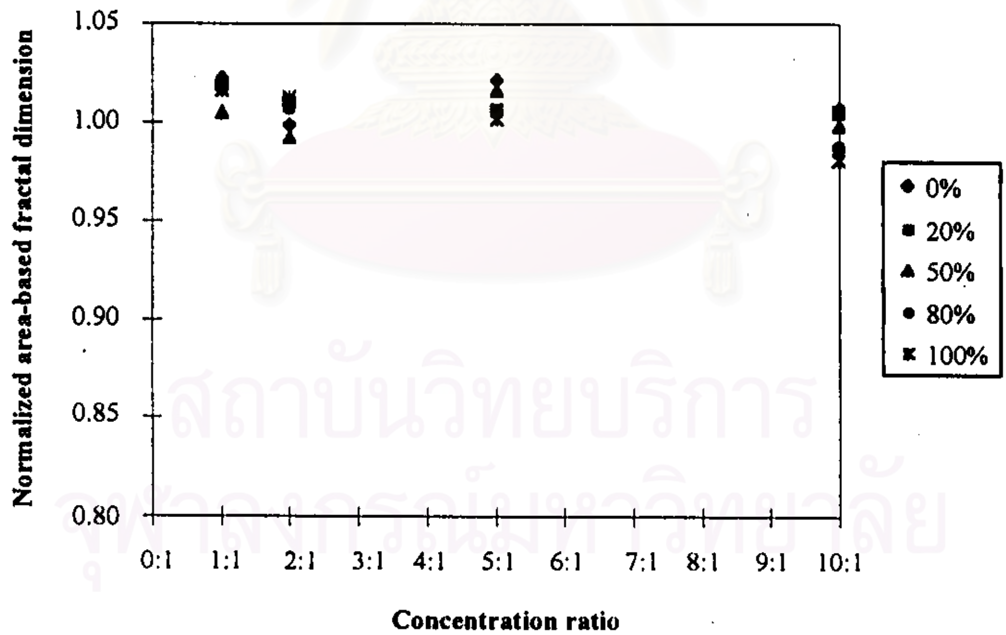

Figure 5.68 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of uniform - uniform dispersion and particle size ratio = 0.04:1.

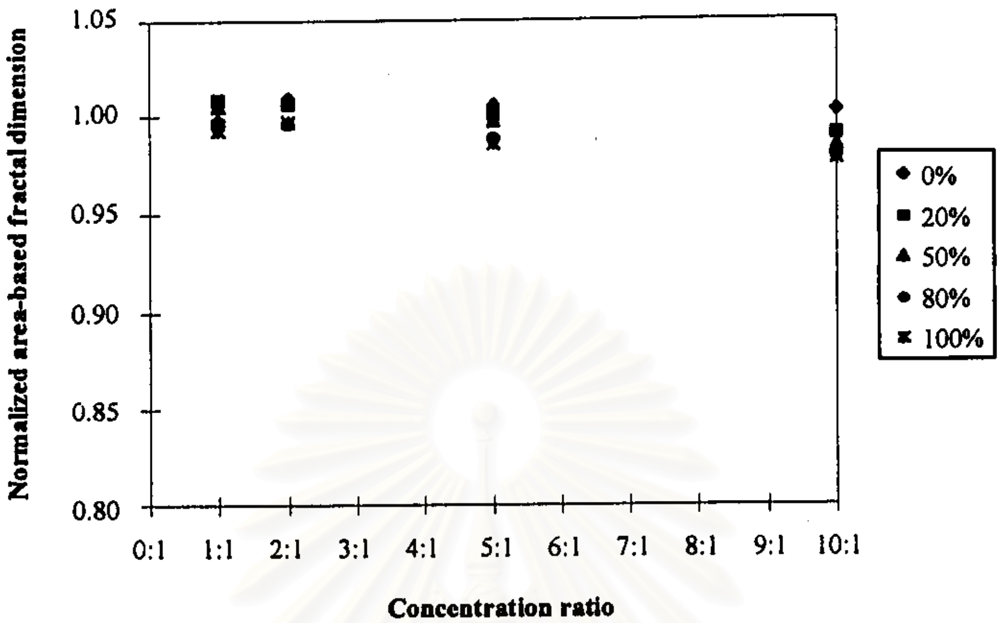

Figure 5.69 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of uniform - uniform dispersion and particle size ratio = 0.10:1.

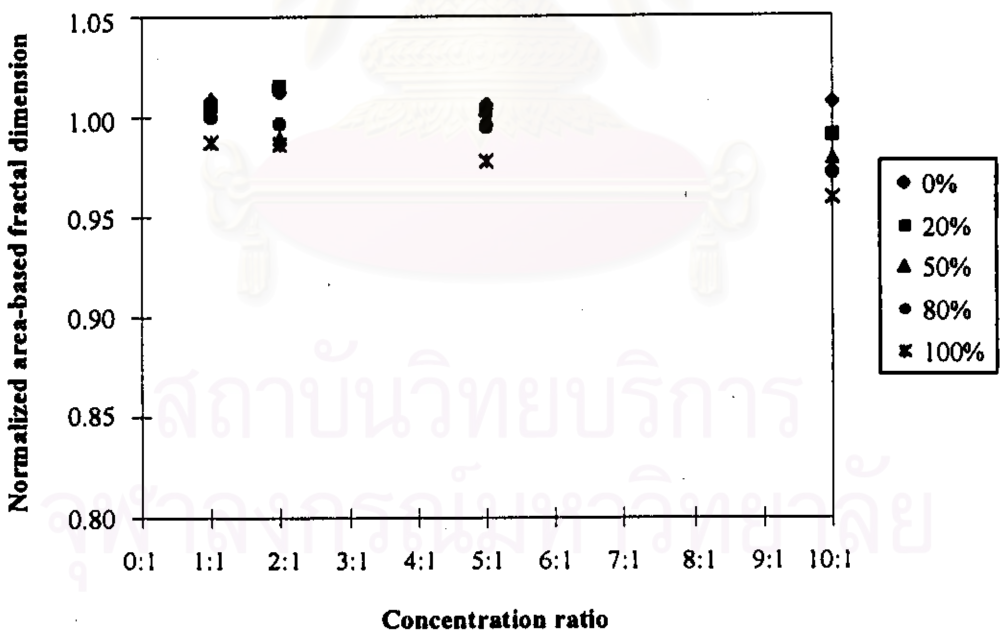

Figure 5.70 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of uniform - uniform dispersion and particle size ratio = 0.20:1.

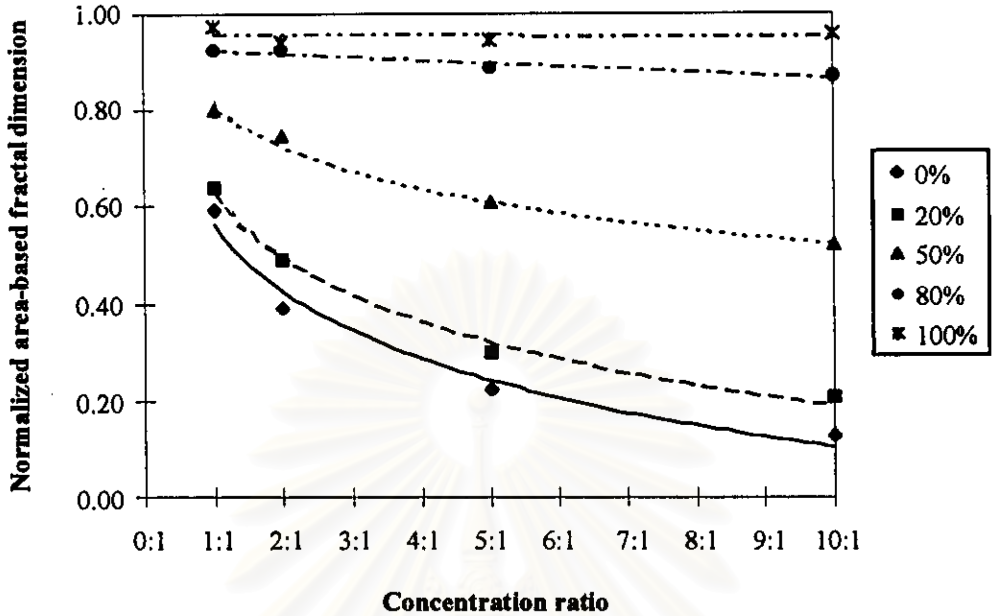

Figure 5.71 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of uniform - normal dispersion and particle size ratio = 0.02:1.

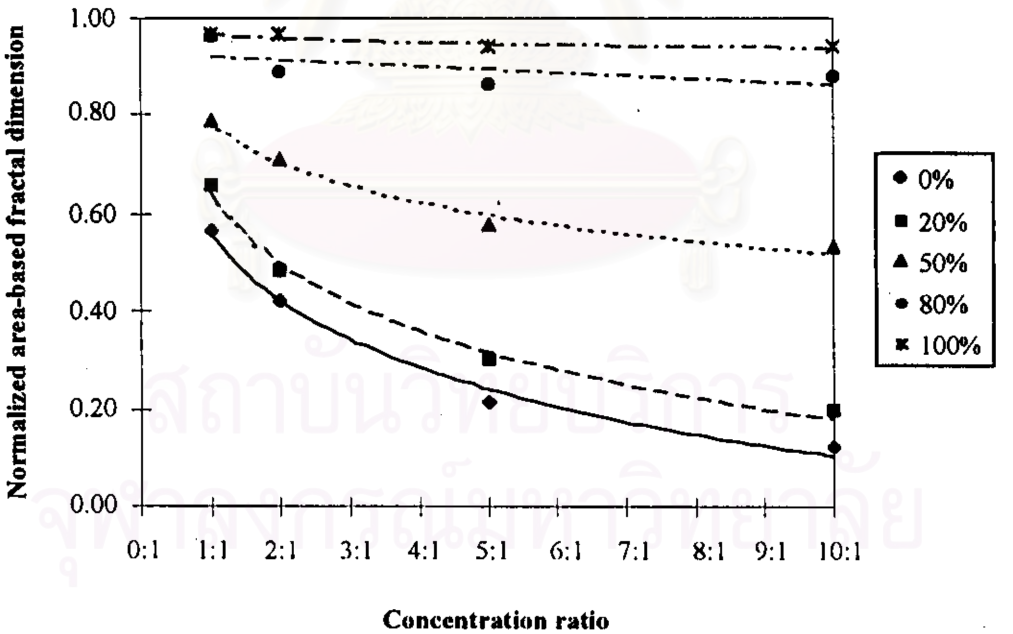

Figure 5.72 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of uniform - normal dispersion and particle size ratio = 0.04:1.

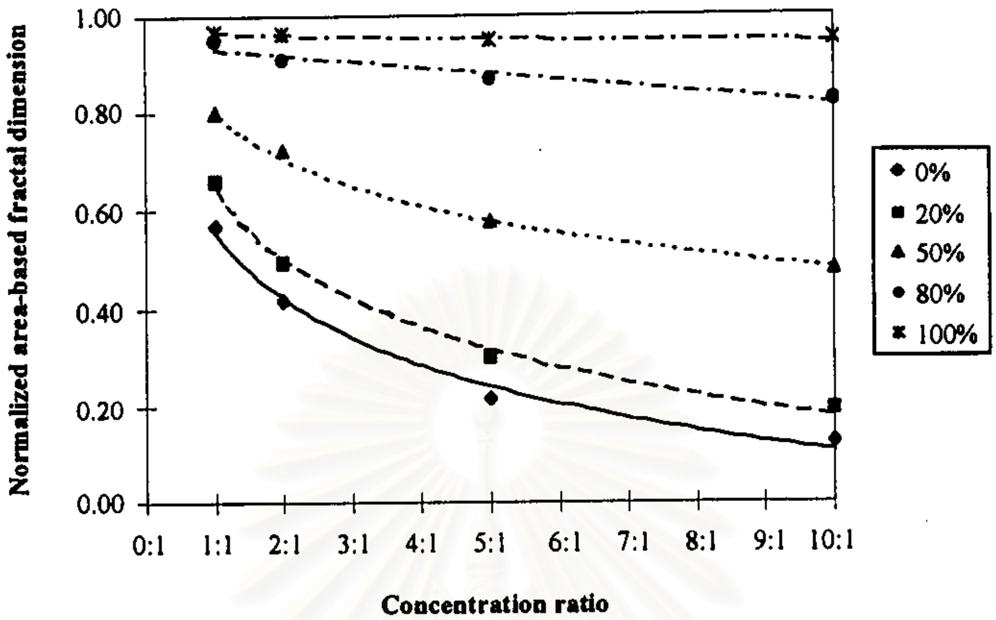

Figure 5.73 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of uniform - normal dispersion and particle size ratio = 0.10:1.

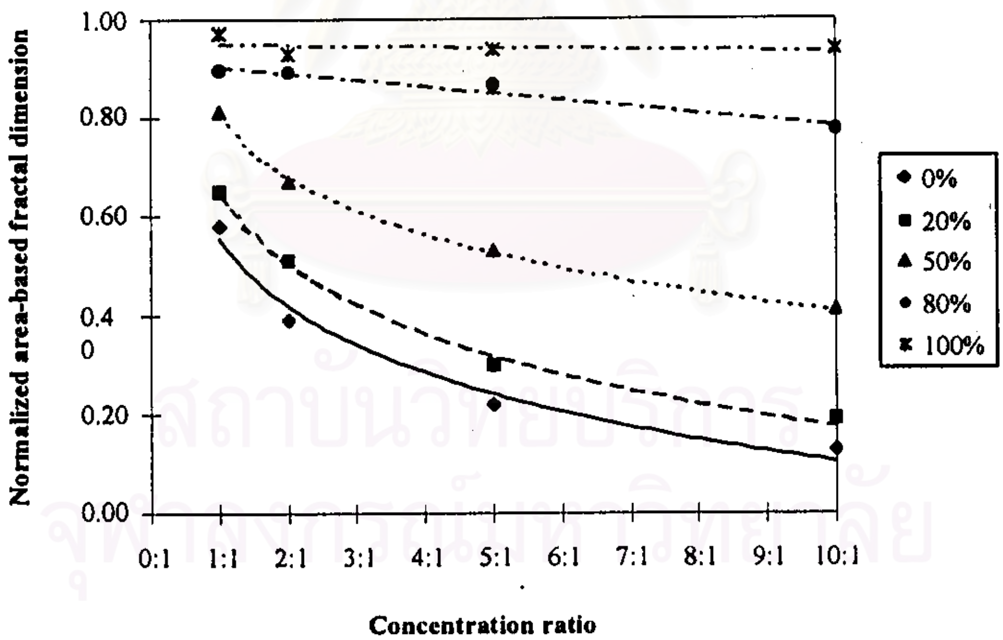

Figure 5.74 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of uniform - normal dispersion and particle size ratio = 0.20:1.

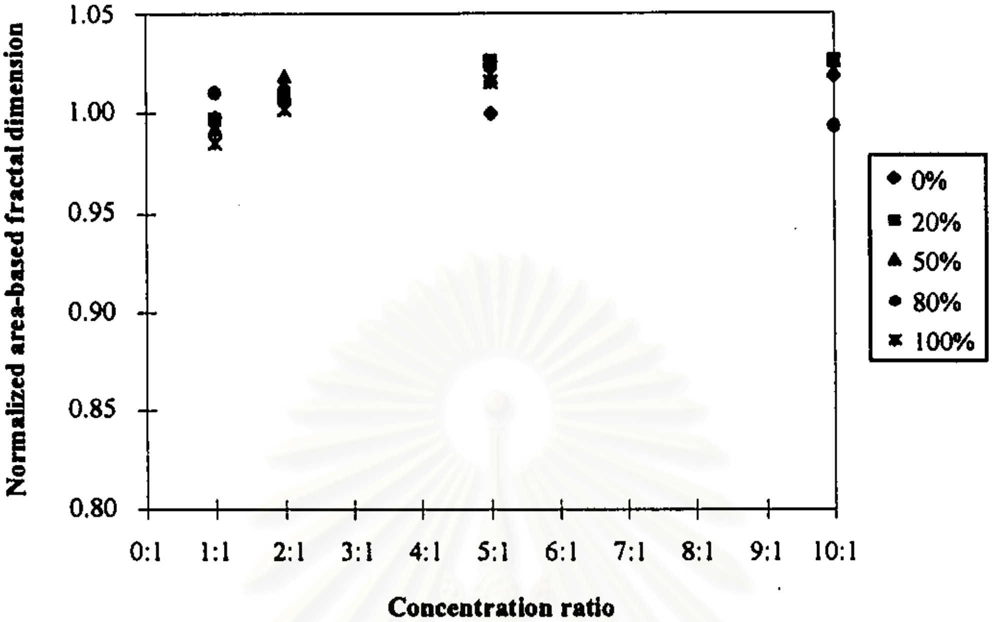

Figure 5.75 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of uniform - normal dispersion and particle size ratio = 0.02:1.

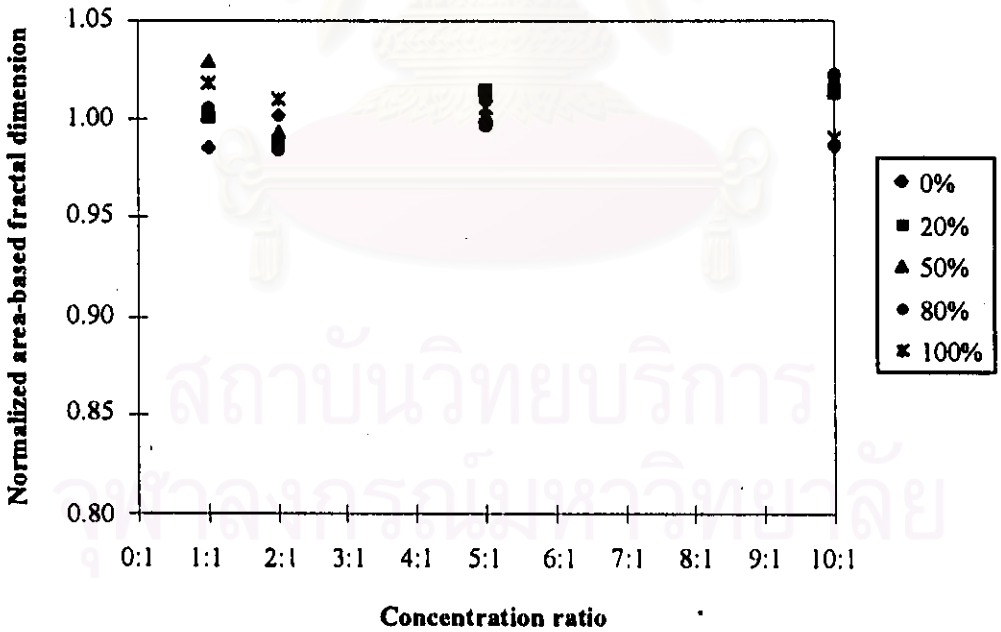

Figure 5.76 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of uniform - normal dispersion and particle size ratio = 0.04:1.

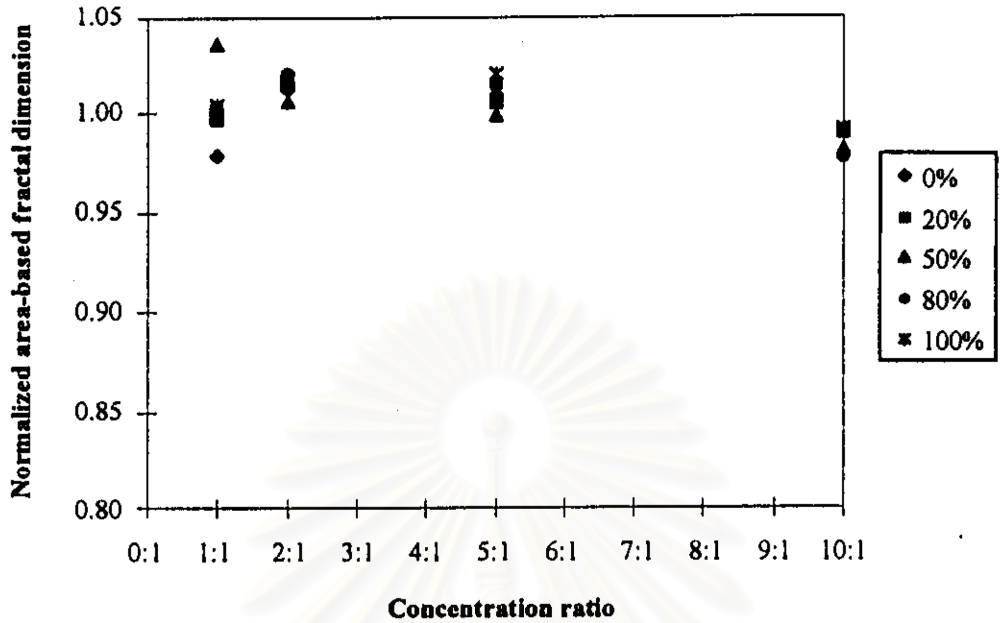

Figure 5.77 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of uniform - normal dispersion and particle size ratio = 0.10:1.

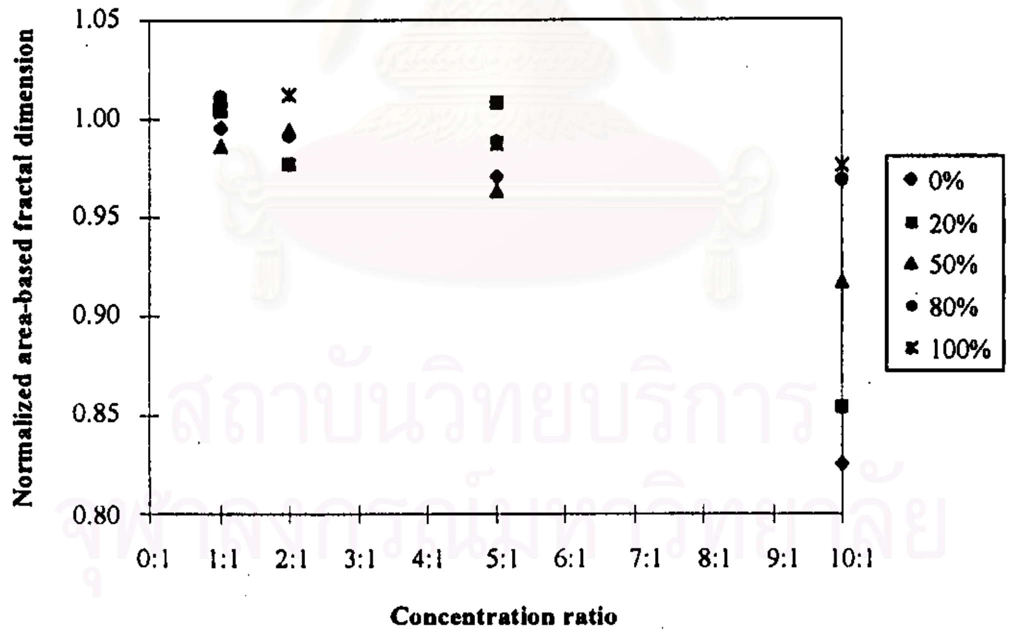

Figure 5.78 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of uniform - normal dispersion and particle size ratio = 0.20:1.

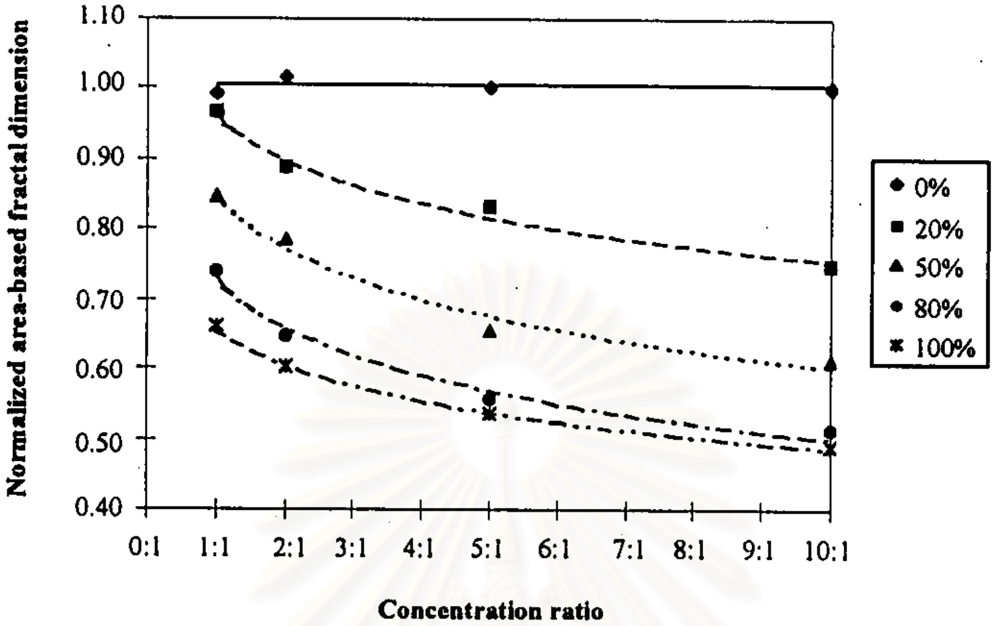

Figure 5.79 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of normal - uniform dispersion and particle size ratio = 0.02:1.

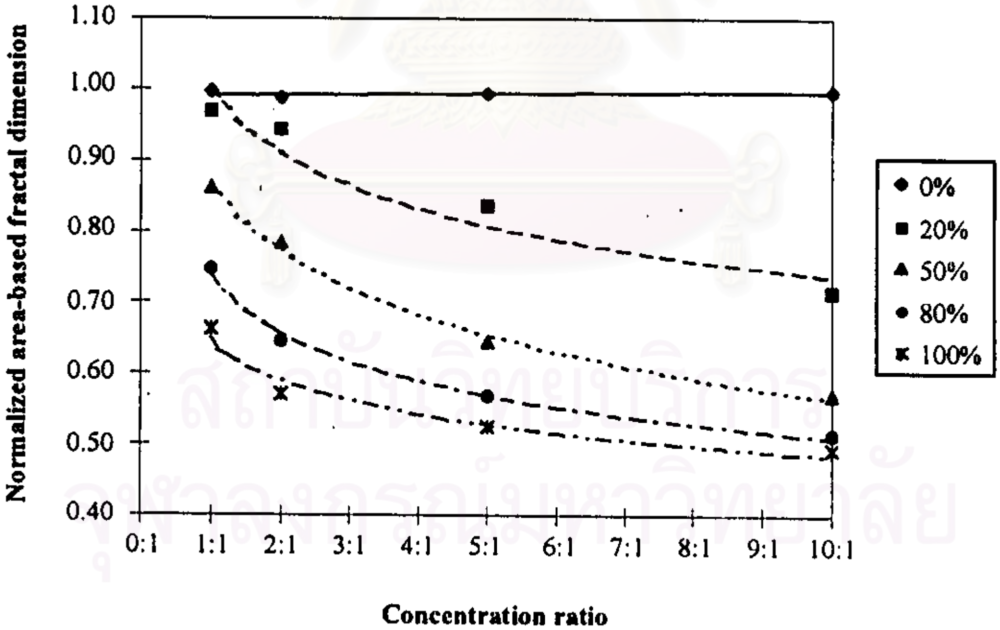

Figure 5.80 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of normal - uniform dispersion and particle size ratio = 0.04:1.

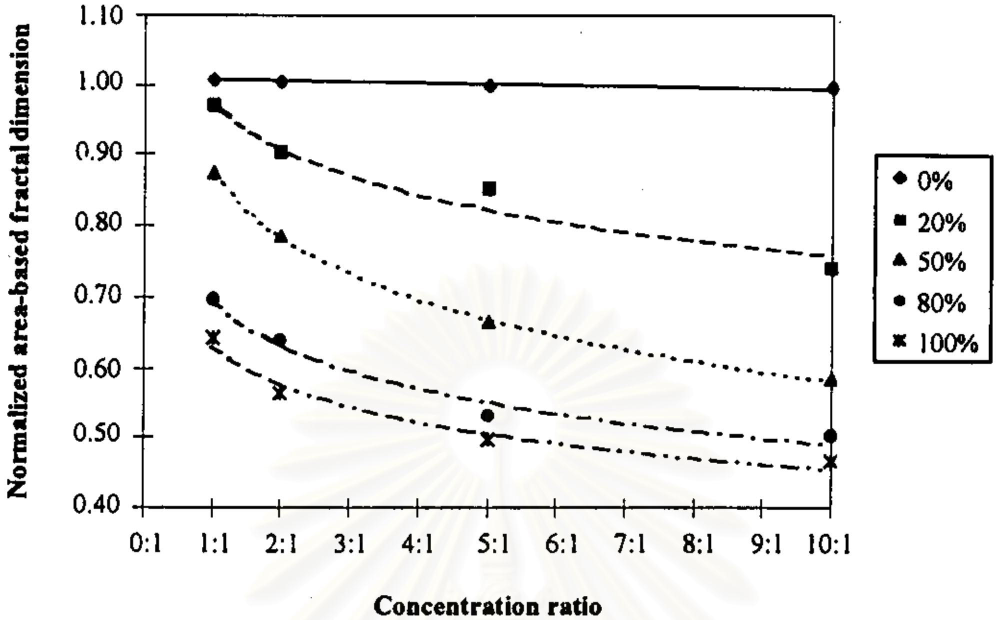

Figure 5.81 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of normal - uniform dispersion and particle size ratio = 0.10:1.

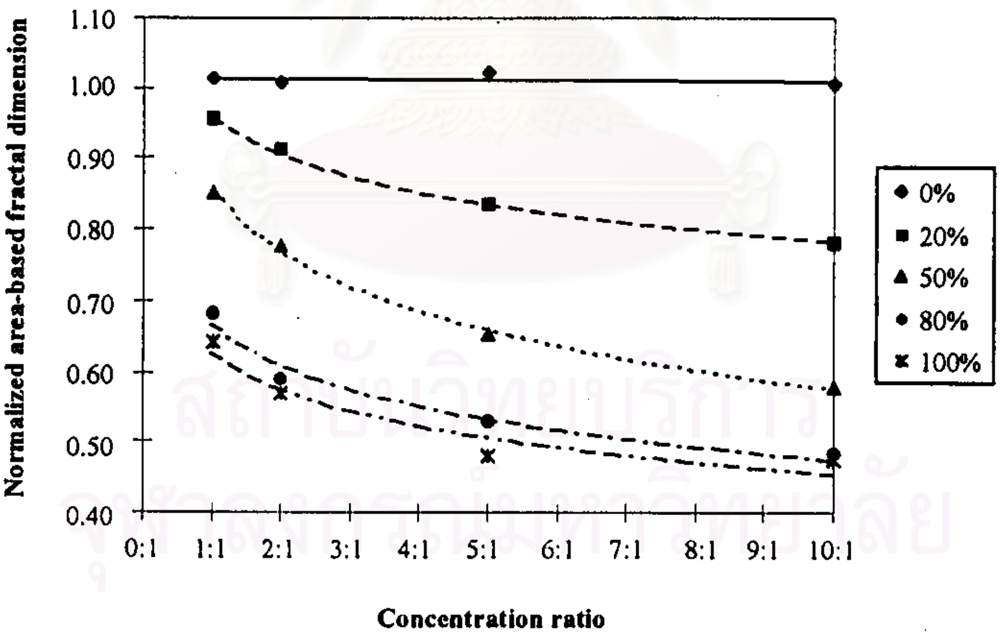

Figure 5.82 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of normal - uniform dispersion and particle size ratio = 0.20:1.

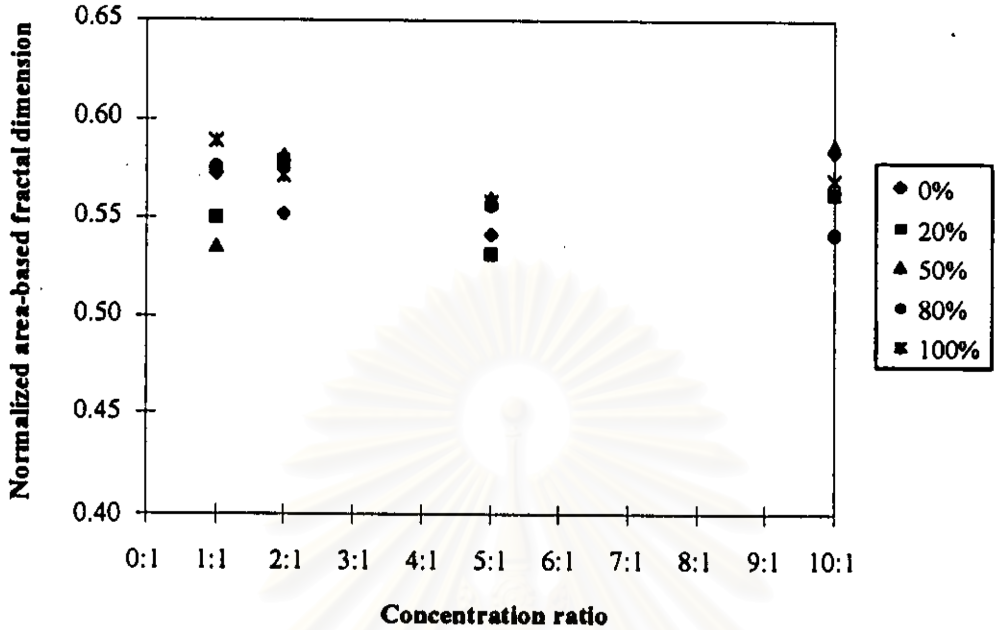

Figure 5.83 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of normal - uniform dispersion and particle size ratio = 0.02:1.

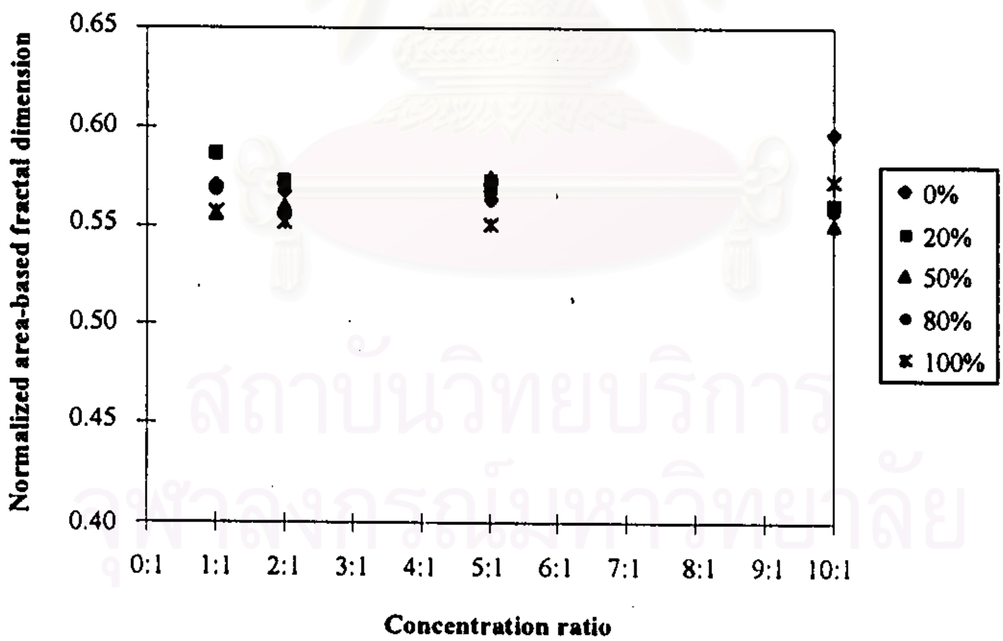

Figure 5.84 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of normal - uniform dispersion and particle size ratio = 0.04:1.

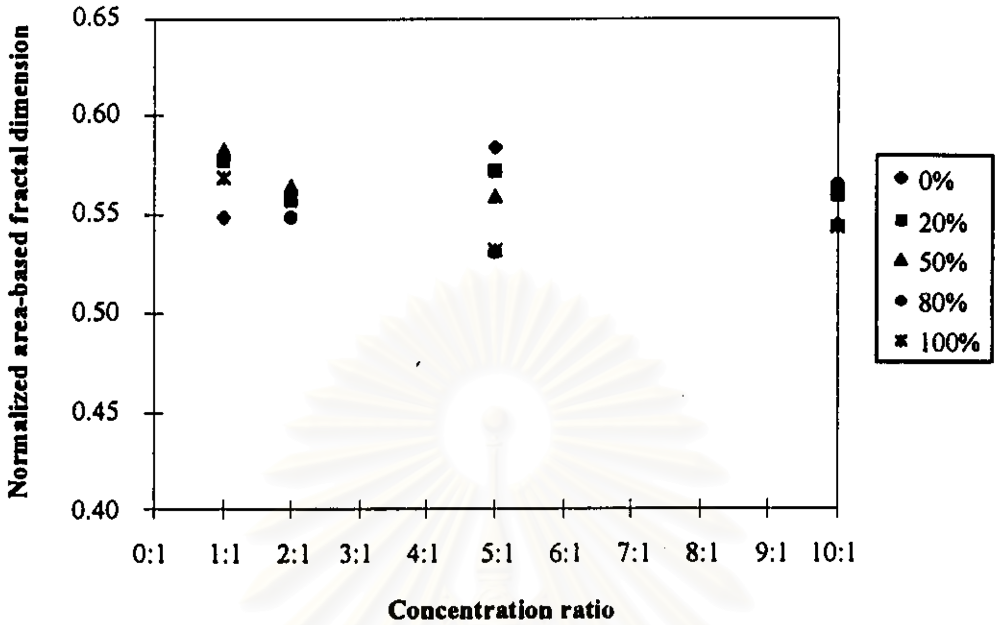

Figure 5.85 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of normal - uniform dispersion and particle size ratio = 0.10:1.

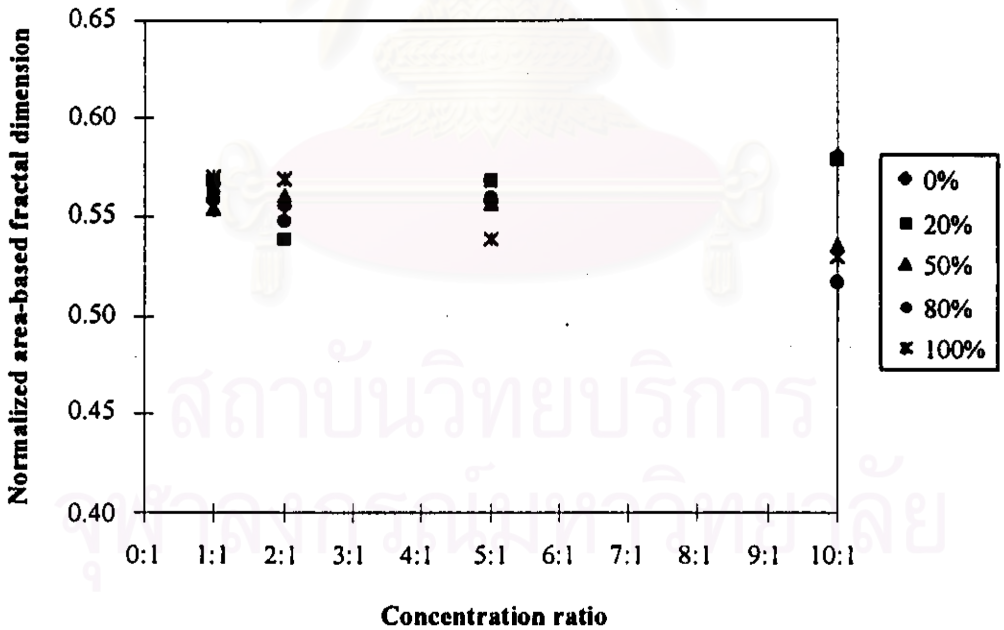

Figure 5.86 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of normal - uniform dispersion and particle size ratio = 0.20:1.

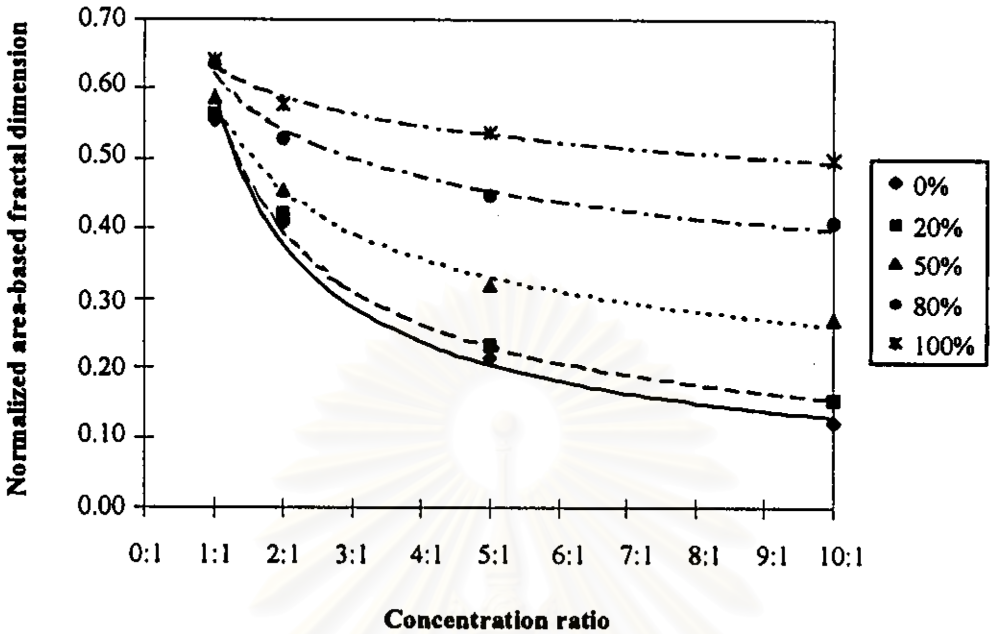

Figure 5.87 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of normal - normal dispersion and particle size ratio = 0.02:1.

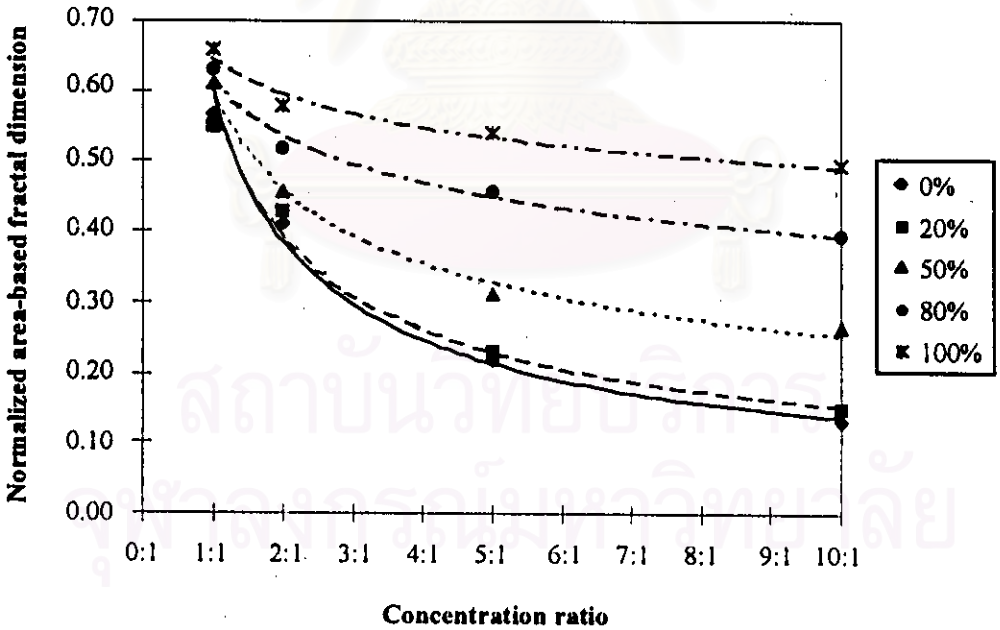

Figure 5.88 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of normal - normal dispersion and particle size ratio = 0.04:1.

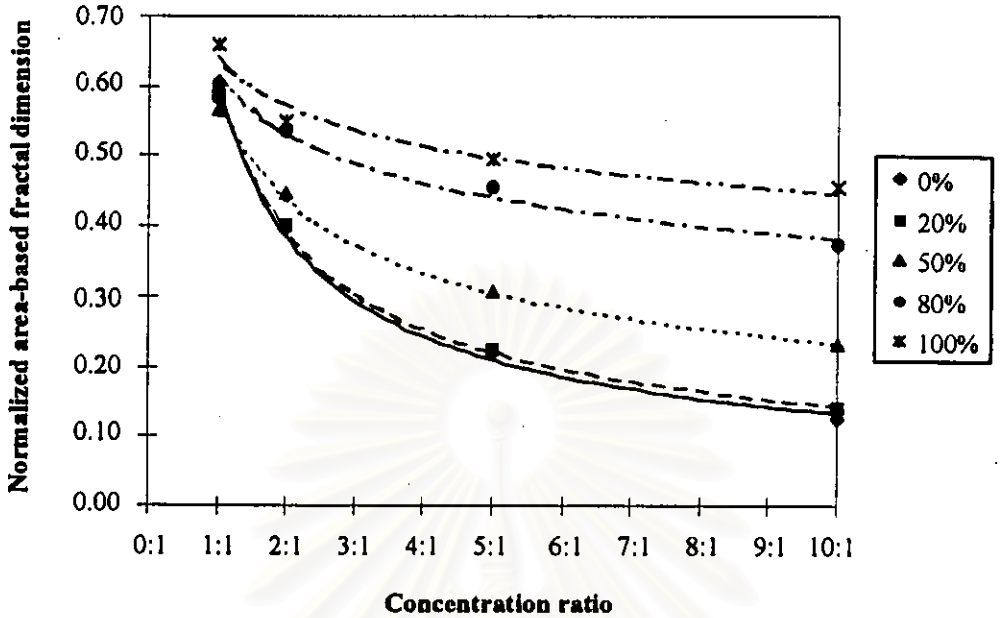

Figure 5.89 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of normal - normal dispersion and particle size ratio = 0.10:1.

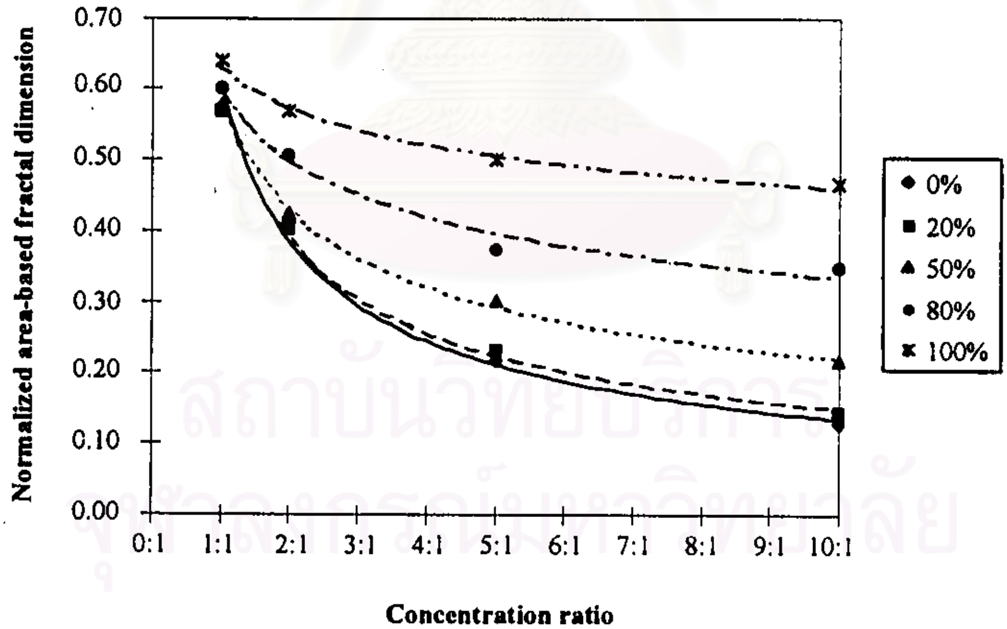

Figure 5.90 Relationship between concentration ratio and normalized area-based fractal dimension of B particles in the case of normal - normal dispersion and particle size ratio = 0.20:1.

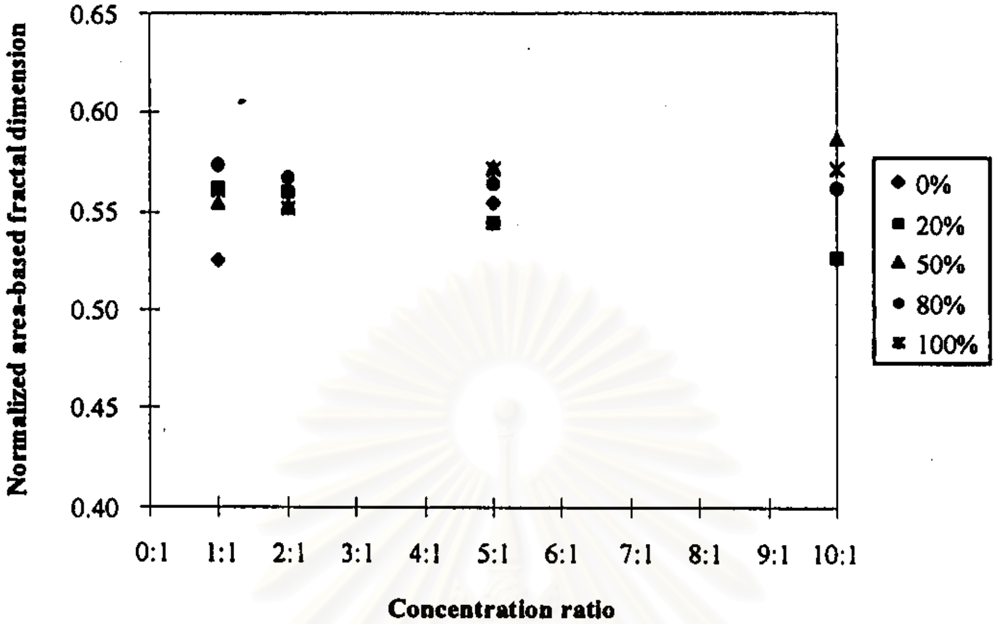

Figure 5.91 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of normal - normal dispersion and particle size ratio = 0.02:1.

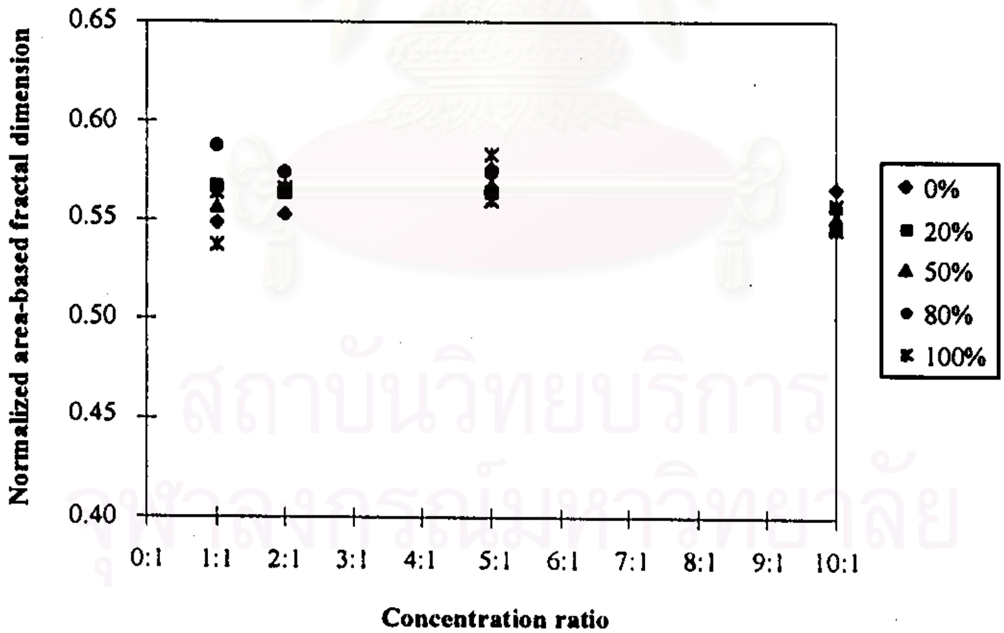

Figure 5.92 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of normal - normal dispersion and particle size ratio = 0.04:1.

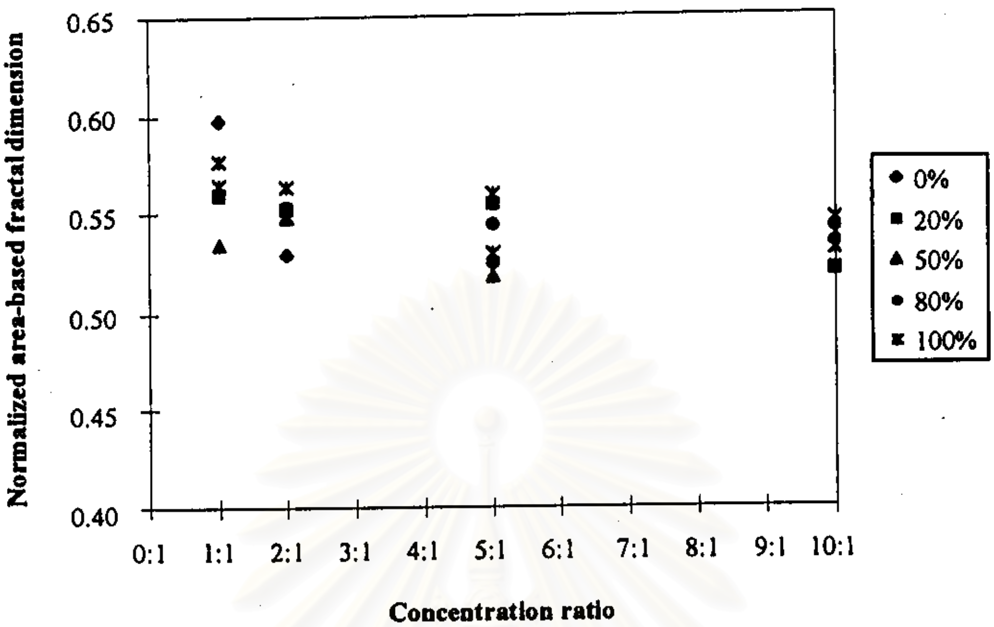

Figure 5.93 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of normal - normal dispersion and particle size ratio = 0.10:1.

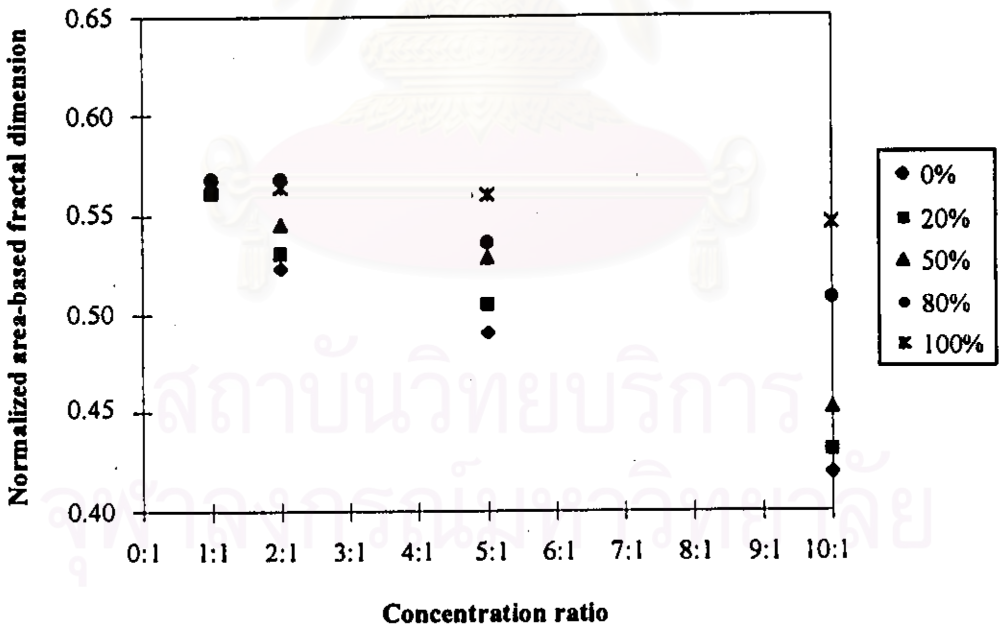

Figure 5.94 Relationship between concentration ratio and normalized area-based fractal dimension of A plus B particles in the case of normal - normal dispersion and particle size ratio = 0.20:1.

As shown in Figures 5.83 to 5.86, because of the normal dispersion and the much greater area of A particles, it is hard to discern the effect of the adhesion probability on the normalized area-based fractal dimension of A plus B particles.

5.2.1.3.4 Normal - normal dispersion

From Figures 5.87 to 5.90, it is found that the normalized area-based fractal dimension of B particles increased, as the adhesion probability rose. This was because the more numerous B particles which followed the normal dispersion was forced in increasing numbers to adhere onto the much fewer A particles. Therefore the effective number of normally dispersed B particles appeared to decline because of the clustering of B particles.

As depicted in Figures 5.91 to 5.94, because the area of one A particle is much greater than that of a B particle, it is hard to discern the effect of the adhesion probability on the normalized area-based fractal dimension of A plus B particles except when the particle size and concentration of B particles were sufficiently large.

5.2.1.4 Coordination number

The coordination number is the most direct indicator of the number of B particles adhering onto each of the A particles. In this section, the relationship between the adhesion probability and the mean and mode of the coordination number was listed in Tables 5.10 to 5.13.

Tables 5.10 to 5.13 show that the observed coordination number (especially the mean) rose in proportion to the adhesion probability of B particles, regardless of the type of dispersion of both A and B particles. At 0% adhesion, every B particle was dispersed freely in the matrix, but all B particles was forced to adhere onto the A particles at 100% adhesion, so the resulting mean value of the

Table 5.10 The effect of adhesion probability, concentration ratio (B:A) and particle size ratio (B:A) on coordination number (mean and mode) in the case of uniform - uniform dispersion.
Particle size of A : 0.5 unit and concentration of A : 500 particles/area.

Particle size ratio (B:A)	Concentration ratio (B:A)	Coordination number									
		Adhesion probability									
		0%		20%		50%		80%		100%	
		MEAN	MODE	MEAN	MODE	MEAN	MODE	MEAN	MODE	MEAN	MODE
0.02:1	1:1	0.00	0.00	0.17	0.00	0.45	0.00	0.78	0.00	1.00	0.00
	2:1	0.00	0.00	0.33	0.00	0.93	0.00	1.53	1.11	2.00	1.47
	5:1	0.00	0.00	0.88	0.00	2.39	1.87	3.90	3.90	5.00	4.64
	10:1	0.00	0.00	1.86	1.33	4.74	4.29	7.78	6.90	10.00	9.36
0.04:1	1:1	0.00	0.00	0.17	0.00	0.44	0.00	0.78	0.00	1.00	0.57
	2:1	0.00	0.00	0.33	0.00	0.91	0.00	1.52	1.11	2.00	1.51
	5:1	0.00	0.00	0.92	0.00	2.32	1.45	3.88	3.23	5.00	4.48
	10:1	0.00	0.00	1.80	1.36	4.76	4.65	7.70	7.28	10.00	9.42
0.1:1	1:1	0.00	0.00	0.18	0.00	0.44	0.00	0.76	0.00	1.00	0.54
	2:1	0.00	0.00	0.33	0.00	0.91	0.00	1.53	1.09	2.00	1.58
	5:1	0.00	0.00	0.90	0.00	2.32	1.84	3.79	3.64	5.00	4.44
	10:1	0.00	0.00	1.82	1.42	4.44	4.30	7.44	7.17	10.00	9.95
0.2:1	1:1	0.00	0.00	0.17	0.00	0.38	0.00	0.75	0.00	1.00	0.61
	2:1	0.00	0.00	0.34	0.00	0.89	0.00	1.49	1.18	2.00	1.72
	5:1	0.00	0.00	0.92	0.00	2.22	1.59	3.68	3.30	5.00	4.96
	10:1	0.00	0.00	1.72	1.46	4.06	3.92	6.78	6.71	10.00	9.70

Table 5.11 The effect of adhesion probability, concentration ratio (B:A) and particle size ratio (B:A) on coordination number (mean and mode) in the case of uniform - normal dispersion.
Particle size of A : 0.5 unit and concentration of A : 500 particles/area.

Particle size ratio (B:A)	Concentration ratio (B:A)	Coordination number									
		Adhesion probability									
		0%		20%		50%		80%		100%	
		MEAN	MODE	MEAN	MODE	MEAN	MODE	MEAN	MODE	MEAN	MODE
0.02:1	1:1	0.00	0.00	0.17	0.00	0.44	0.00	0.78	0.00	1.00	0.23
	2:1	0.00	0.00	0.34	0.00	0.92	0.00	1.55	0.21	2.00	0.28
	5:1	0.00	0.00	0.90	0.00	2.42	1.71	3.88	3.15	5.00	4.18
	10:1	0.00	0.00	1.92	1.39	4.76	3.97	7.83	7.13	10.00	9.62
0.04:1	1:1	0.00	0.00	0.17	0.00	0.46	0.00	0.78	0.00	1.00	0.00
	2:1	0.00	0.00	0.37	0.00	0.93	0.00	1.54	0.21	2.00	0.65
	5:1	0.00	0.00	0.89	0.00	2.30	1.70	3.94	3.07	5.00	4.18
	10:1	0.00	0.00	1.84	1.38	4.73	4.40	7.70	7.44	10.00	9.59
0.1:1	1:1	0.00	0.00	0.18	0.00	0.46	0.00	0.79	0.00	1.00	0.47
	2:1	0.00	0.00	0.35	0.00	0.87	0.00	1.50	0.26	2.00	1.04
	5:1	0.00	0.00	0.89	0.00	2.30	1.74	3.85	3.28	5.00	4.56
	10:1	0.00	0.00	1.84	1.35	4.48	4.10	7.46	7.14	10.00	9.94
0.2:1	1:1	0.00	0.00	0.17	0.00	0.47	0.00	0.74	0.00	1.00	0.39
	2:1	0.00	0.00	0.36	0.00	0.90	0.00	1.53	0.20	2.00	1.11
	5:1	0.00	0.00	0.89	0.12	2.21	1.70	3.71	3.33	5.00	4.52
	10:1	0.00	0.00	1.72	1.33	4.16	3.90	6.83	6.92	10.00	9.54

Table 5.12 The effect of adhesion probability, concentration ratio (B:A) and particle size ratio (B:A) on coordination number (mean and mode) in the case of normal - uniform dispersion.
Particle size of A : 0.5 unit and concentration of A : 500 particles/area.

Particle size ratio (B:A)	Concentration ratio (B:A)	Coordination number									
		Adhesion probability									
		0%		20%		50%		80%		100%	
		MEAN	MODE	MEAN	MODE	MEAN	MODE	MEAN	MODE	MEAN	MODE
0.02:1	1:1	0.00	0.00	0.19	0.00	0.48	0.00	0.78	0.00	1.00	0.35
	2:1	0.00	0.00	0.36	0.00	0.92	0.00	1.54	0.24	2.00	0.74
	5:1	0.00	0.00	0.92	0.00	2.33	1.63	3.79	3.28	5.00	5.04
	10:1	0.00	0.00	1.85	1.28	4.48	4.18	7.41	7.13	10.00	9.56
0.04:1	1:1	0.00	0.00	0.17	0.00	0.46	0.00	0.78	0.00	1.00	0.26
	2:1	0.00	0.00	0.34	0.00	0.97	0.00	1.55	0.22	2.00	0.71
	5:1	0.00	0.00	0.92	0.13	2.38	1.82	3.89	3.37	5.00	3.92
	10:1	0.00	0.00	1.93	1.38	4.74	3.95	7.79	7.75	10.00	9.59
0.1:1	1:1	0.00	0.00	0.17	0.00	0.47	0.00	0.78	0.00	1.00	0.12
	2:1	0.00	0.00	0.35	0.00	0.95	0.11	1.56	0.55	2.00	0.71
	5:1	0.00	0.00	0.95	0.00	2.43	1.62	3.89	3.54	5.00	4.53
	10:1	0.00	0.00	1.91	1.34	4.83	4.35	7.88	7.09	10.00	8.93
0.2:1	1:1	0.00	0.00	0.18	0.00	0.46	0.00	0.79	0.00	1.00	0.64
	2:1	0.00	0.00	0.36	0.00	0.93	0.12	1.52	0.25	2.00	0.75
	5:1	0.00	0.00	0.88	0.14	2.26	1.78	3.73	3.39	5.00	4.56
	10:1	0.00	0.00	1.69	1.22	4.18	4.12	6.85	6.88	10.00	9.20

Table 5.13 The effect of adhesion probability, concentration ratio (B:A) and particle size ratio (B:A) on coordination number (mean and mode) in the case of normal - normal dispersion.

Particle size of A : 0.5 unit and concentration of A : 500 particles/area.

Particle size ratio (B:A)	Concentration ratio (B:A)	Coordination number									
		Adhesion probability									
		0%		20%		50%		80%		100%	
		MEAN	MODE	MEAN	MODE	MEAN	MODE	MEAN	MODE	MEAN	MODE
0.02:1	1:1	0.00	0.00	0.19	0.00	0.45	0.00	0.78	0.00	1.00	0.59
	2:1	0.00	0.00	0.36	0.00	0.88	0.00	1.56	1.10	2.00	1.50
	5:1	0.00	0.00	0.91	0.00	2.33	1.88	3.89	3.37	5.00	4.27
	10:1	0.00	0.00	1.90	1.36	4.70	4.10	7.74	7.38	10.00	9.91
0.04:1	1:1	0.00	0.00	0.19	0.00	0.46	0.00	0.79	0.00	1.00	0.00
	2:1	0.00	0.00	0.36	0.00	0.95	0.00	1.56	1.17	2.00	1.56
	5:1	0.00	0.00	0.91	0.00	2.34	1.71	3.87	3.57	5.00	4.28
	10:1	0.00	0.00	1.88	1.37	4.84	4.60	7.80	7.22	10.00	9.96
0.1:1	1:1	0.00	0.00	0.19	0.00	0.49	0.00	0.77	0.00	1.00	0.55
	2:1	0.00	0.00	0.38	0.00	0.93	0.00	1.55	1.14	2.00	1.72
	5:1	0.00	0.00	0.93	0.00	2.31	1.72	3.84	3.65	5.00	4.58
	10:1	0.00	0.00	1.82	1.32	4.52	4.11	7.56	6.06	10.00	10.19
0.2:1	1:1	0.00	0.00	0.18	0.00	0.44	0.00	0.76	0.00	1.00	0.66
	2:1	0.00	0.00	0.35	0.00	0.90	0.00	1.52	1.26	2.00	1.66
	5:1	0.00	0.00	0.88	0.00	2.22	1.67	3.61	3.52	5.00	4.48
	10:1	0.00	0.00	1.76	1.49	4.12	4.11	6.78	6.50	10.00	9.76

Table 5.14 Comparison between estimated and specified values of the adhesion probability in the case of uniform - uniform dispersion

Particle size of A : 0.5 unit and concentration of A : 500 particles/area.

Particle size ratio (B:A)	Concentration ratio (B:A)	Specified value of the adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.00	17.20	45.40	78.20	100.00
	2:1	0.00	16.50	46.52	76.60	100.00
	5:1	0.00	17.60	47.80	78.00	100.00
	10:1	0.00	18.60	47.40	77.80	100.00
0.04:1	1:1	0.00	16.60	44.40	78.20	100.00
	2:1	0.00	16.62	45.34	76.12	100.00
	5:1	0.00	18.40	46.40	77.60	100.00
	10:1	0.00	18.00	47.60	77.00	100.00
0.1:1	1:1	0.00	17.60	44.20	76.40	100.00
	2:1	0.00	16.44	45.34	76.72	100.00
	5:1	0.00	18.00	46.40	75.80	100.00
	10:1	0.00	18.20	44.40	74.40	100.00
0.2:1	1:1	0.00	16.80	38.40	75.40	100.00
	2:1	0.00	16.96	44.44	74.70	100.00
	5:1	0.00	18.40	44.40	73.60	100.00
	10:1	0.00	17.20	40.60	67.80	100.00

Table 5.15 Comparison between estimated and specified values of the adhesion probability in the case of uniform - normal dispersion.
Particle size of A : 0.5 unit and concentration of A : 500 particles/area.

Particle size ratio (B:A)	Concentration ratio (B:A)	Specified value of the adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.00	18.56	47.80	78.24	100.00
	2:1	0.00	18.06	45.92	76.78	100.00
	5:1	0.00	18.43	46.51	75.87	100.00
	10:1	0.00	18.52	44.79	74.12	100.00
0.04:1	1:1	0.00	17.32	45.84	78.00	100.00
	2:1	0.00	17.24	48.46	77.60	100.00
	5:1	0.00	18.38	47.66	77.78	100.00
	10:1	0.00	19.29	47.44	77.95	100.00
0.1:1	1:1	0.00	16.88	46.96	77.72	100.00
	2:1	0.00	17.28	47.34	77.84	100.00
	5:1	0.00	18.94	48.58	77.74	100.00
	10:1	0.00	19.14	48.25	78.79	100.00
0.2:1	1:1	0.00	18.12	46.36	78.88	100.00
	2:1	0.00	17.88	46.64	76.22	100.00
	5:1	0.00	17.62	45.11	74.50	100.00
	10:1	0.00	16.90	41.76	68.45	100.00

Table 5.16 Comparison between estimated and specified values of the adhesion probability in the case of normal - uniform dispersion.
Particle size of A : 0.5 unit and concentration of A : 500 particles/area.

Particle size ratio (B:A)	Concentration ratio (B:A)	Specified value of the adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.00	18.56	47.80	78.24	100.00
	2:1	0.00	18.06	45.92	76.78	100.00
	5:1	0.00	18.43	46.51	75.87	100.00
	10:1	0.00	18.52	44.79	74.12	100.00
0.04:1	1:1	0.00	17.32	45.84	78.00	100.00
	2:1	0.00	17.24	48.46	77.60	100.00
	5:1	0.00	18.38	47.66	77.78	100.00
	10:1	0.00	19.29	47.44	77.95	100.00
0.1:1	1:1	0.00	16.88	46.96	77.72	100.00
	2:1	0.00	17.28	47.34	77.84	100.00
	5:1	0.00	18.94	48.58	77.74	100.00
	10:1	0.00	19.14	48.25	78.79	100.00
0.2:1	1:1	0.00	18.12	46.36	78.88	100.00
	2:1	0.00	17.88	46.64	76.22	100.00
	5:1	0.00	17.62	45.11	74.50	100.00
	10:1	0.00	16.90	41.76	68.45	100.00

Table 5.17 Comparison between estimated and specified values of the adhesion probability in the case of normal - normal dispersion.
Particle size of A : 0.5 unit and concentration of A : 500 particles/area.

Particle size ratio (B:A)	Concentration ratio (B:A)	Specified value of the adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.00	19.20	45.40	77.60	100.00
	2:1	0.00	17.80	44.20	77.86	100.00
	5:1	0.00	18.20	46.60	77.80	100.00
	10:1	0.00	19.00	47.00	77.40	100.00
0.04:1	1:1	0.00	18.60	46.00	78.60	100.00
	2:1	0.00	17.80	47.60	78.16	100.00
	5:1	0.00	18.20	46.80	77.40	100.00
	10:1	0.00	18.80	48.40	78.00	100.00
0.1:1	1:1	0.00	18.60	48.60	76.80	100.00
	2:1	0.00	19.00	46.60	77.66	100.00
	5:1	0.00	18.60	46.20	76.80	100.00
	10:1	0.00	18.20	45.20	75.60	100.00
0.2:1	1:1	0.00	17.80	44.00	75.60	100.00
	2:1	0.00	17.60	45.20	75.94	100.00
	5:1	0.00	17.60	44.40	72.20	100.00
	10:1	0.00	17.60	41.20	67.80	100.00

coordination number should be exactly as the values predicted from the specified adhesion probability and concentration ratio.

Tables 5.14 to 5.17 summarize the value of the adhesion probability that are estimated from the mean values of the coordination number. Obviously, the cases of intermediate probability show estimated values that are somewhat lower because the adhering B particles are not allowed to overlap.

5.2.2 Effect of concentration ratio

In all simulations the concentration of A particles was kept constant at 500 particles/area, while the concentration ratio, which is defined as the ratio of concentration of B to concentration of A was varied as 1:1, 2:1, 5:1 and 10:1. The effects of the concentration ratio on the degree of mixedness, count-based fractal dimension, area-based fractal dimension and coordination number were investigated to identify suitable indices that quantify the degree of dispersion of the binary additive system.

The results have already been shown and occasionally discussed along with the effect of the adhesion probability in 5.2.1. What follows is more discussion.

5.2.2.1 Degree of mixedness

Here the effect of the concentration ratio on the degree of mixedness of B particles is investigated.

5.2.2.1.1 Uniform - uniform dispersion

From Figures 5.15 to 5.18, it can be seen that the degree of mixedness of B tended to diminish as the B : A concentration ratio was heightened. When the concentration of B particles increased, the average number of B particles adhering onto each A particle increased, resulting in larger clusters. This led to a slight decrease in the degree of mixedness. Even at 0% adhesion, the degree of mixedness also dropped when the concentration ratio was raised. This is consistent with Figure 5.1 which shows that the degree of mixedness depended not only on the adhesion probability and particle size but also on the concentration of B particles.

5.2.2.1.2 Uniform - normal dispersion

Figures 5.19 to 5.22 show that the degree of mixedness of B declined, as the B : A concentration ratio increased. The reason was mentioned in 5.2.2.1.1. Furthermore, the degree of mixedness at 100 % adhesion dropped more swiftly than that at 80% adhesion. The reason was also given in 5.2.1.1.2.

5.2.2.1.3 Normal - uniform dispersion

For the same reason as that mentioned in 5.2.2.1.1, the degree of mixedness of B also fell off, as the concentration ratio grew higher. Because of the normal dispersion of A particles, the degree of mixedness dwindled more rapidly than case 5.2.2.1.1, in which A particles were uniformly dispersed. These results were depicted in Figures 5.23 to 5.26.

5.2.2.1.4 Normal - normal dispersion

From Figures 5.27 to 5.30, it can be seen that the degree of mixedness of B dropped fast, as the concentration ratio increased. This may be attributed to the size increase of the normally dispersed clusters and to the fact that both A and B particles were of normal dispersion.

5.2.2.2 Count-based fractal dimension

In this section, the count-based fractal dimension is used to quantify the degree of dispersion of the binary additive system. The effects of concentration ratio on the normalized count-based fractal dimension of B particles only and of A plus B particles are investigated.

5.2.2.2.1 Uniform - uniform dispersion

As seen from Figures 5.31 to 5.34, the rise in the B : A concentration ratio resulted in an increase in the normalized count-based fractal dimension of B particles except at 0% adhesion. At 0% adhesion, all B particles were uniformly dispersed in the matrix. So they behaved like the single additive system and the normalized count-based fractal dimension of B remained essentially constant around 1.0. At a higher adhesion probability, the clustering of B particles around A particles seemed like localized or microscale normal dispersion. This tendency was consistent with the result shown in Figure 5.4.

Figures 5.35 to 5.38 show that the normalized count-based fractal dimension of A plus B particles decrease swiftly when the B : A concentration ratio increased from 1:1 to 5:1. At the ratio 1:1, there were 500 A particles/area and 500 B particles/area, but the observed count-based fractal dimension was normalized by that of the ideal single-component uniform dispersion at 500 particles/area (concentration of B). So the value of the normalized count-based fractal dimension was greater than 1.0 at each adhesion probability. Similarly, at concentration ratios 2:1 and 5:1 ,there were 500 A particles/area together with 1000 and 2500 B particles/area, respectively but they were normalized by the corresponding ideal value at 1000 and 2500 particles/area. So the normalized count-based fractal dimension of A plus B particles at 2:1 and 5:1 dropped rapidly. At the ratio 10:1, there were 500 A particles/area and

5000 B particles/area and the fractal dimension was normalized by the corresponding value at 5000 particles/area, so the normalized value changed only slightly.

5.2.2.2.2 Uniform - normal dispersion

Figures 5.39 to 5.42 reveal that the normalized count-based fractal dimension of B increased, as the concentration ratio increased. At 0% and 20% adhesion, the normalized count-based fractal dimension increased rapidly with the concentration ratio. This may be explained by the fact that the normalized count-based fractal dimension of the ideal single-component normal dispersion at high concentrations tended to increase with concentration. At 50%, 80% and 100%, a large number of B particles were forced to adhere onto the A particles that followed uniform dispersion. So the normalized count-based fractal dimension of B particles at 50%, 80%, and 100% increased only slightly with the concentration ratio.

Figures 5.43 to 5.46 show the effect of the concentration ratio on the normalized count-based fractal dimension of A plus B particles. The normalized count-based fractal dimension dropped rapidly at first. After that, it dropped slowly as the concentration ratio further increased. The reason was given in 5.2.2.2.1.

5.2.2.2.3 Normal - uniform dispersion

Figures 5.47 to 5.50 show that the rise in the concentration ratio caused an increase in the normalized count-based fractal dimension of B particles, except at 0% and 100% adhesion. This is because of the uniform dispersion of B particles in the matrix. And at 100% adhesion, all B particles were forced to adhere onto A particles which followed the normal dispersion, so the normalized count-based fractal dimension decreased slightly. At 20% adhesion, the normalized count-based fractal dimension increased slightly, as the concentration ratio increased. This is because a large number of B particles remained uniformly dispersed in the matrix. At 80% adhesion, a rise in the concentration ratio resulted in a fast increase in the normalized count-based fractal dimension. This is because only a small percentage of B particles remained uniformly dispersed. The effect of concentration on the nonideal single-component dispersion can then used to explain the above behavior.

Figures 5.51 to 5.54 show the effect of the concentration ratio on the normalized count-based fractal dimension of A plus B particles. It can be seen that at an intermediate adhesion probability the normalized count-based fractal dimension initially decreased and then increased as the concentration ratio further increased.

5.2.2.2.4 Normal - normal dispersion

From Figures 5.55 to 5.58, it can be seen that the normalized count-based fractal dimension of B particles grew greater as the concentration ratio rose. At 0% up to 80% adhesion, the normalized count-based fractal dimension increased speedily with the concentration ratio. At 100% adhesion, every B particle was obliged to adhere onto some A particles, so the normalized count-based fractal dimension rose slightly, as the concentration ratio increased.

As shown in Figures 5.59 to 5.62, the normalized count-based fractal dimension of A plus B particles initially declined and then rose, as the concentration ratio further increased.

5.2.2.3 Area-based fractal dimension

In this work, the area-based fractal dimension was used to quantify the state of dispersion as the B : A concentration ratio increased from 1:1 to 10:1. From Figure 5.3, it can be seen that the increased concentration of particles that follow the ideal normal dispersion caused a decrease in the area-based fractal dimension. Relationship between the area-based fractal dimension and the concentration ratio is discussed as follows.

5.2.2.3.1 Uniform - uniform dispersion

In the case of 0% adhesion probability, the normalized area-based fractal dimension of B remained essentially constant around 1.0, regardless of the concentration ratio because all B particles were uniformly dispersed in the matrix. At higher adhesion probability, the absolute number of B particles which were forced to adhere onto the A particles grew larger when the concentration ratio increased. This is the cause of the reduction of the normalized area-based fractal dimension. The relations were shown in Figures 5.63 to 5.66.

Similarly, Figures 5.67 to 5.70 show the effect of the concentration ratio on the normalized area-based fractal dimension of A plus B particles. The normalized area-based fractal dimension of A plus B also declined slowly for the same reason given above.

5.2.2.3.2 Uniform - normal dispersion

From Figures 5.71 to 5.74, it can be seen that the normalized area-based fractal dimension of B dropped rapidly as the concentration ratio increased with the adhesion probability being 0%, 20% and 50%. In contrast, the normalized area-based fractal dimension decreased slowly at 80% and 100% adhesion as the concentration ratio rose. This is because most B particles adhered onto the A particles which follow the uniform dispersion.

Figures 5.75 to 5.78 show the relationship between the concentration ratio and the normalized area-based fractal dimension of A plus B particles. It is difficult to discern the effect of the concentration ratio on the normalized area-based fractal dimension except at high concentrations and for large particle size of B.

5.2.2.3.3 Normal - uniform dispersion

The effects of the B : A concentration ratio on the normalized area-based fractal dimension of B particles were shown in Figures 5.79 to 5.82. At 0% adhesion, all B particles were uniformly dispersed in the matrix; thus the normalized area-based fractal dimension did not vary with a rise in the concentration ratio. When the adhesion probability was greater than 0%, the normalized area-based fractal dimension dropped rapidly, as the concentration ratio increased.

As regards the effect of the concentration ratio on the normalized area-based fractal dimension of A plus B particles, Figures 5.83 to 5.86 show little effect of the concentration ratio. It is because an A particle occupied a much greater area than a B particle. So the result was dominated by A particles that followed the normal dispersion.

5.2.2.3.4 Normal - normal dispersion

From Figures 5.87 to 5.90, it can be seen that the normalized area-based fractal dimension of B dropped rapidly as the concentration ratio increased because both A and B particles followed the normal dispersion.

Figures 5.91 to 5.94 show the effect of the concentration ratio on the normalized area-based fractal dimension of A plus B particles. At low concentrations and for small particle size of B, this effect was difficult to discern. This is because an A particle occupies a much larger area than a relatively small B particle.

5.2.2.4 Coordination number

From Tables 5.10 to 5.13 , it can also be seen that both the mean and mode of the coordination number increased as the B : A concentration ratio rose. This is because at the same adhesion probability the number of B particles which adhere onto the A particles should rise in proportion to the increase in the concentration of B relative to A.

5.2.3 Effect of particle size ratio

In this part, the particle size ratio of A particles remains constant at 0.5 unit, while the particle size of B particles is presented as the B : A particle size ratio. The B : A particle size ratios investigated are 0.02:1, 0.04:1, 0.1:1 and 0.2:1. The effects of the size ratio on the degree of mixedness, count-based fractal dimension, area-based fractal dimension and coordination number (mean and mode) as indicators of the adhesion probability of B particles on A particles are investigated.

5.2.3.1 Degree of mixedness

5.2.3.1.1 Uniform - uniform dispersion

Figure 5.95 shows that the degree of mixedness of B dwindled when the B : A particle size ratio increased. Especially, at a high B : A concentration ratio and/or high adhesion probability, the degree of mixedness dropped swiftly. At a small particle size ratio or low B : A concentration ratio, however, it is unsuitable to use the degree of mixedness of B to differentiate the adhesion probability.

5.2.3.1.2 Uniform - normal dispersion

From Figure 5.96, it can be seen that the degree of mixedness of B declined when the particle size ratio was increased from 0.02:1 to 0.20:1. At a high B : A concentration ratio, the degree of mixedness tended to decrease rapidly. This may be because the dispersion of B particles was normal dispersion. However, at a small B : A particle size ratio and/or low B : A concentration ratio, it is again unsuitable to use the degree of mixedness of B to differentiate the adhesion probability.

5.2.3.1.3 Normal - uniform dispersion

Figure 5.97 reveals that a decrease in the degree of mixedness of B was caused by an increase in the B : A particle size ratio. At the 100% adhesion probability and a high B : A concentration ratio, the degree of mixedness tended to declined remarkably. This is because the A particles was of normal dispersion and all B particles were forced to adhere onto A particles at 100% adhesion probability.

5.2.3.1.4 Normal - normal dispersion

Figure 5.98 shows that the degree of mixedness of B dwindled when the B : A particle size ratio increased. Furthermore, at a low B : A concentration ratio, it is hard to discern its effect on the degree of mixedness, even though the adhesion probability and the B : A particle size ratio were high. At a high concentration ratio, the degree of mixedness of B decreased rapidly, as the particle size ratio was increased. This may be because both A and B particles were of normally dispersed.

From Figures 5.95 to 5.98, it may be concluded that the degree of mixedness is a poor indicator of the adhesion probability at low B : A concentration ratio and/or small B : A particle size ratio.

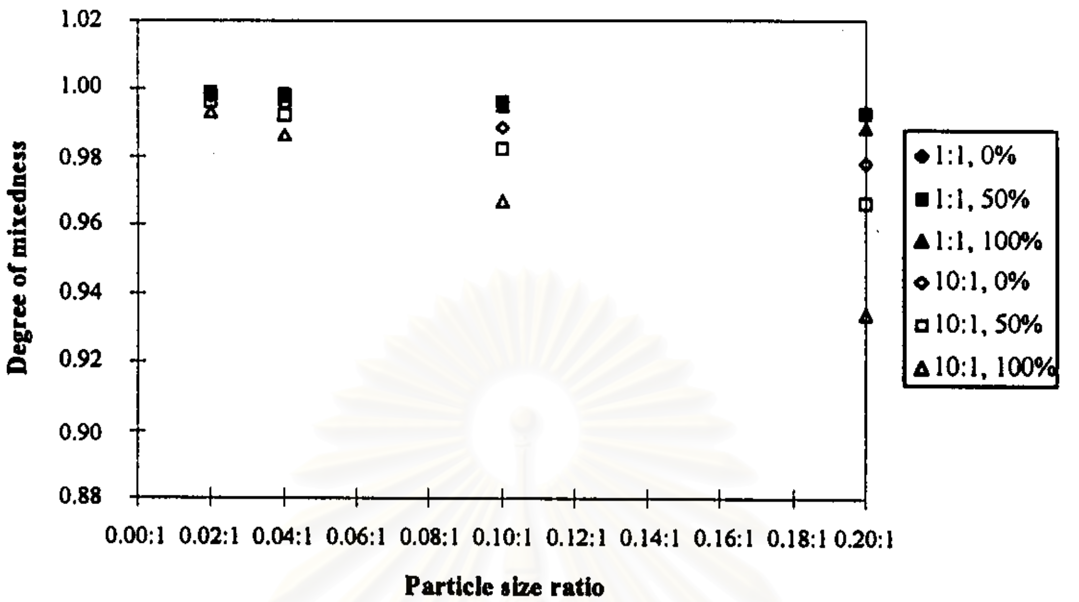

Figure 5.95 Relationship between particle size ratio and degree of mixedness of B particles in the case of uniform - uniform dispersion.

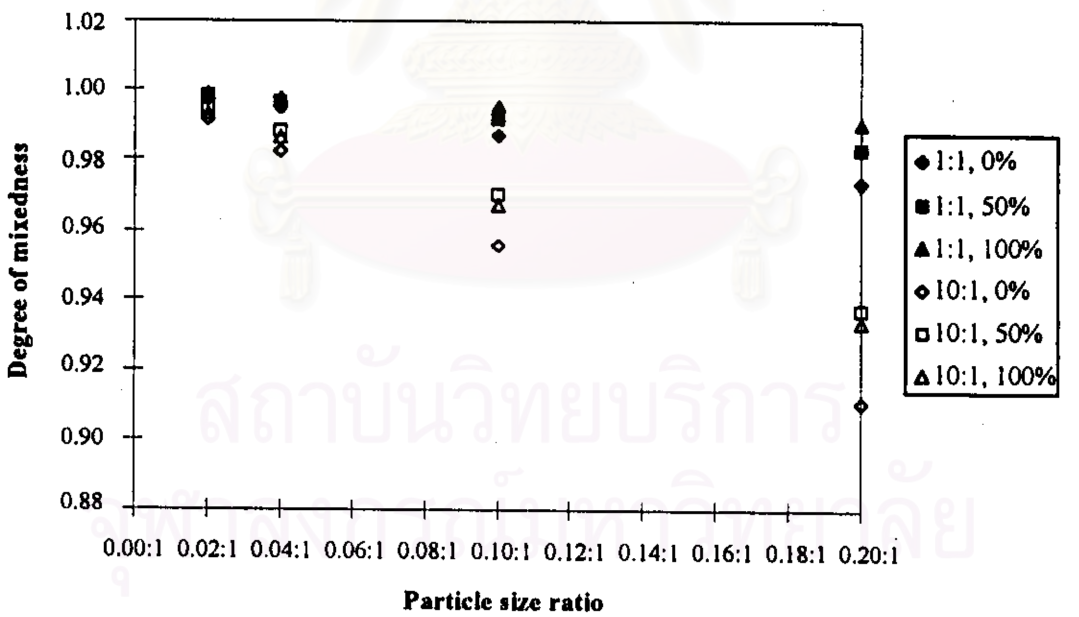

Figure 5.96 Relationship between particle size ratio and degree of mixedness of B particles in the case of uniform - normal dispersion.

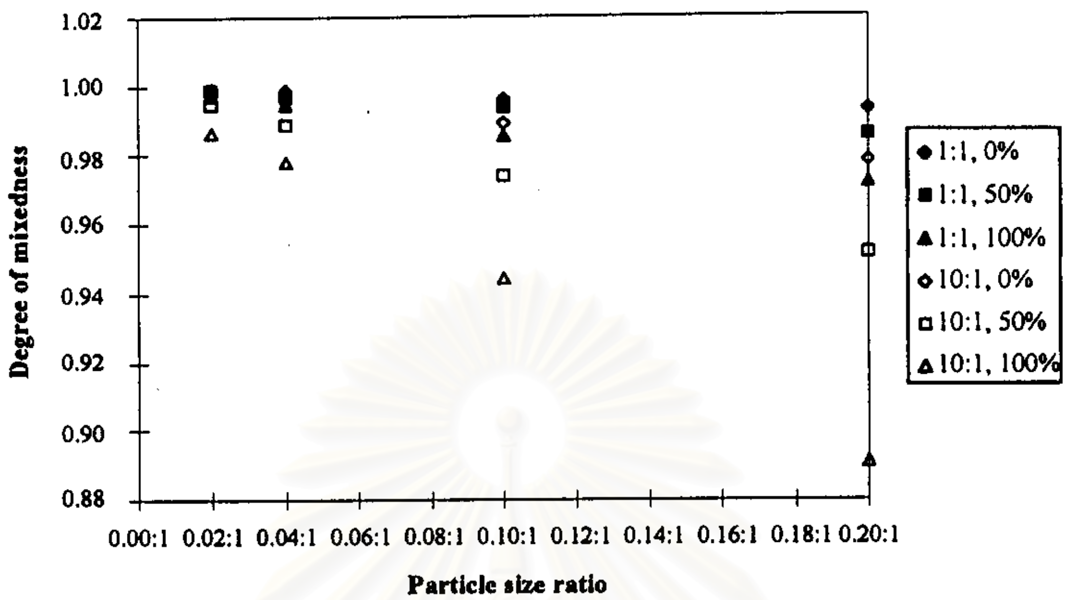

Figure 5.97 Relationship between particle size ratio and degree of mixedness of B particles in the case of normal - uniform dispersion.

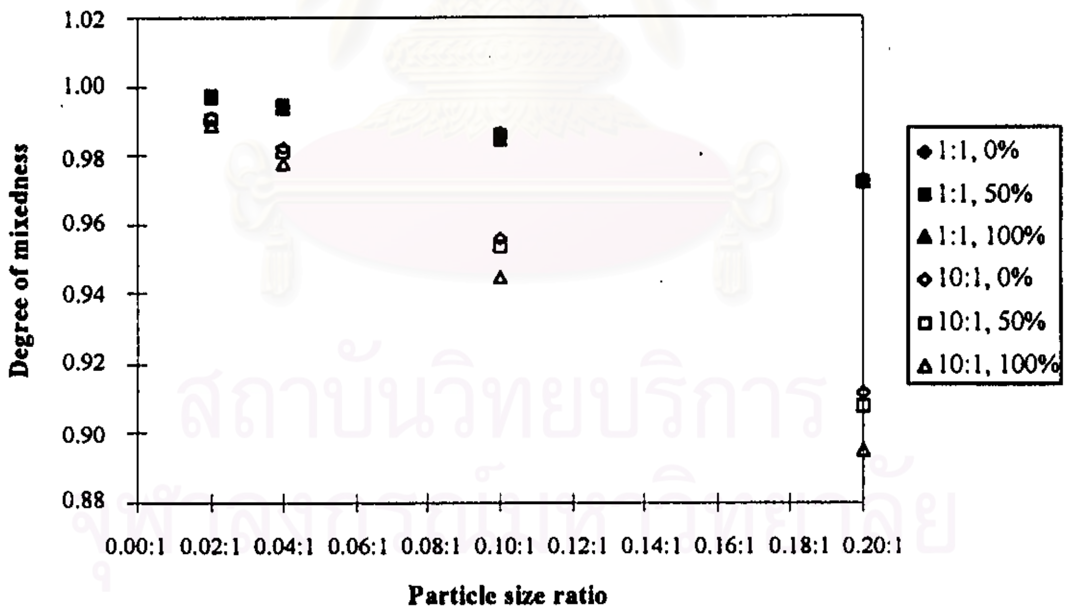

Figure 5.98 Relationship between particle size ratio and degree of mixedness of B particles in the case of normal - normal dispersion.

5.2.3.2 Count-based fractal dimension

The purpose here is to see how the normalized count-based fractal dimension as indicator of the adhesion probability is effected by the B : A particle size ratio only the fractal dimension of B particles will be investigated.

Figures 5.99 to 5.102 show the effect of the particle size ratio on the normalized count-based fractal dimension of B at a combination of the concentration ratio and the adhesion probability.

5.2.3.2.1 Uniform - uniform dispersion

Figure 5.99 shows that the normalized count-based fractal dimension of B increased only slightly as the particle size ratio increased, except for the case of 0% adhesion. At 0% adhesion, the uniform dispersion of B particles in the binary additive systems behaved the same as that in the single additive systems, so the normalized count-based fractal dimension did not depend on the B : A particle size ratio nor the B : A concentration ratio and remained constant around 1.0. At 50% adhesion the concentration ratio had less effect on the fractal dimension than at 100% adhesion. However, at the same concentration ratio, there was a significant difference between 50% and 100% adhesion, regardless of the particle size ratio.

5.2.3.2.2 Uniform - normal dispersion

Figure 5.100 reveals a slight rise in the normalized count-based fractal dimension, as the B : A particle size ratio increased from 0.02:1 to 0.20:1, except for the case of 0% adhesion. At 0% adhesion, the dispersion of B particles was normal dispersion, so the normalized count-based fractal dimension of B particles remained constant around 0.83 and 0.89, when the B : A concentration ratio were 1:1 and 10:1, respectively. At the same concentration ratio, there was again a significant differece between 50% and 100% adhesion regardless of the particle size ratio.

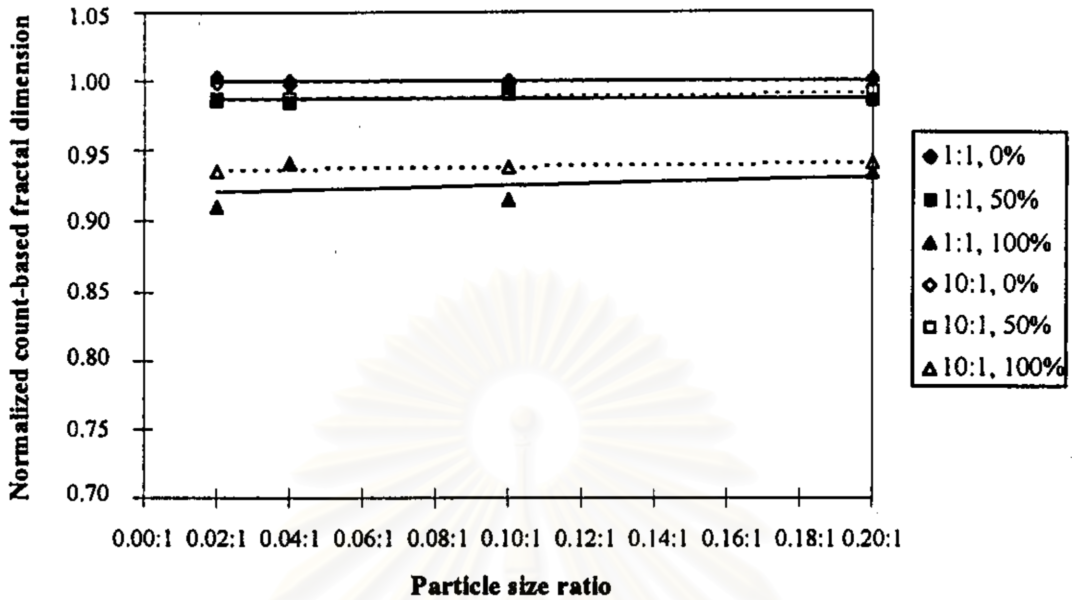

Figure 5.99 Relationship between particle size ratio and normalized count-based fractal dimension of B particles in the case of uniform - uniform dispersion.

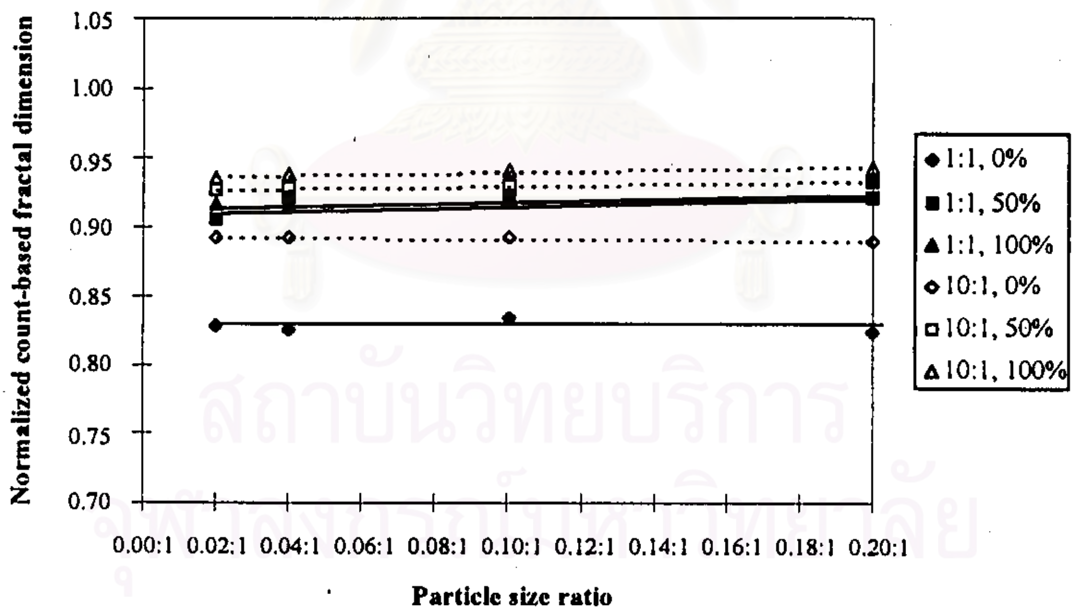

Figure 5.100 Relationship between particle size ratio and normalized count-based fractal dimension of B particles in the case of uniform - normal dispersion.

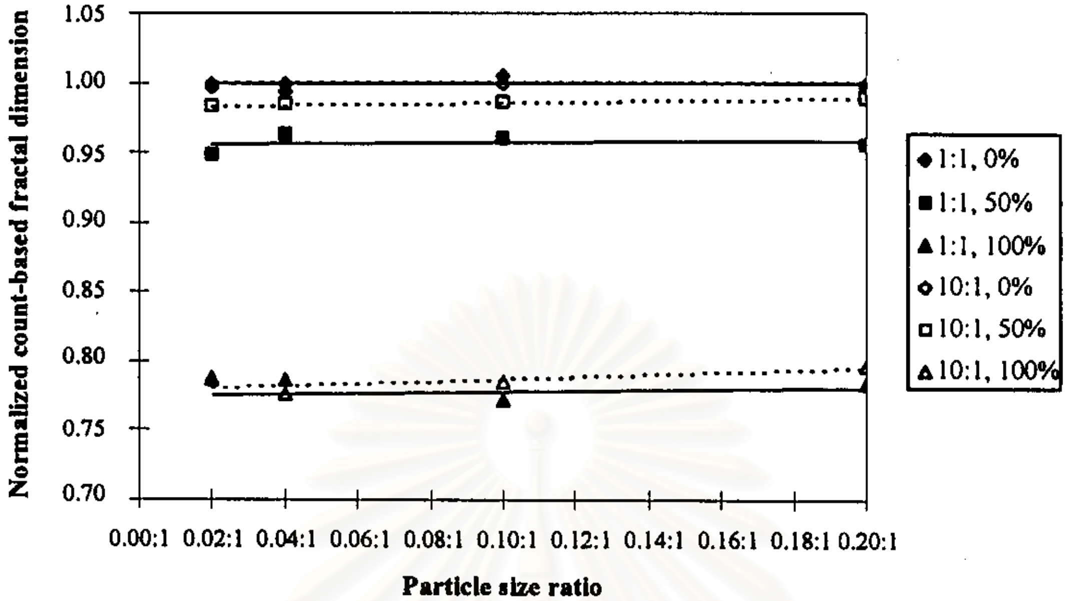

Figure 5.101 Relationship between particle size ratio and normalized count-based fractal dimension of B particles in the case of normal - uniform dispersion.

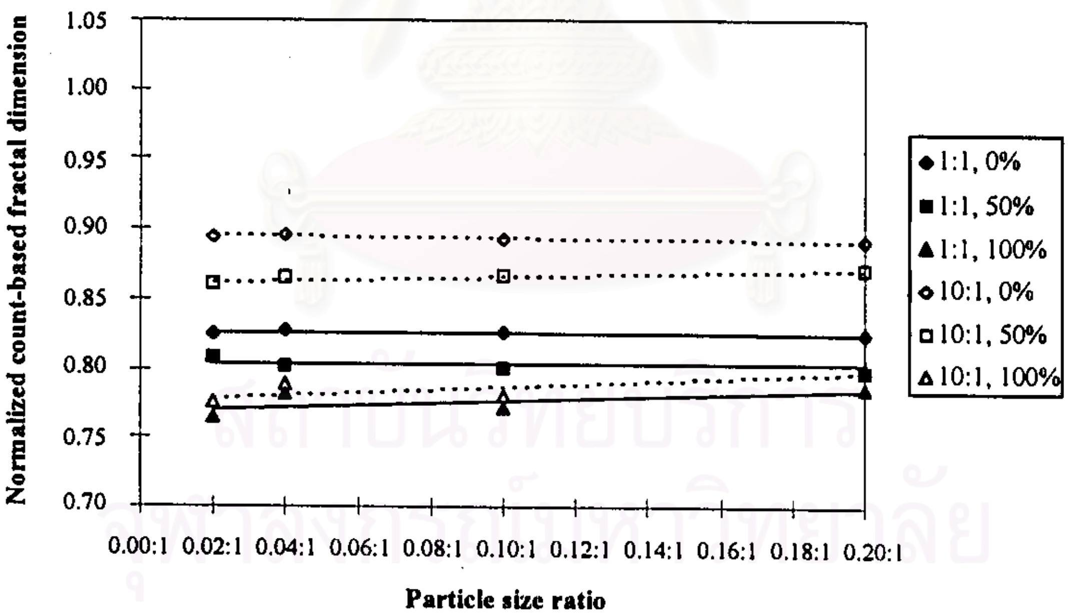

Figure 5.102 Relationship between particle size ratio and normalized count-based fractal dimension of B particles in the case of normal - normal dispersion.

5.2.3.2.3 Normal - uniform dispersion

From Figure 5.101, it can be seen that the increase in the normalized count-based fractal dimension of B particles increased slightly as the particle size ratio increased, except for the case of 0% adhesion. Because the dispersion of B particles was uniform dispersion, so the normalized count-based fractal dimension of B remained constant around unity regardless of the B : A particle size ratio and the B : A concentration ratio. At the same concentration ratio, there was again a significant difference between 50% and 100% adhesion regardless of the particle size ratio.

5.2.3.2.4 Normal - normal dispersion

Figure 5.102 reveals that the normalized count-based fractal dimension of B particles increased slightly, as the particle size ratio increased from 0.02:1 to 0.20:1, except for the case of 0% adhesion. At 0% adhesion, the normalized count-based fractal dimensions of B particles which followed the normal dispersion were 0.83 and 0.89 respectively, regardless of the particle size ratio. At the same concentration ratio, there was again a significant difference between 50% and 100% adhesion.

It may be concluded that the normalized count-based fractal dimension of B is a fairly good indicator of the adhesion probability.

5.2.3.3 Area-based fractal dimension

In this part, the particle size of A particles remains constant at 0.5 unit, while the B : A particle size ratio were 0.02:1, 0.04:1, 0.10:1 and 0.20:1. Relationship between the particle size ratio and the normalized area-based fractal dimension of B particles is depicted and discussed here. This is because each A particles have a much greater area than B particles, so the A particles dominates the effect shown by B particles.

5.2.3.3.1 Uniform - uniform dispersion

Figure 5.103 shows that the normalized area-based fractal dimension of B particles remained constant around 1.0 regardless of the particle size ratio and the concentration ratio when the adhesion probability was 0%. This is because the free dispersion of B particles was uniform dispersion and it behaved like the uniform dispersion of the single additive systems. At 50% and 100% adhesion, the normalized area-based fractal dimension decreased only slightly as the particle size ratio increased. This is because adhesion of B particles onto A particles appeared as conglomerates. When the relative particle size of B particles was larger, the conglomerative effect became more pronounced.

5.2.3.3.2 Uniform - normal dispersion

Figure 5.104 reveals that the B : A particle size ratio had little effect on the normalized area-based fractal dimension of B at 0% adhesion. At 0% adhesion, the normalized area-based fractal dimension of B particles which followed the normal dispersion remained constant around 0.58 and 0.12, when the concentration ratio of B particles were 1:1 and 10:1, respectively. At the same B : A concentration ratio, the normalized area-based fractal dimension can differentiate clearly between 0%, 50% and 100% adhesion probability, regardless of the B : A particle size ratio.

5.2.3.3.3 Normal - uniform dispersion

The normalized area-based fractal dimension did not depend on the B : A particle size ratio at 0% adhesion, and its value remained essentially constant around 1.0. When the adhesion probability was 50% or 100%, the normalized area-based fractal dimension decreased slightly as the particle size ratio increased. At the same concentration ratio, the normalized area-based fractal dimension could differentiate clearly between 0%, 50% and 100% adhesion probability.

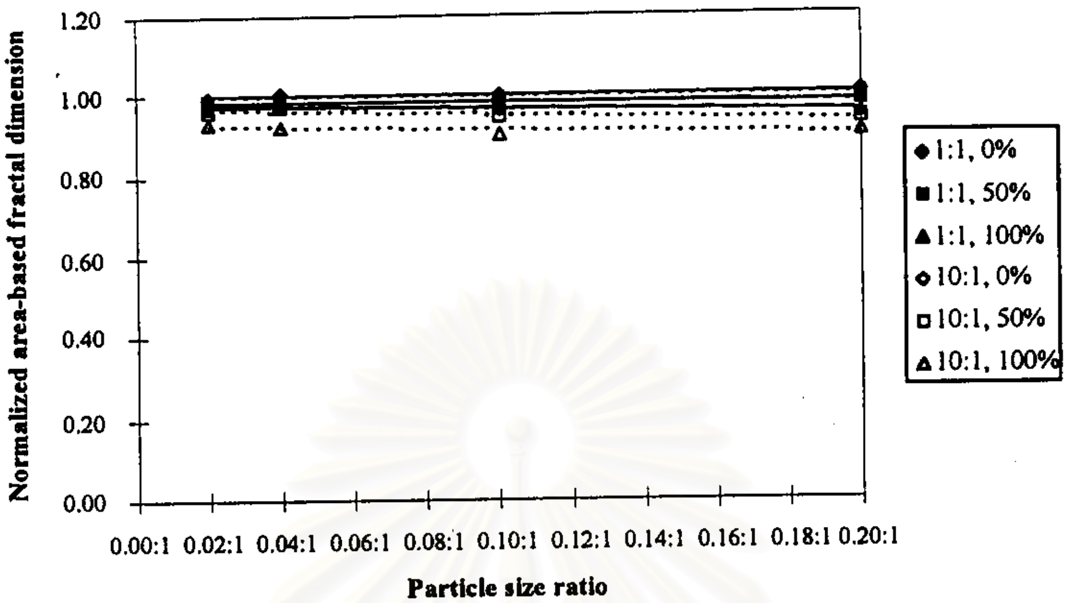

Figure 5.103 Relationship between particle size ratio and normalized area-based fractal dimension of B particles in the case of uniform - uniform dispersion.

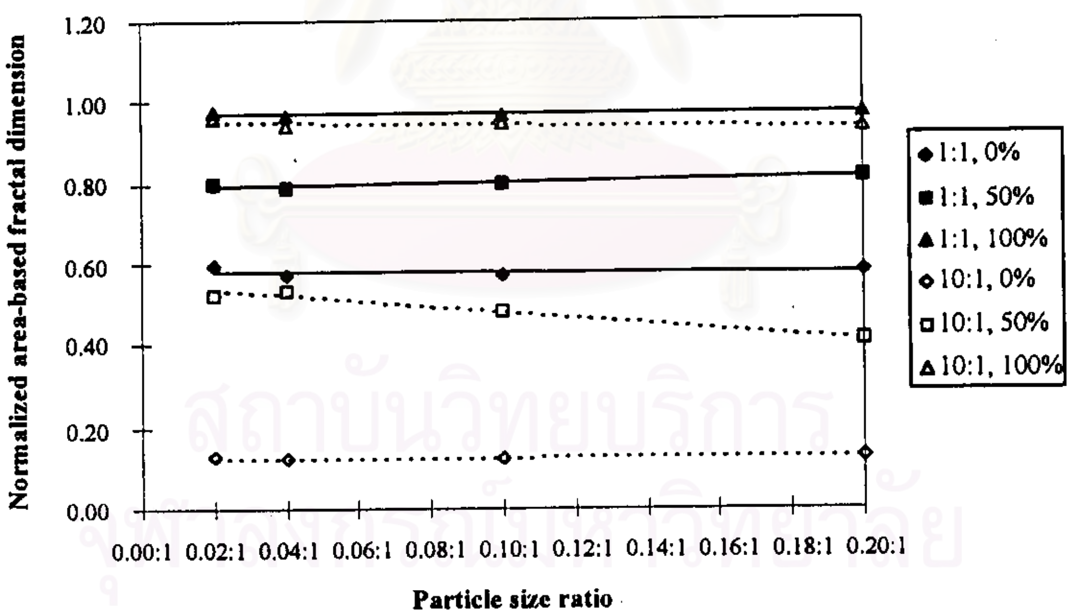

Figure 5.104 Relationship between particle size ratio and normalized area-based fractal dimension of B particles in the case of uniform - normal dispersion.

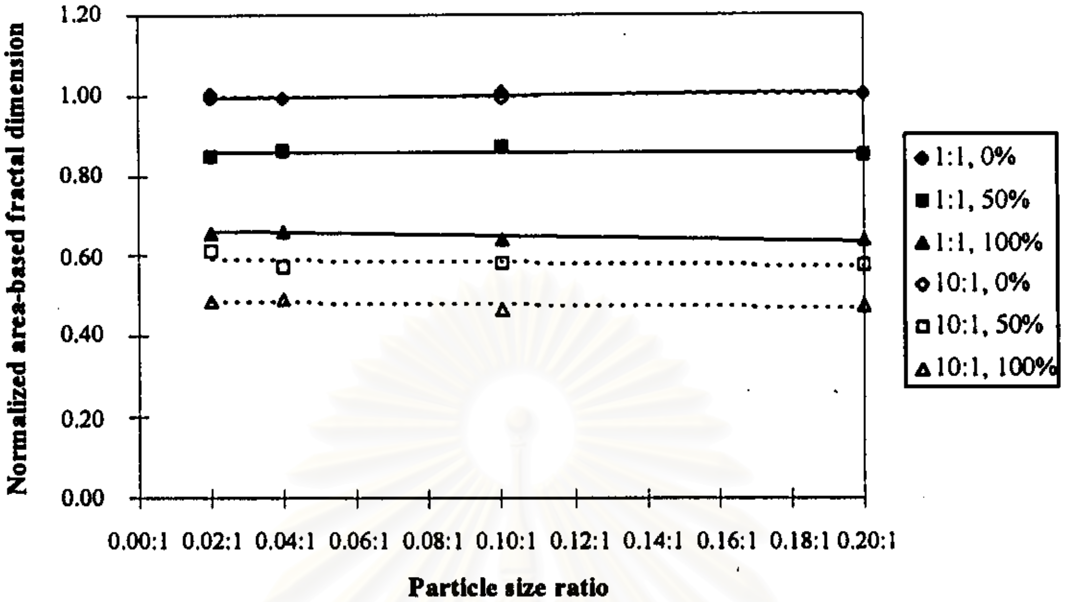

Figure 5.105 Relationship between particle size ratio and normalized area-based fractal dimension of B particles in the case of normal - uniform dispersion.

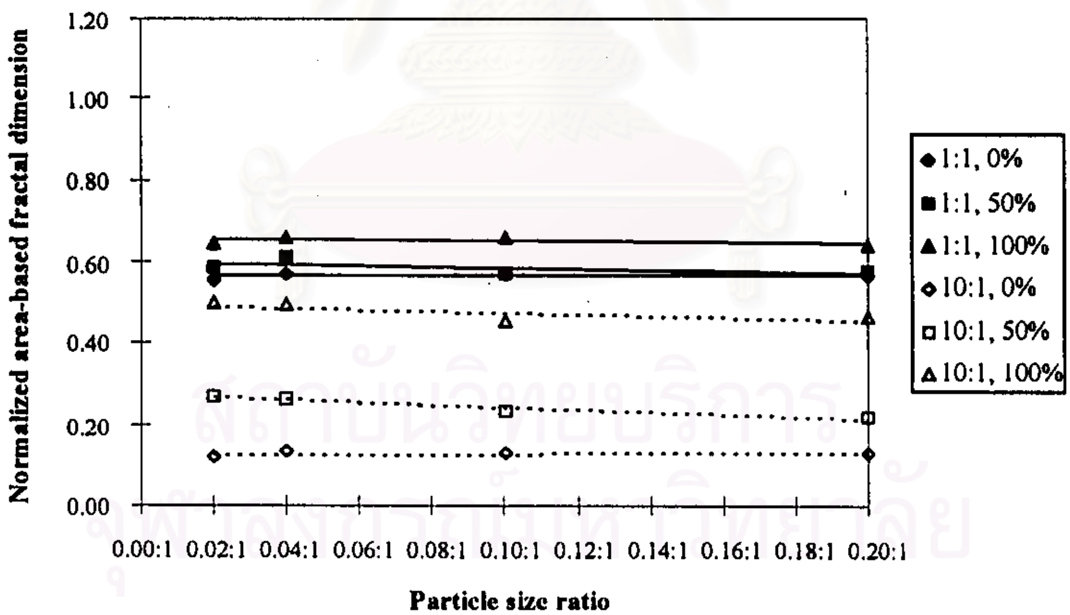

Figure 5.106 Relationship between particle size ratio and normalized area-based fractal dimension of B particles in the case of normal - normal dispersion.

5.2.3.3.4 Normal - normal dispersion

From Figure 5.106, it can be seen that the normalized area-based fractal dimension of B particles at 0% adhesion remained constant around 0.58 and 0.12, regardless of the particle size ratio. At 50% and 100% adhesion, the normalized area-based fractal dimension decreased only slightly as the B : A particle size ratio was changed from 0.02:1 to 0.20:1.

From Figures 5.103 to 5.106, it may be concluded that the normalized area-based fractal dimension of B particles at 0% adhesion do not depend on the B : A particle size ratio and remained essentially constant around 1.0 when the dispersion of B particles is uniform dispersion. When the dispersion of B particles is normal dispersion, the normalized area-based fractal dimension at 0% adhesion depends on the B : A concentration ratio. When the adhesion probability greater than 0% adhesion, the concentration ratio has more effected on the normalized area-based fractal dimension than the particle size ratio. At the same B : A concentration ratio, the normalized area-based fractal dimension can clearly differentiate the different adhesion probability.

5.2.3.4 Coordination number

As expected, Tables 5.10 to 5.13 reveal that the particle size ratio should have no effect on the coordination number. This is true when the concentration ratio were 1:1, 2:1 and 5:1. At the highest concentration ratio of 10:1, the mean of the coordination number declined slightly as the the particle size ratio increased. This is because the number of overlapping B particles that were discarded became higher as the particle size ratio increased. However, the mode of the coordination number was not affected by the particle size ratio.

From Tables 5.10 to 5.13, it may be concluded that the coordination number is very useful to identify the average number of B particles adhering onto one of the A particles, but it reveals nothing about the types of dispersion of B and A particles.

5.3 Application of the present work to the interpretation of published results

Naorat P.(1996) has found that kneading temperature is one of the factors that affect the dispersion state of a pigment in a polymer, namely, a higher temperature (from 170 to 210 °C) led to improved dispersibility.

In this work, the normalized count-based fractal dimension obtained from experimental results (Naorat P. 1996) is compared with the normalized count-based fractal dimension obtained from the present computer-simulated results. The experimental values of the normalized count-based fractal dimension are listed in Table 5.18 for the case of carbon black and iron oxide pigment in polystyrene.

Table 5.18 The experimental normalized count-based fractal dimension in the case of carbon black and iron oxide.

Pigment	Kneading temperature (°C)	Speed of screw (rpm)	Feed rate (g/min)	Number of particles counted	Normalized count-based fractal dimension
Carbon black	170	81	4.5	160	0.964
	210	81	4.5	193	0.996
Iron oxide	170	81	4.5	88	0.914
	210	81	4.5	113	0.935

Obviously, the normalized count-based fractal dimension indicates that carbon black kneaded at 210 °C was more uniformly dispersed than at 170 °C. So was iron oxide. This is because the viscosity of the polymer melt became lower at a higher temperature. When carbon black and iron oxide were compared at the same kneading temperatures, the former was more uniformly dispersed than the latter because carbon black is organic, non-polar and more compatible with the polymer matrix.

If the pigment is uniformly randomly dispersed, the normalized fractal dimension should be essentially one. Thus the closer the experimental normalized fractal dimension to unity, the more nearly uniform the dispersion.

Alternatively, the simulated results of the binary component system may be used to interpret the experimental results. Consider a binary system of A and B particles that are identical in all characteristics except their names. The composition of A and B is a % and b %, respectively. The only difference is that A follows an ideal normal random dispersion (N type) while B follows an ideal uniform random dispersion (U type) in the mixture. Figure 5.107 shows the simulated results of the relationship between the normalized count-based fractal dimension and the total particle concentration for this ideal binary component system. Similarly, Figure 5.108 shows the corresponding results between the normalized area-based fractal dimension and the total particle concentration.

The purpose here is to demonstrate how the experimental results may be interpreted. At 170 ^{o}C kneading temperature, the experimental normalized count-based fractal dimension is reported by Naorat P.(1996) to be 0.964. From Figure 5.107, at the same 160 total particle concentration, it is found that a binary mixture of identical A and B particles consisting of 28% A of N type dispersion and 72% B of U type dispersion would have the same fractal dimension of 0.964. In other words, the obtained experimental dispersion is equivalent to one in which 28% of the particles are normally randomly dispersed with the remaining 72% being uniformly randomly dispersed. When the same interpretation is applied to the rest of Table 5.18, the results shown in Table 5.19 are obtained.

Obviously, Figure 5.108 may be used to interpret the normalized area-based fractal dimension obtained experimentally.

Table 5.19 Relationship between normalized count-based fractal dimension obtained from experiment results and N-U ratio (normal dispersion : uniform dispersion).

Pigment	Kneading temperature (oC)	Number of particles	Normalized count-based fractal dimension	N-U ratio (normal : uniform) (% N)
Carbon black	170	160	0.964	28
	210	193	0.996	2
Iron oxide	170	88	0.914	40
	210	113	0.935	35

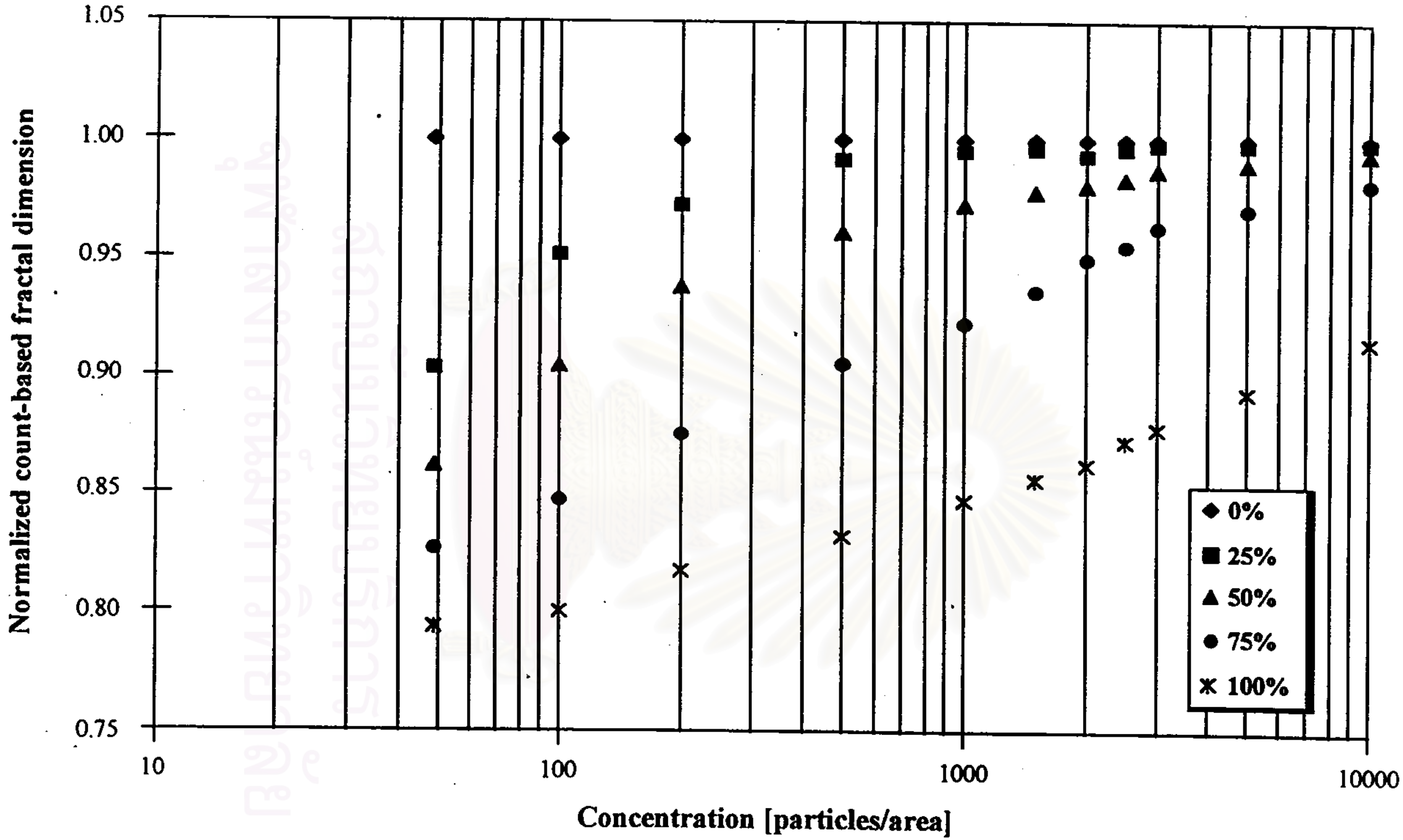

Figure 5.107 Relationship between the total concentration and normalized count-based fractal dimension (D = 0.5 unit) at each N-U ratio.

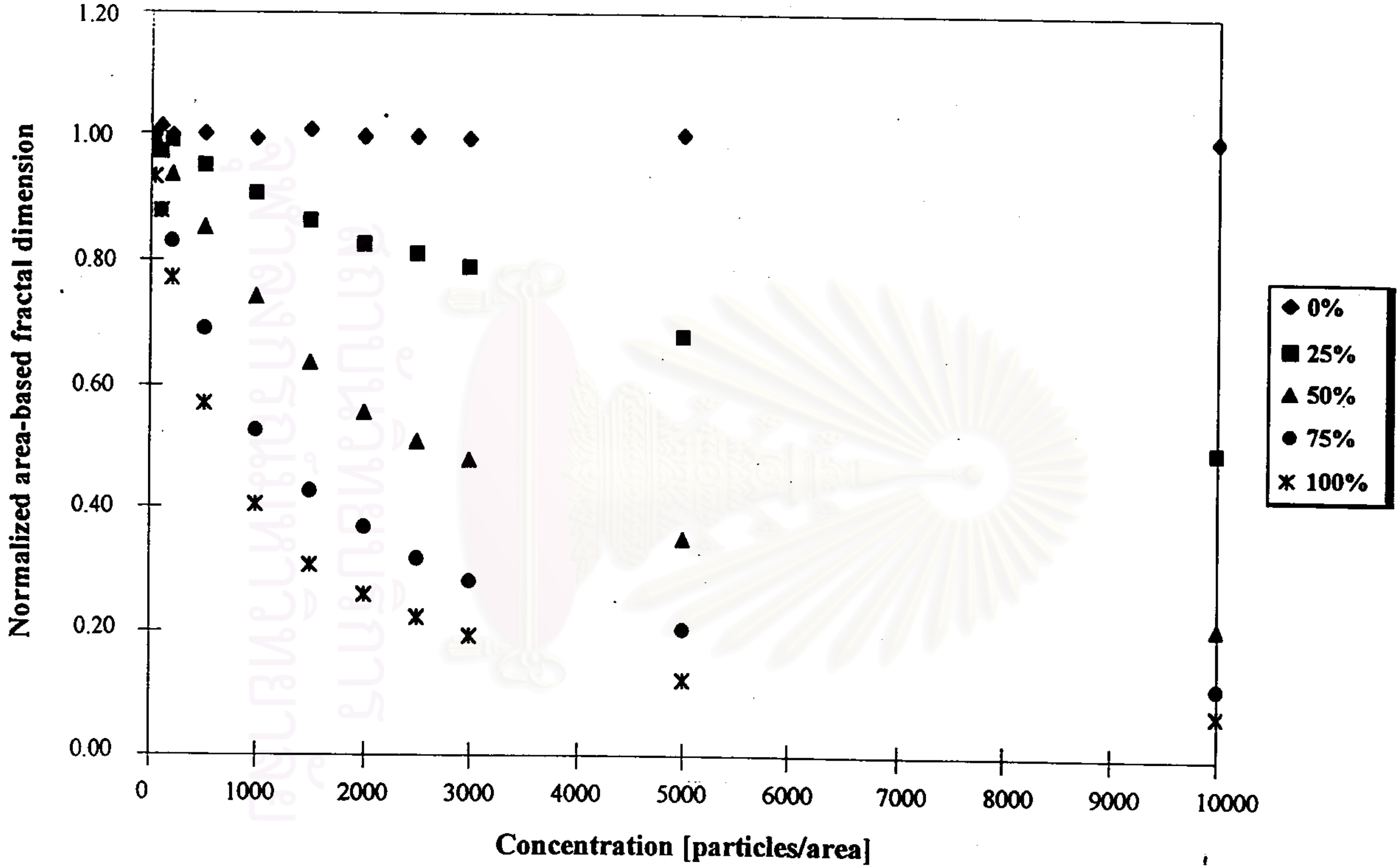

Figure 5.108 Relationship between the total concentration and normalized area-based fractal dimension (D = 0.5 unit) at each N-U ratio.