CHAPTER IV

SIMULATION TECHNIQUE

Simulation is a powerful technique for solving a wide variety of problems. To simulate is to imitate the behavior of a system or phenomenon under study. The basic idea behind dynamic simulation is simple, namely, to model the given system by means of mathematical equations, and then determine its time-dependent behavior. The simplicity of the approach, when combined with the computational power of a high-speed digital computer, makes simulation a powerful tool. Normally, simulation is used when either an exact analytic expression for the behavior of the system under investigation is not available, or the analytic solution is too time-consuming or costly to obtain.

In modeling natural phenomena, two different approaches are available : deterministic and stochastic. Deterministic models are those in which each variable and parameter can be assigned a definite number, or a series of definite number, for any given set of conditions. In contrast, in stochastic or random models, uncertainty is introduced. The variables or parameters used to describe the structure of the elements (and the constraints) may not be precisely known. The former approach are less demanding computationally than the latter and could frequently be solved analytically.

To represent random variables, we require a source of randomness. A random number generator and its appropriate use play the central role of any simulation experiments involving a stochastic system. Methods of generating random numbers are discussed separately in Appendix A.

4.1 Simulation assumptions

In this work, the following assumptions were used :

1) All A and B particles are spherical.

2) Dispersion state is limited to two-dimensional.

3) No overlap of particles is allowed.

4) Core particles which are larger and less numerous, are called " particles A".

5) Adhering particles which are smaller and more numerous, are called " particles B".

In this work, the simulation and analysis of the dispersion state is divided in two separate parts. They are the generation part and the analysis part. The algorithm of each of these two parts is described below.

4.2 The algorithm for the generation of the dispersion state

A simplified flow chart of the simulation algorithm is given in Figure 4.1. The simulation is carried out according to the following steps :

1) Input data, including the concentrations of additive particles A and B, particle sizes of A and B ,and value of adhesion probability (%).

2) Input seeds for random number generation.

3) Generate A particles according to the selected type of dispersion state (either uniform or normal random, based on equations (3.1) and (3.2) or (3.3) and (3.4)).

4) Check and eliminate A particles that overlap themselves, keeping only the desired number of A particles.

5) Input seeds for random number generation.

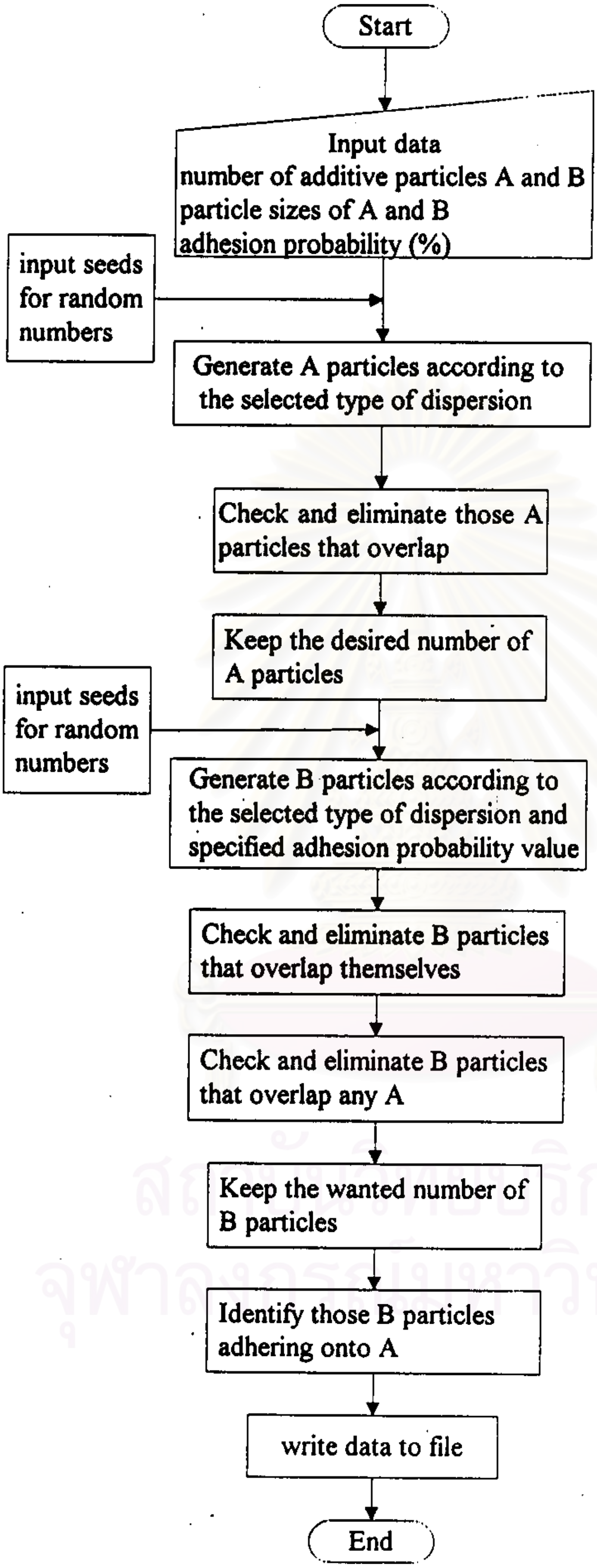

Figure 4.1 Simplified flow chart for the simulation of idealized dispersion states.

6) Generate sequentially B particles so that on the overall a percentage of which are dispersed in the matrix according to the selected type of dispersion state (uniform or normal random, based either on equations (3.1) and (3.2) or (3.3) and (3.4)). The rest of the B particles are uniformly dispersed onto core particles according to the specified adhesion probability [equations (3.5), (3.6) and (3.7)].

7) Check and eliminate B particles that overlap themselves.

8) Check and eliminate B particles that overlap any A particle, keeping only the wanted number of B particles.

9) Identify those B particles adhering onto A.

10) Write data to file.

4.3 The algorithm for the analysis of the dispersion state

A flow chart of the algorithm is shown in Figure 4.2. The analysis algorithm is carried out according to the following steps.

1) Read a previously generated file.

2) Divide the total square area into 50 x 50 subsections.

3) Count the numbers of subsections which are occupied by A particles alone, B particles alone, and A plus B particles.

4) Calculate the coefficients of variation for A alone, B alone, and A plus B particles based on equations (3.15), (3.16), (3.17), and (3.18).

5) Calculate the degree of mixedness of A alone, B alone ,and A plus B particles based on equations (3.8), (3.9), (3.10) and (3.11).

6) Repeat steps 2, 3, 4 and 5 after changing the number of subsections to 40 x 40, 32 x 32, 25 x 25, 20 x 20, 16 x 16, 10 x 10, 8 x 8, 5 x 5 and 4 x 4 ,respectively. Write the data to file.

The data, which are obtained in the analysis program, are next used to determine the fractal dimensions (area-based fractal dimension and count-based fractal dimension), the degree of mixedness, and the mode and mean of the coordination number. Methods for determining these indices are demonstrated in Appendix D.

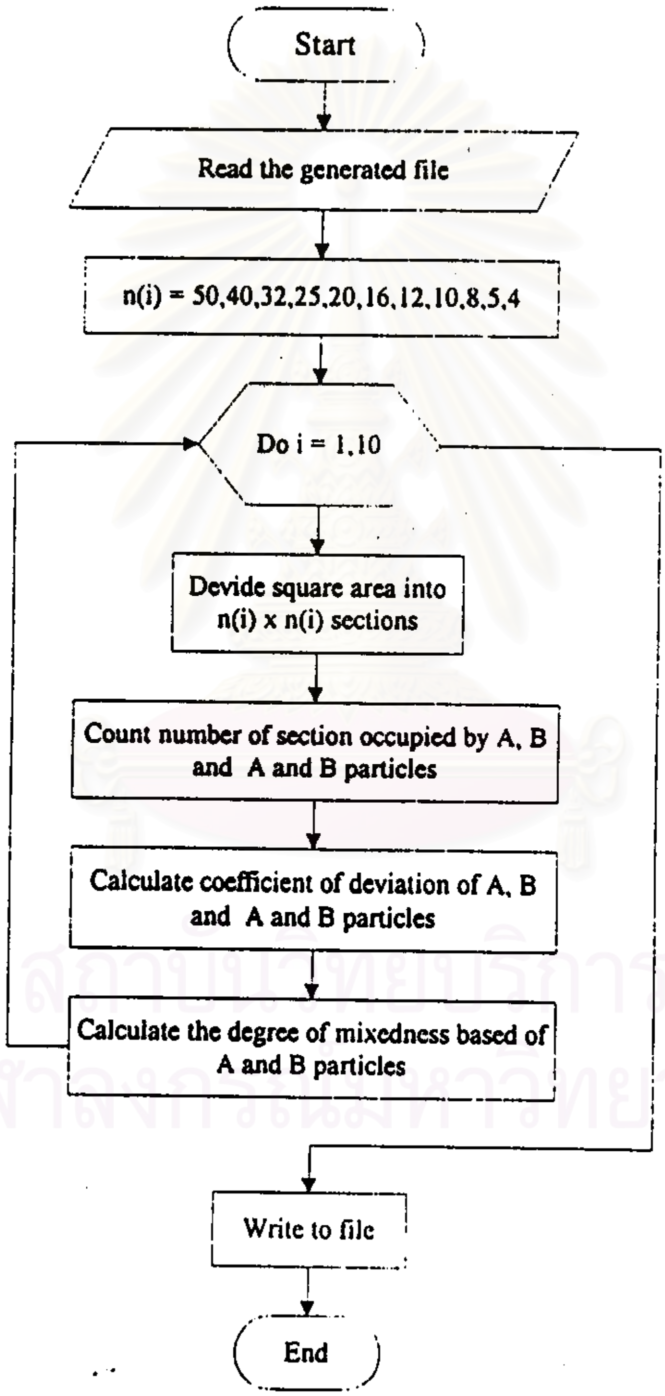

Figure 4.2 Simplified flow chart for the analysis of dispersion state.

4.4 Simulation condition investigated

In this work, the above Monte-Carlo technique was first applied to simulate for evaluation the idealized dispersion state of the single additive system. The simulation conditions of the idealized dispersion state are summarized as follows:

1) Type of dispersion of particle:	Uniform, Normal
2) Particle size :	0.1, 0.2, 0.5
3) Area size :	100 x 100 square
4) Concentration [particles/area] :	50, 100, 200, 500, 1000, 1500, 2000, 2500, 3000, 5000 and 10000

Then the work was extended to binary additive systems. Major factors that could affect the dispersibility of additives in an ordered material were investigated. They were type of random dispersion (uniform, normal) of core particles and of adhering particles, concentration ratio, particle size ratio and adhesion probability of adhering particles. The factors were varied as follows.

1) Type of dispersion of core particles :	Uniform, Normal
2) Particle size of core particles :	0.5
3) Area size :	100 x 100 square
4) Concentration of core particles [particles/area] :	500
5) Type of dispersion of adhering particles :	Uniform, Normal
6) Particle size ratio of adhering particle : core particle :	0.02:1, 0.04:1, 0.10:1, 0.20:1

7) Concentration ratio of

adhering particle : core particle : 1:1, 2:1, 5:1, 10:1

8) Adhesion probability of adhering particles (%) : 0, 20, 50, 80, 100