CHAPTER 5

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 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.

In modelling 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 numbers, 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 B. In some cases, it is necessary to repetitively solve a set of model equations over the same time period or over the same set of conditions, intrinsically a stochastic problem, but with appropriate instantaneous values for the random inputs and/or random parameters, so that data for sample statistics, such as sample means, standard deviations and frequency distributions, of any outputs of interest can be collected and analyzed. This technique of problem solving was given the code name Monte Carlo, because it was based on a gambling-like principle.

The phenomenon of convective diffusional deposition of a polydisperse aerosol on a dust loaded fiber is overwhelming complex. Furthermore, the accumulation of deposited particles with time causes the boundary conditions to alter, and the distribution of incoming particle sizes make the problem extremely tough. Analytical solutions of the above phenomenon are impossible. Therefore we had to resort the Monte Carlo technique in our stochastic simulation.

5.1 Simulation Technique

This investigation is devoted to a stochastic analysis of the convective diffusional deposition of polydispere aerolols on a dust loaded fiber. To simulate the system of yield the required

information for analysis, three kinds of distributions were used to describe stochastic variables. They are

(1) Normal distribution,

(2) Uniform distribution, and

(3) Log-normal distribution.

In many a physical process, the stochastic variables may be decomposed into two components : deterministic plus random noise. Generally, the noise component is either a normal or truncated normal random variable.

The arrival position of an aerosol particle at the surface of Kuwabara's cell is random but evenly distributed; therefore, it can be represented by a uniform random variable. The normal random variable was shown by Chandrasekhar (1943) to depict the Brownian motion of an aerosol particle. On the other hand, the size distribution of the polydisperse aerosol studied here is a log-normal distribution.

Mutually indepedent random numbers that belong to the above three distributions were generated using subroutines investigated by Tanthapanichakoon (1978). Their listings are given in Appendix B.

As described in Section 4.2 the behavior of a fibrous air filter can be simplified and represented by that a single typical fiber. Figure 5.1 is a schematic diagram of the representative fiber surrounded by Kuwabara's cell. The dimensionless radius of the cell, R_c, is related to α by

$$R_c = \frac{1}{\sqrt{\alpha}} \qquad (5.1.1)$$

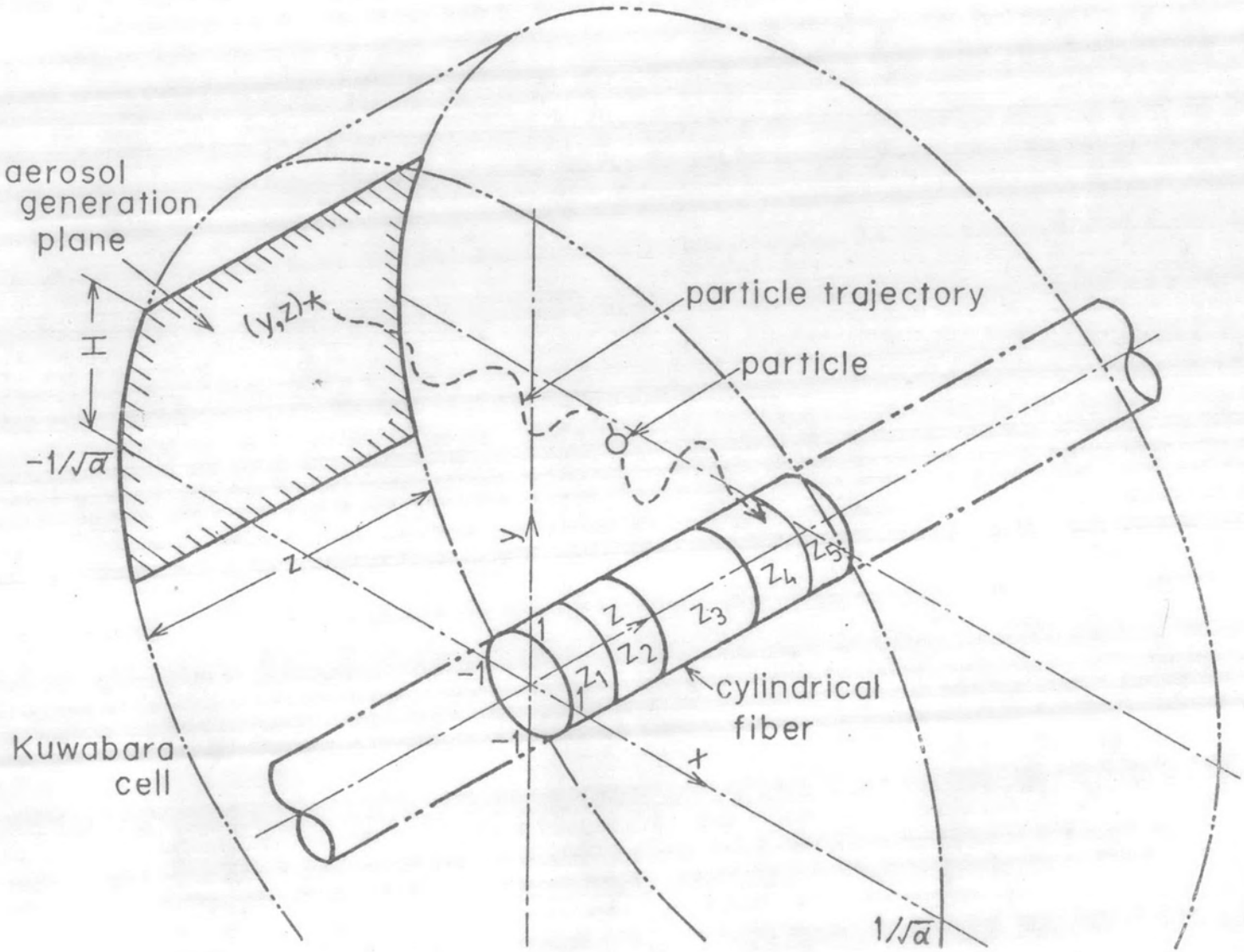

Figure 5.1 Schematic diagram of Kuwabara's cell

Because the total length a fiber is very much longer than one particle diameter, end effects due to the finite length of the fiber should be negligible. To cut down the amount of computer time associated with the usage of a very long fiber, however, a relative short fiber with special provision for minimizing end effects was used. The total length of the fiber is then subdivided into 5 sections, I, II, III, IV, V, with lengths Z_1, Z_2, Z_3, Z_4 and Z_5, respectively (Figure 5.1). However, the effective length of the fiber was actually Z_3; whereas the length of the generation plane Z_{gen}, which overlaps the cell surface was $Z_{gen} = Z_{tot} = Z_1 + Z_2 + Z_3 + Z_4 + Z_5$ with $Z_1 = Z_5$, and $Z_2 = Z_4$. In this way, the deposition of particles and growth of dendrites within the effective length Z_3 was expected to resemble those obtained from using a very long fiber. Naturally, the shorter the fiber, the less amount of information for statistical analysis. This drawback was not serious in Monte Carlo simulation because a large number of independent samples were analyzed.

To simulate the convective diffusional deposition process, the following general procedure was used.

1) The starting point of an incoming particle was chosen randomly on a control surface, called the generation plane, which has height 2H and length Z_{tot}.

Two mutaully independent uniform random numbers were generated using subroutine RANDOM, which has been tested quite extensively by Tanthapanichakoon (1978). The value of the first uniform random

number S_1 always lay between -H and +H, and that of the second number S_2 ranged from $-Z_1$ to $Z_{tot} - Z_1$. Then the starting coordinates are $(X_o, Y_o, Z_o) = (-(\frac{1}{\alpha} - S_1^2)^{\frac{1}{2}}, S_1, S_2)$, since $X_o^2 + Y_o^2 = \frac{1}{\alpha} - S_1^2 + S_2^2 = \frac{1}{\alpha} = R_c$.

2) The diameter of the incoming particle, which belongs to a log-normal distribution with a specified geometric standard deviation, σ_g; is generated as follows. A standard normal random number, n, was produced using subroutine RND (Tanthapanichakoon, 1978). Then the particle diameter, d_p, is

$$d_p = \exp(n.\ln \sigma_g + \ln d_{pm}) \qquad (5.1.2)$$

3) The convective Brownian movement of the particle at each successive time interval $\Delta\tau$ was simulated using the equations described in Section 5.3.

At each time interval, three mutually uncorrelated standard normal random numbers, n_x, n_y and n_z were generated using subroutine RND. These were used as the components of the random normal vector n_{i-1}; and the next position vector P_i was calculate.

4) The new position vector P_i was then checked to see whether the particle had collided against the fiber surface or any of the previously captured particles. If collision had occured the coordinates of the location of capture, the size of the captured particle and other pertinent information were stored, and step 5) was executed next. (It might be necessary to adjust the location of capture in order that the distance between the centers of two contacting particles was equal to the sum of radii of the two particles or

the distance between the center of the captured particle and the fiber surface was exactly the radius of that particle). If no collision had occured, steps 3) and 4) were repeated until the particle was captured, moved out of the rear boundary of Kawabara's cell, or strayed far beyond the length Z_{tot} of the fiber.

5) Steps 1), 2), 3) and 4) were repeated until one of the dendrites on the fiber surface reached a pre-assigned height, for example, of ten particle layers, This then constituted an independent sample, or record, of the Monte-Carlo simulation.

Because of the stochastic nature of the phenomenon, the results contained in a sample represent just one realization of the infinite possibilities of the problem. To obtain more reliable and definitive information on the phenomenon, a large number of independent samples under the same filtration conditions were required to yield an average picture of the situation.

In addition to the above simulation procedure; the following measures were taken to reduce the frequency of checking for possible collision between the incoming particle and fiber or one of the dendrites.

a) The "effective" radius R_{eff} of the dust loaded fiber, which is defined as the radius of the clean fiber plus the height of the tallest dendrite and one geometric mean, $d_{p,\,mean}$, of the particle diameter (a deterministic value), was first compared to the distance C between the latest position of the particle and

the central axis of the fiber. If R_{eff} was smaller than C, there was, obviously, no need to check for capture of particle.

b) The total length Z_{tot} of the fiber was divided into equal partitions of width $d_{p,\ mean}$. Whenever R_{eff} was found greater than C in step a), the partition to which the particle belonged and a number of adjacent partitions, the number being related to the size of the current particle, were searched to see whether there were already any captured particles in them. If not, it was unnecessary to check for possible collision between particles, except collision against the fiber surface. Otherwise, step c) was next executed.

c) Each partition of b) was further diveded angle-wise into a number of angular divisions. The size of each angular division was chosen such that it would be able to contain the largest possible particle on the fiber surface. No checking for possible capture would be necessary if no captured particles already existed in the same angular division as the present particle or in any of the two adjacent angular divisions.

Another important measure was employed to reduce the computer time. It was based on the concept that, in the absence of Brownian motion, the trajectory of any incoming particle in Kuwabara's flow could be resolved uniquely from its entrance height. In other words, it was convenient to determine a priori the position along some trajectory that an incoming particle would reach at time τ as a function of its entrance height ($\tau = 0$ when a particle first entered the cell).

We devided the height of the generation plane into a set of equally spaced points, and we constructed in advance for each trajectory passing through such a point a corresponding set of points on it that a particle would reach at time τ_i (i = 1, 2, ..., j) in the absence of Brownian motion (see Figure 5.2).

Since the displacement contributed by Brownian motion was additive and governed by equation (4.3.3) when the air velocity u remained nearly constant, it was possible to move an incoming particle to some new position much closer to the fiber surface in "one big step", as follows :

$$P_{new} = fn\ (P_{ini},\ \tau) + 2\sqrt{\tau/Pe}\ .n \qquad (5.1.3)$$

where P_{ini} is the initial or starting position vector of the particle, P_{new} is its new position vector after a passage of time τ due to convective Brownian movement, fn is a vector function of P_{ini} and τ, giving the location on the trajectory passing through P_{ini} that the particle would have reached at time τ in the absence of Brownian motion, Pe is the Peclet number, and n is a standard normal random vector generated by subroutine RND.

The above measures appeared to reduce considerably the required computational time and made it possible to carry out a stochastic simulation of fifty independent samples with approximately 120-240 minutes of computer time on an IBM 370/138 computer of Chulalongkorn University. A flow chart of the computational procedure is shown in Figure 5.3.

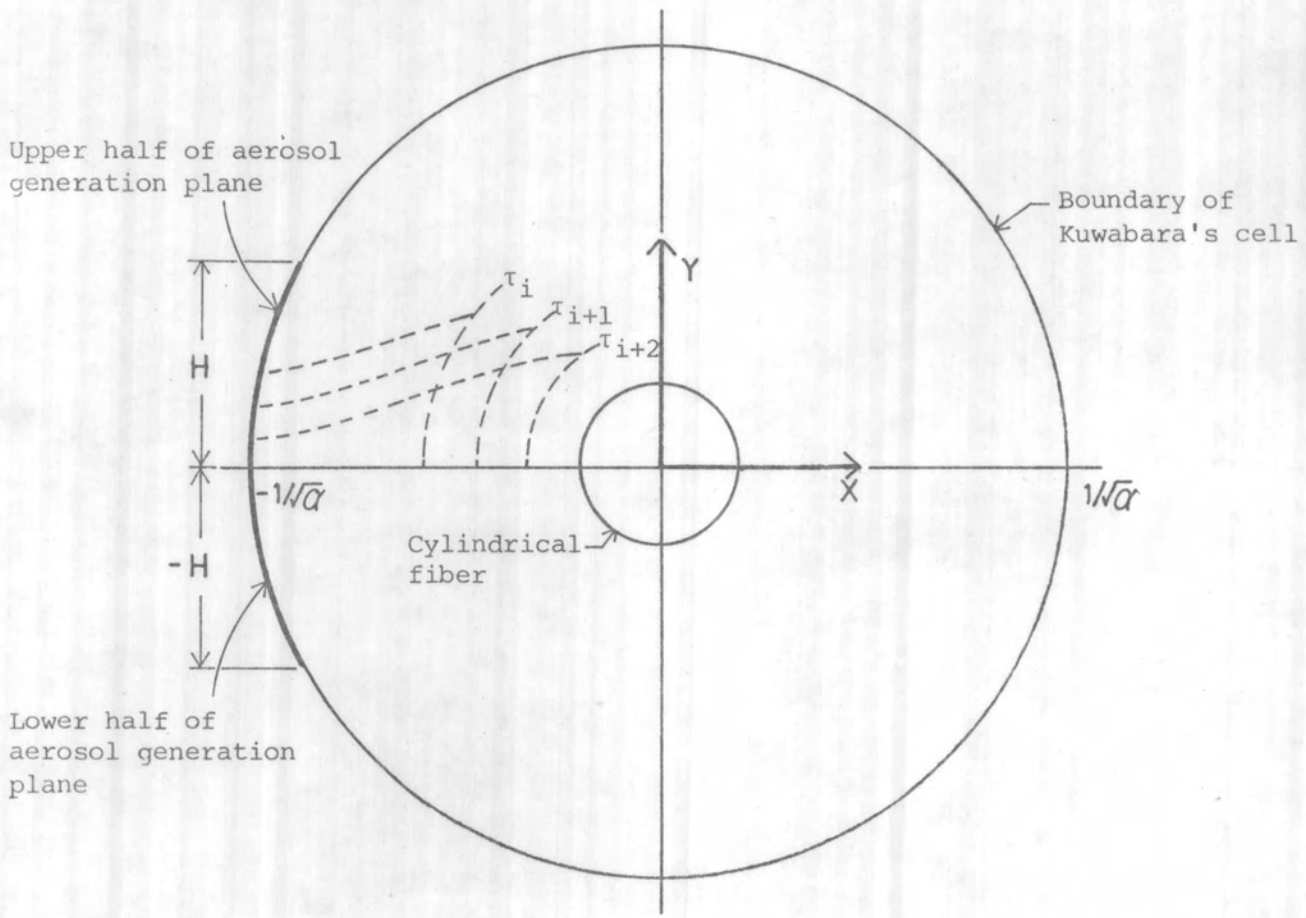

Figure 5.2 Cross section of Kuwabara's cell at (z - z) showing schematically would be trajectories in the absence of Brownian diffusion for times $\tau_i + \tau_{i+1} + \tau_{i+2}$, i = 1, 2, 3, ...

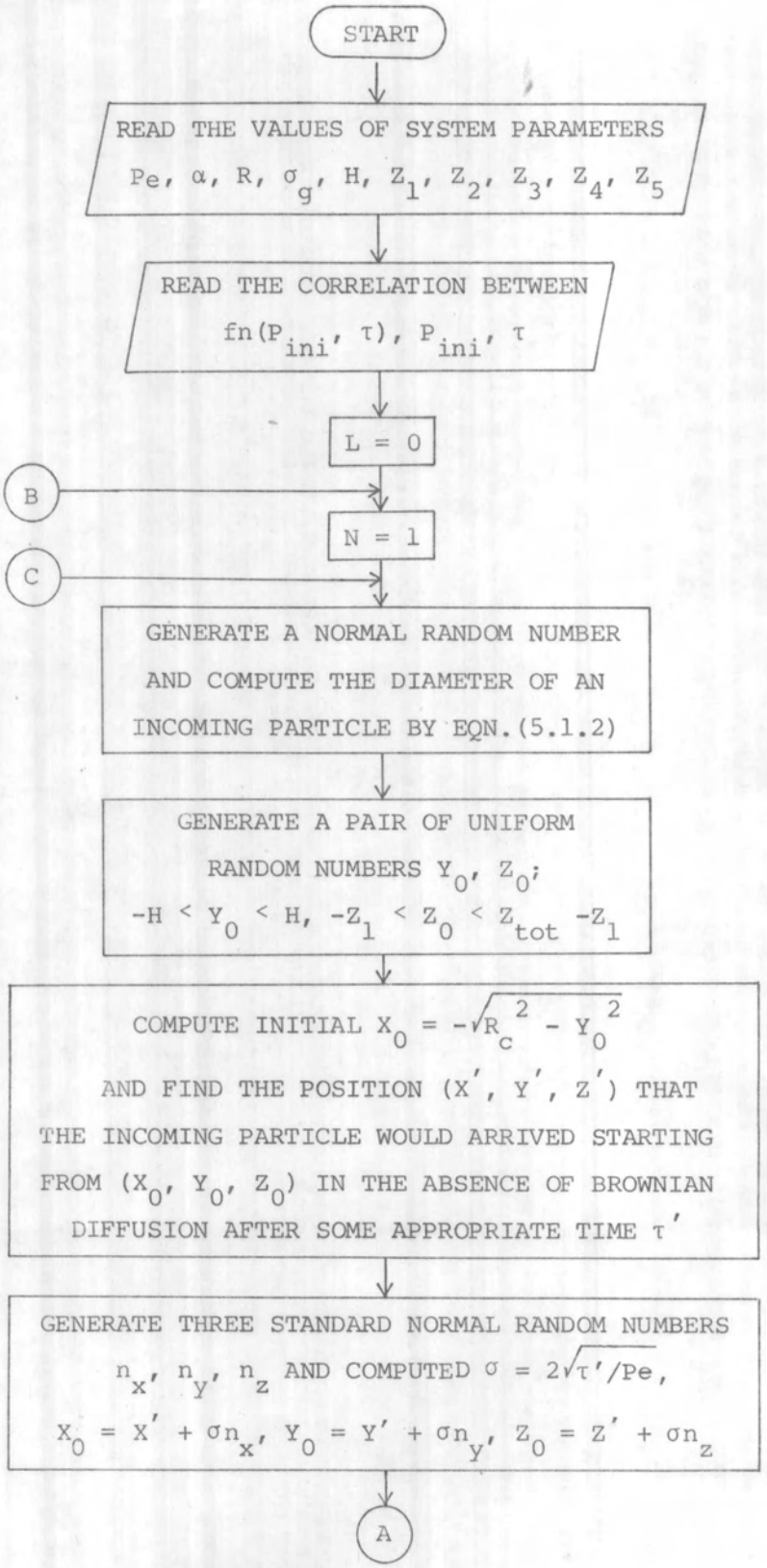

Figure 5.3 Flow chart of computational procedure

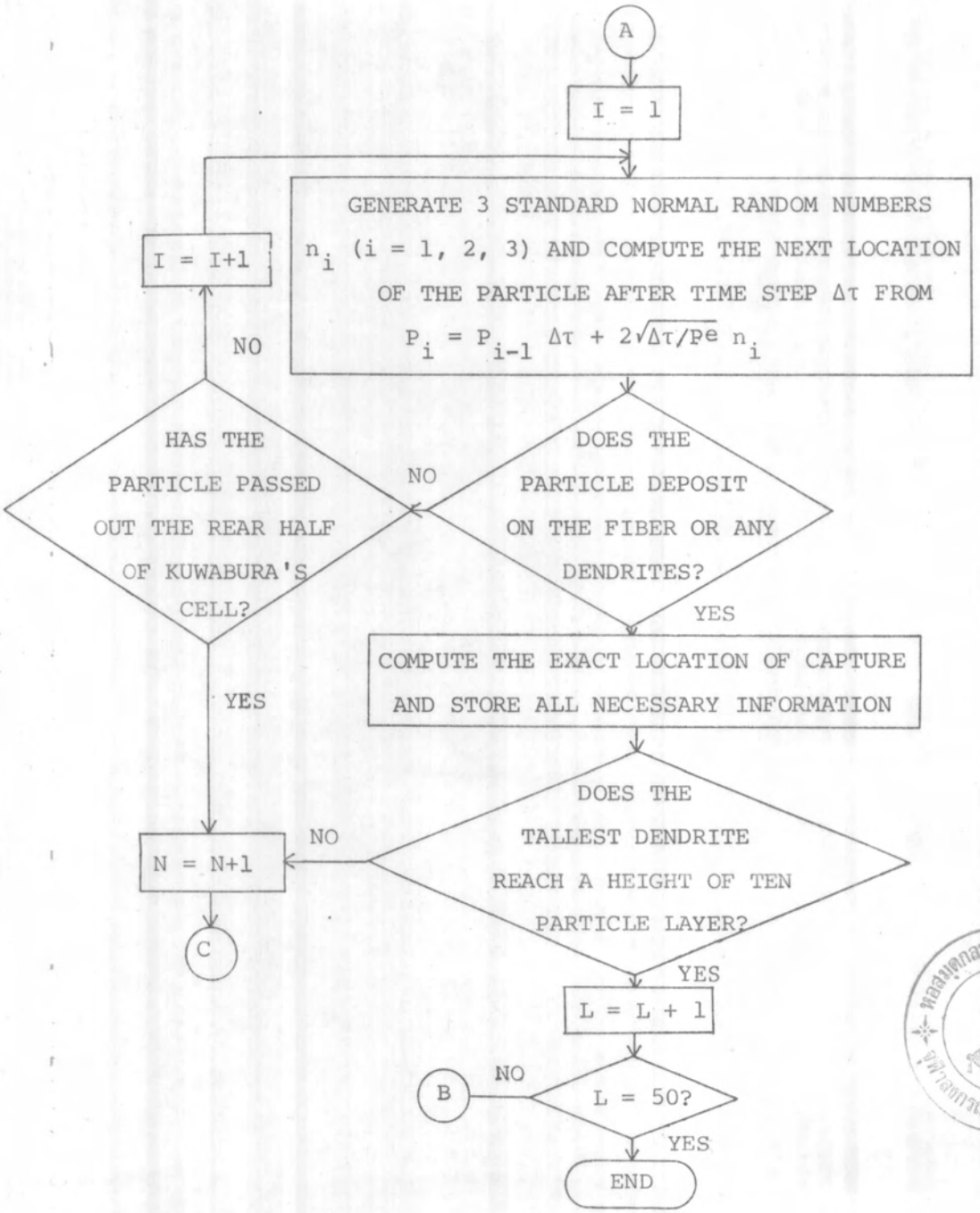

Figure 5.3 (Continued)

5.2 Simulation Conditions

Monte Carlo simulations are carried out under various filtration conditions. However, the packing density of the filter α and the particle density ρ_p were fixed at 0.03 and 1 g/cm^3, respectively. The conditions investigated are listed in Table 5.1. The recommended value of $\Delta\tau = 0.5$ by Kanaoka et al. (1981) was adopted in this study since both studies were concerned with convective diffusional deposition of aerosols on a dust loaded fiber and the stochastic model used here was just an extension of Kanaoka's.

5.3 Sample Size

The sample size here refers to the number of independent samples, or records, obtained via Monte Carlo simulation technique for a given filtration condition. In theory, the larger the sample size used, the better the estimates of the ensemble statistics of the outputs of interest. Obviously, there exists an upper limit for the sample size beyond which little improvement in the precision of these estimates could be obtained.

Because it took a considerable amount of computer time (2-5 minutes) to obtain each sample of the present stochastic process, a compromise of 50 samples was selected as the sample size in this study. Thus it generally toke about 120-240 minutes to investigate a different filtration condition.

It should be noted that, even though 24 different filtration conditions are listed in Table 5.1, some of them had been investigated

Table 5.1 Fitration Conditions Investigated

Interception parameter R [-]	0.1*, 0.2	(Deterministic value)
Peclet number Pe [-]	200*, 1,000*, 5,000, 25,000	
Geometric standard deviation σ_g [-]	1.1*, 1.2, 1.4	
Packing density of filter α [-]	0.03	
Particle density ρ_p [kg/m^3]	1,000	
Length of fiber section		
I, Z_1 [-]	0.6	
II, Z_2 [-]	1.0	
III, Z_3 [-]	4.0	
IV, Z_4 [-]	1.0	
V, Z_5 [-]	0.6	
Radius of fiber R_f [-]	1.0	
Height of half generation plane H [-]	2.0	
Number of samples L [-]	50	

*Investigated by Tanthapanichakoon in a separate work (1982).

earlier in a recent report by Tanthapanichakoon (1982). They are inclued here for the sake of comparision and completness.