CHAPTER IV
SIMULATION PROCEDURE

The optimal values of the essential parameters e_N and e'_N of the deterministic dendritic growth model are determined in this study by comparison with the stochastic results of dendritic growth for convective Brownian diffusion as well as for inertial impaction. This chapter presents the simulation procedure using the stochastic model and the deterministic model of dendritic growth, as well as the procedure of parameter estimation.

4.1 The simulaiton procedure using the stochastic model

The stochastic variable may be composed of deterministic and random components. The deterministic velocity component is described by the equation of motion of a particle. The random position at the aerosol generation plane of Kuwabara's cell is represented by a uniform random number. Furthermore, the dimensionless radius of the Kuwabara's cell R_c is related to the packing density α by

$$R_c = \frac{1}{\sqrt{\alpha}} \qquad (4.1)$$

The total length of the fiber is subdivided into 5 sections with length Z_1, Z_2, Z_3, Z_4, Z_5, respectively (Figure 4.1). However, the effective length of the fiber is Z_3, which is expected to resemble those obtained from using a very long fiber. Here the length of the generation plane Zgen is equal to $Z_1 + Z_2 + Z_3 + Z_4 + Z_5$ with Z_1=Z_5, and Z_2=Z_4.

Based on the stochastic model described in Equation (3.4), (3.5), (3.22), (3.23), (3.24),and (3.25), the simulation is carried out according to the following procedure.

1. The starting point K_0 of an incoming particle was chosen randomly on the generation plane, which overlaps the cell surface and has height of 2H and width of Z. Two mutually independent uniform random number, Y_0 and Z_0,

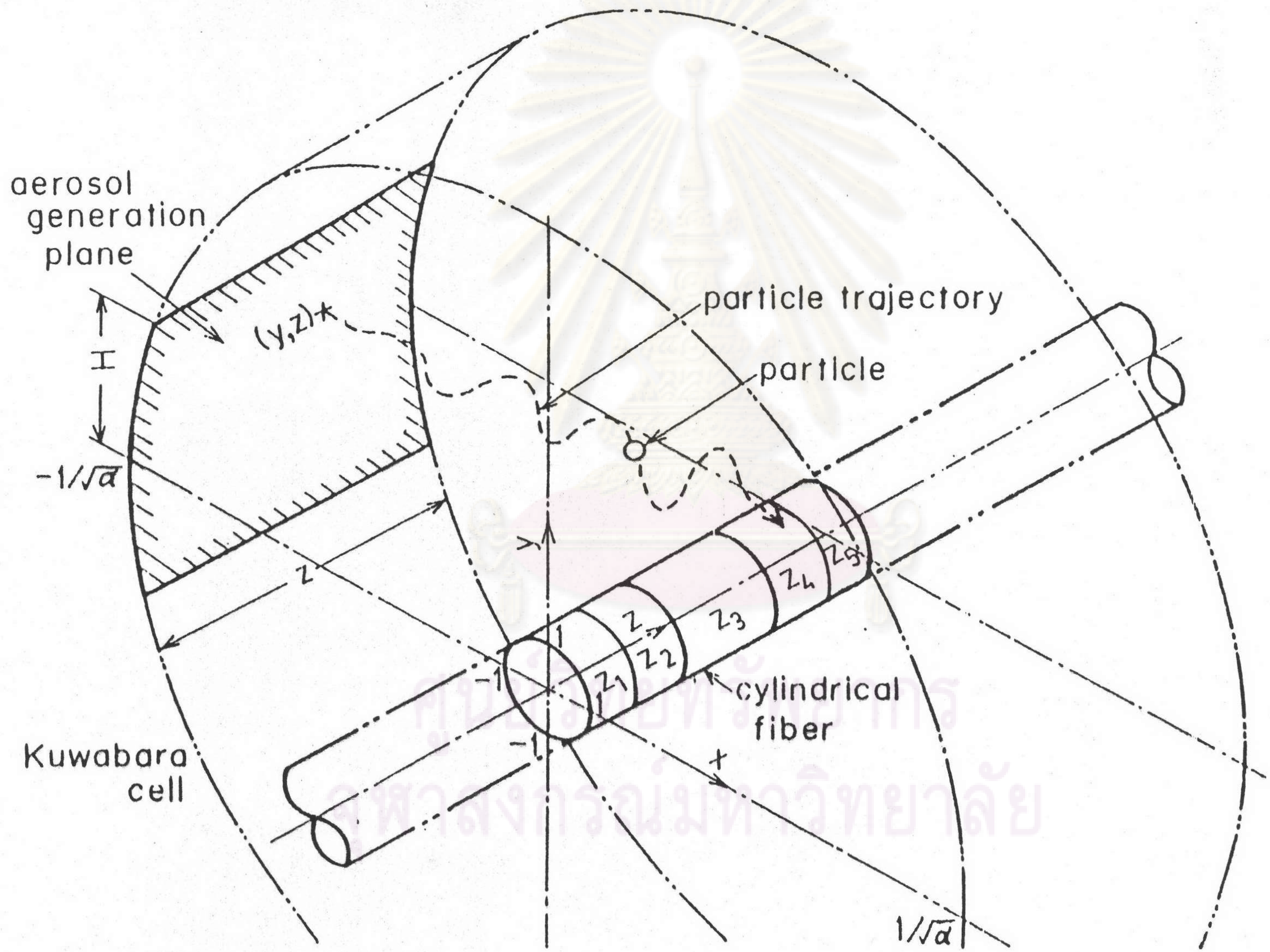

Figure 4.1. Schematic diagram of Kuwabara's cell

($-H \leq y_0 \leq H$, $0 \leq z_0 \leq Z$), are generated by using subroutine RANDOM (Tanthapanichakoon, 1978) to give $K_0=(-\sqrt{R_c^2 - y_0^2}, y_0, z_0)$.

2. For convective Brownian diffusional deposition, the movement of the particle at each successive time interval, Δt, is simulated by using the equation (3.23), then the next position vector K_i can be calculated. The random component in equation (3.23) uses three mutually uncorrelated standard normal random numbers, nx, ny, and nz, which are generated by using subroutine RND (Tanthapanichakoon, 1978). In contrast, in the case of inertial impaction deposition, the next position vector K_i of the particle at each time step, was calculated by using the equation (3.24) and (3.25).

3. The new position vector K_i at the end of the each time step is checked to see whether the particle has collided on the fiber surface or with any of the previously captured particles. If collision has occured the coordinates of the location of capture is stored, and step 4 is executed next. If no collision has occured, step 2 and 3 are repeated until the particle either is captured or moves out of the boundary of Kuwabara's cell.

4. Steps 1, 2, and 3 are repeated until one of the dendrites on the fiber surface grows up to a predetermined height of ten-particle layer.

5. Steps 1, 2, 3, and 4 are repeated for a number of samples to yield enough information for stochastic analysis.

A flow chart of the computational procedure is given in Figure 4.2. Monte Carlo simulations are carried out under various filtration conditions. However, the packing density of the filter α and the particle density ρ_p are fixed at 0.03 and 1000 respectively. Time step Δt and fiber length Z are the two most important parameters which control the accuracy and computational time of the simulation. A short time step and a longer fiber length would enhance accuracy but consume very large computer memory and much computational time. Their suitable values in previous study (Kanaoka et al., 1983) are adopted in this study. A compromise of 50 samples is selected in this study. The simulation conditions are listed in Table 4.1 for convective Brownian diffusion and in Table 4.2 for inertial impaction.

Table 4.1 Stochastic simulation conditions
for convective diffusion

Interception parameter R (-)	0.05, 0.1, 0.13, 0.15, 0.17, 0.2
Peclet number Pe (-)	200, 500, 1000, 2500, 5000
Packing density of filter α (-)	0.03
Length of test fiber section 0 Z_1 (-)	0.4
I Z_2 (-)	0.6
II Z_3 (-)	1.6
III Z_4 (-)	0.6
IV Z_5 (-)	0.4
Half height of generation plane H (-)	2.0
Step size Δt (-)	0.5
Number of simulation L (-)	50

Table 4.2 Stochastic simulation conditions
for inertial impaction

Interception parameter R (-)	0.05, 0.1, 0.13, 0.15, 0.17, 0.2
Stokes number St (-)	0, 0.6, 1.0, 1.4, 2.0
Packing density of filter α (-)	0.03
Length of test fiber section 0 Z_1 (-)	0.4
I Z_2 (-)	0.6
II Z_3 (-)	1.6
III Z_4 (-)	0.6
IV Z_5 (-)	0.4
Half height of generation plane H (-)	2.0
Step size Δt (-)	0.1
Number of simulation L (-)	50

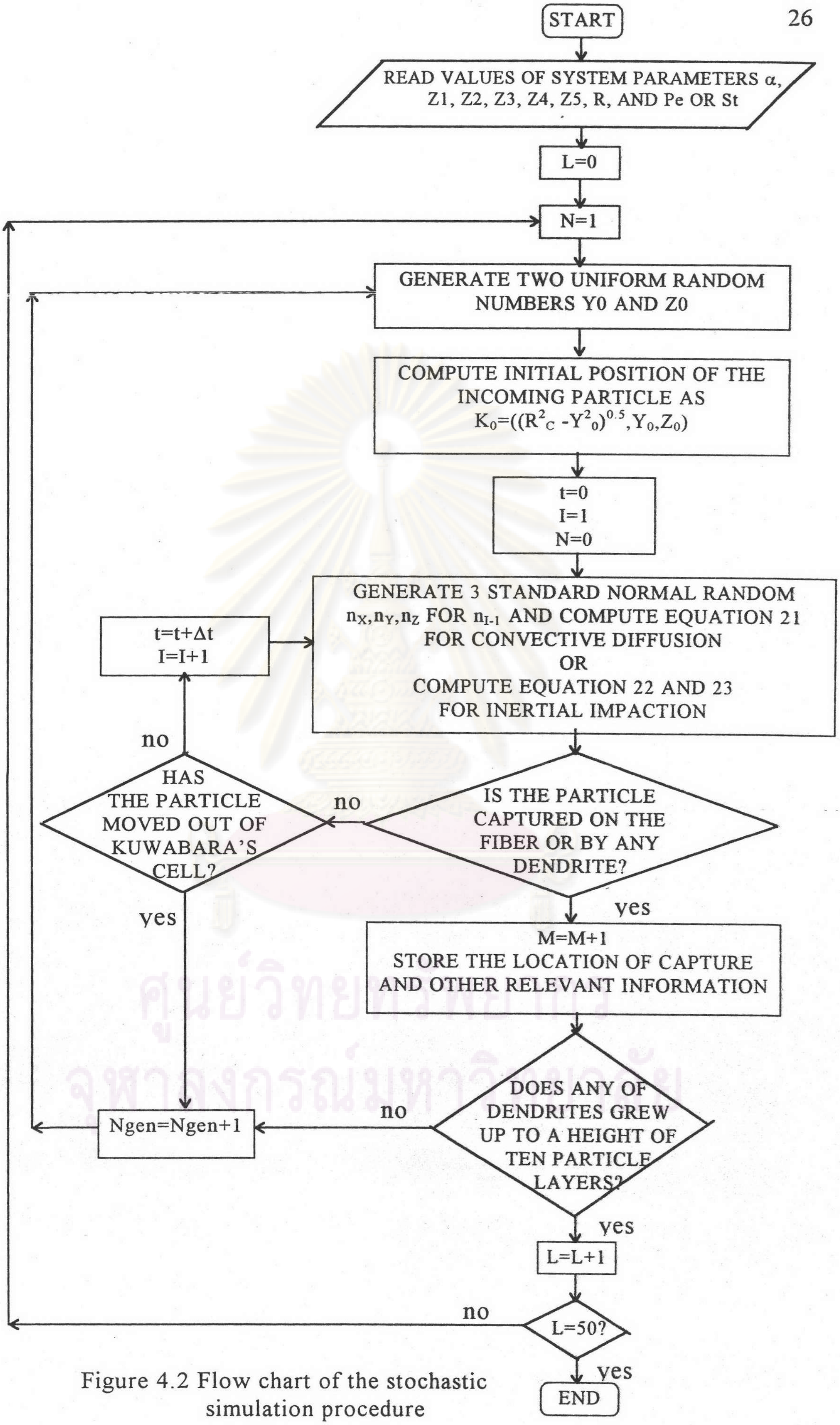

Figure 4.2 Flow chart of the stochastic simulation procedure

4.2 The simulation procedure of the deterministic model

The simple deterministic dendritic growth model (Wiwut Tanthapanichakoon et al., 1993) which is based on the population balance model is adopted in this study. The net rate of birth and growth of dendrites are given in equation (3.23) and (3.24). These equations are solved by Runge-Kutta 4th-order method. Using the deterministic model described above, the calculation is carried out according to the following procedures.

1. The parameters e_N and e'_N are estimated before-hand by curve-fitting method.

2. The clean fiber efficiency is calculated at first. For convective diffusion, the clean fiber efficiency is calculated using Fuchs's equation which is given in equations (3.16) and (3.17). In contrast, the clean fiber efficiency is calculated using limiting trajectory of a particle for the case of inertial impaction.

3. The collection efficiency raising factor was calculated using equation (3.38).

4. The birth of dendrites of size 1 and the growth of dendrites of size N on a fiber at each incoming particle interval dN_{gen} are calculated using Runge-Kutta 4th-order method to solve equations (3.26) and (3.29), respectively. If the number concentration of the largest size of dendrites P_{NMAX} reaches a predetermined value of 0.02, the largest dendrite size is allowed to increase by one (NMAX=NMAX+1). The maximum allowable size of dendrites is 100.

5. The dust load and collection efficiency are calculated using equations (3.36) and (3.34), respectively.

6. Step 4, and 5 are repeated until the total number of incoming particles reaches a predetermined number of interest.

A flow chart of the computational procedure is given in Figure 4.3. The simulation conditions for convective diffusion and inertial impaction are listed in Tables 4.3 and 4.4 , respectively.

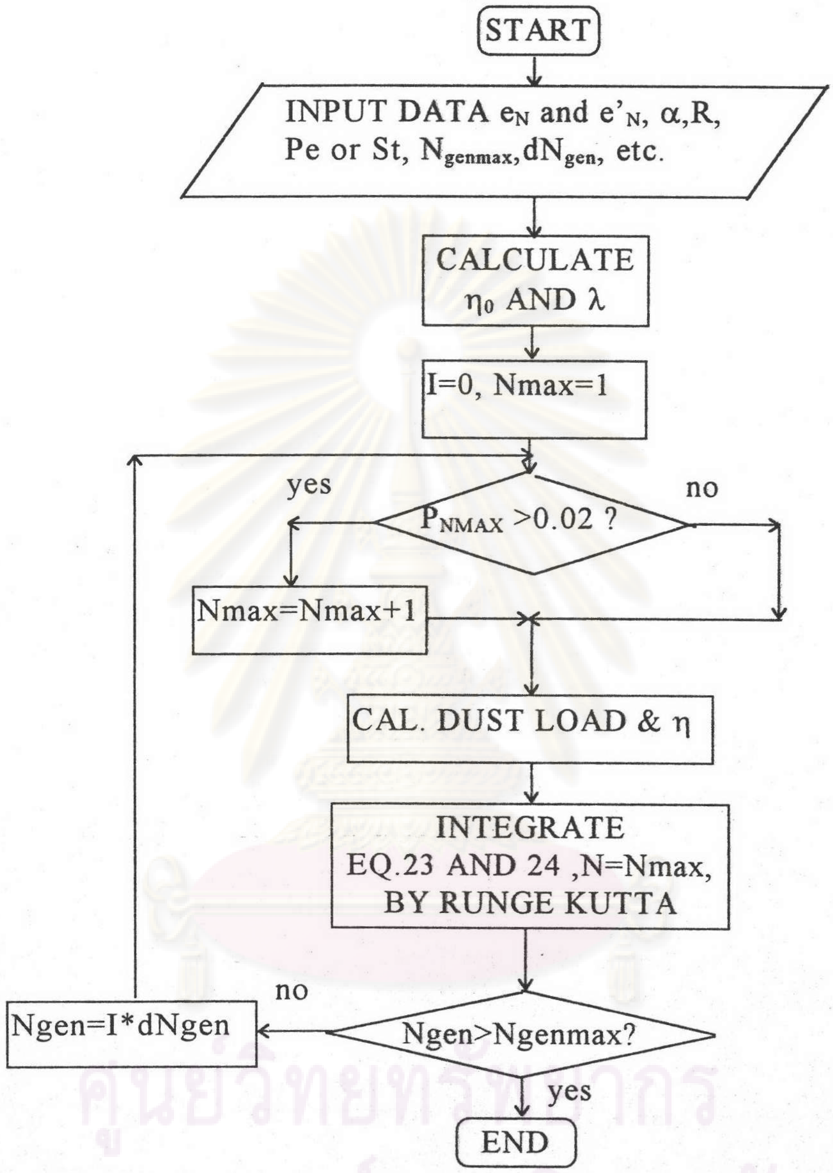

Figure 4.3 Flow chart of the deterministic simulation procedure

4.3 The procedure of the parameter estimation

To predict the growth of dendrites, it is necessary to know the parameters e_N and e'_N. The parameters e_N and e'_N are determined by minimizing the following sum of squares of the differences between the present model and the previous stochastic model (Kanaoka et al., 1983).

$$S(e_N, e_N') = \sum_{j=1}^{N}\sum_{i=1}^{M}\left(\frac{(P_i^j - Psto_i^j)^2}{Psto_i^j}\right) + \omega NM\left(1 - \frac{\lambda}{\lambda_{sto}}\right)^2 \quad (4.2)$$

where ω is a weight factor. Typically $\omega = 0.1$.

A non-linear simplex method is used in a curve-fitting program for estimating the parameters of the deterministic model. It will be used to minimize the objective function shown in equation (4.2). The estimation of the parameter e_N and e'_N is carried out according to the following procedures.

1. The simplex method must be started, not with a single point, but with N+1 points, defining an initial simplex, where N is the number of search dimensions. First, one of these points, the starting point A_0 of the parameters e_N and e'_N are guessed. The difference between e_N and e'_N is estimated with the aid of equation (3.38). The other N points can be given by

$$A_i = A_0 + \sigma I_i \quad (4.3)$$

where I_i is a unit vector, and σ is constant of 0.1

2. The optimal values of the parameters e_N and e'_N were determined using subroutine SIMPLEX (Nelder et al., 1965). During optimization, the simplified deterministic model is simulated, and the results of dendritic growth is compared with the corresponding stochastic results using equation (4.2). The temination criteria for optimization is:

$$|S_{high} - S_{low}| \le 0.001$$

Parameter estimation are carried out for various filtration conditions of convective Brownian diffusion as well as inertial impaction.

The simulation conditions for convective diffusion and inertial impaction are listed in Tables 4.3 and 4.4, respectively.

Table 4.3 Deterministic simulation conditions for convective diffusion

Interception parameter R (-)	0.05, 0.1, 0.13, 0.15, 0.17, 0.2
Peclet number Pe (-)	200, 500, 1000, 2500, 5000
Packing density of filter α (-)	0.03
Total fiber length Z(-)	3.6
Step size Δt (-)	0.05

Table 4.4 Deterministic simulation conditions for inertial impaction

Interception parameter R (-)	0.05, 0.1, 0.13, 0.15, 0.17, 0.2
Stoke number St (-)	0.0, 0.6, 1.0, 1.4, 2.0
Packing density of filter α (-)	0.03
Total fiber length Z(-)	3.6
Step size Δt (-)	0.05