CHAPTER IV

MODELING AND SIMULATION TECHNIQUE

Mathematical simulation means the study of a system or its parts by manipulation of its mathematical representation or its physical model. The simulation has many benefits. It is possible to study existing system more quickly, economically and thoroughly than in the real system. Furthermore, with a suitable mathematical representation, it is possible to test extreme ranges of operating conditions, some of which might be impractical or unsafe to test in a real plant.

A mathematical representation, namely mathematical model, is a mathematical abstraction of a real system. Models can be classified into three different categories, depending on how they are derived: first, theoretical models which are developed by using the principle of chemistry and physics, second, empirical models which are obtained from a mathematical (statistical) analysis of system data, and finally, models that compromise between the both categorized models with one or more parameters to be evaluated from plant data called semi-empirical models. In the last classification, certain theoretical model parameters such as heat transfer coefficient and similar fundamental relations usually must be evaluated from physical experiments or from process operating data.

In this chapter, a comprehensive model of the pneumatic conveying dryer with two periods of drying, namely surface evaporation model and internal moisture diffusion controlled model, is proposed. The model is derived from two separate theoretical models proposed by S. Matsumoto and D.C.T. Pei (1984a, 1984b). The heat and mass transfer and solid transport equations which are derived from transport phenomena is presented with the simulation technique. In addition, the fundamental correlations of air properties are summarized in an appendix.

4.1 Model assumptions

The following assumptions are made in the modeling.

1. The whole system is at steady state.
2. Air temperature and humidity are uniform over the cross section of the dryer, but vary along the drying path.
3. Solid particles are distributed uniformly over the cross section of dryer.
4. Solid particles are essentially spherical and can be represented by a mean size.
5. The wall of the dryer is thermally insulated and there is no heat loss to the surroundings.
6. Air and solid flow co-currently upward in uniform suspension.
7. Air behaves like an ideal gas.
8. The moisture content within the solid particles is quite uniform only during the surface evaporation period.
9. The moisture content within the solid particles at the start of the internal moisture diffusion controlled period is quite uniform.
10. The internal moisture diffusion coefficient is not a function of the local moisture content.

11. The equilibrium moisture content is approximately a linear function of the humidity of drying air.

$$W_{eq} = \alpha H + \beta. \tag{4.1}$$

4.2 Mathematical model

The present comprehensive mathematical model is based on the two separate models proposed by S. Matsumoto and D.C.T Pei (1984a, 1984b). Based on the above assumptions, mass (water) and energy (enthalpy) balances around a dryer element of length ΔZ, as shown in Figure 4.1, are taken on both the solid and gas phases to obtain the equations of change for the moisture content, humidity, and solid and air temperatures along the drying path.

4.2.1 Moisture balance of solid phase

$$\begin{Bmatrix}\text{Rate of accumulation}\\ \text{of moisture}\end{Bmatrix} = \begin{Bmatrix}\text{Rate of moisture}\\ \text{in with solid}\end{Bmatrix} - \begin{Bmatrix}\text{Rate of moisture}\\ \text{out with solid}\end{Bmatrix} - \begin{Bmatrix}\text{Drying rate}\\ \text{of moisture}\end{Bmatrix}$$

$$0 = G_s AW\big|_{z=z} - G_s AW\big|_{z=z+\Delta z} - R_d a_v A\Delta Z$$

Divided through by $A\Delta Z$ and applying the definition of derivative, the equation becomes

$$G_s \frac{dW}{dZ} = -R_d a_v A. \tag{4.2}$$

It is noted that the solid surface area per unit dryer volume, a_v, is defined as follows:

$$a_v = \frac{\text{The amount of grains in the element * Surface area of each grain}}{\text{The volume the element}}$$

Thus, $$a_v = \left\{ \frac{\left[\left(\frac{\Delta Z}{u_s} * G_s \right) \Big/ \left(\frac{\pi}{6} d_p^2 * \rho_s \right) \right] * \pi d_p^2}{\frac{\pi}{4} D^2 \Delta Z} \right\} = \frac{24 G_s}{\pi \rho_s u_s d_p D^2}.$$

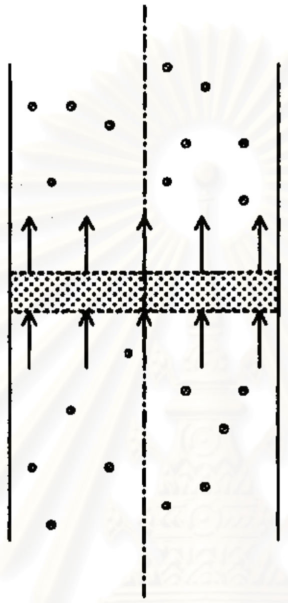

Figure 4.1 Diagram of pneumatic conveying dryer

4.2.2 Water vapor balance of gas phase

$$\begin{Bmatrix} \text{Rate of accumulation} \\ \text{of water vapor} \end{Bmatrix} = \begin{Bmatrix} \text{Rate of water} \\ \text{vapor in with air} \end{Bmatrix} - \begin{Bmatrix} \text{Rate of water} \\ \text{vapor out with air} \end{Bmatrix} + \begin{Bmatrix} \text{Drying rate} \\ \text{of moisture} \end{Bmatrix}$$

$$0 = G_a AH\big|_{z=z} - G_a AH\big|_{z=z+\Delta z} + R_d a_v A \Delta Z$$

Similarly, we obtain

$$G_a \frac{dH}{dZ} = R_d a_v A \tag{4.3}$$

and $$\frac{dH}{dZ} = -\frac{G_s}{G_a} \frac{dW}{dZ}. \tag{4.4}$$

4.2.3 Energy balance of solid phase

$$\begin{Bmatrix}\text{Rate of accumulation}\\ \text{of energy}\end{Bmatrix}=\begin{Bmatrix}\text{Rate of energy in by}\\ \text{mass flow of wet solid}\end{Bmatrix}-\begin{Bmatrix}\text{Rate of energy out by}\\ \text{mass flow of wet solid}\end{Bmatrix}$$

$$+\begin{Bmatrix}\text{Rate of heat transfer}\\ \text{from gas phase}\end{Bmatrix}-\begin{Bmatrix}\text{Rate of energy consumption}\\ \text{to evaporate moisture}\end{Bmatrix}$$

$$0 = G_s i_s\big|_{z=z} - G_s i_s\big|_{z=z+\Delta z} + h_p(T_a - T_s)a_v A\Delta Z$$
$$-(\lambda_s + C_w T_s + C_v(T_a - T_s))R_d a_v A\Delta Z$$

Thus

$$G_s \frac{di_s}{dZ} = \{h_p(T_a - T_s) - [\lambda_s + C_w T_s + C_v(T_a - T_s)]R_d\}a_v A \qquad (4.5)$$

The enthalpy of wet solid is defined as

$$i_s = (C_s + C_w W)T_s$$

$$di_s = (C_s + C_w W)dT_s + C_w T_s dW .$$

Substitution into equation (4.5) gives

$$(C_s + C_w W)\frac{dT_s}{dZ} = \{h_p(T_a - T_s) - [\lambda_s + C_v(T_a - T_s)]R_d\}\frac{a_v A}{G_s}. \qquad (4.6)$$

4.2.4 Energy balance of gas phase

$$\begin{Bmatrix}\text{Rate of accumulation}\\ \text{of energy}\end{Bmatrix}=\begin{Bmatrix}\text{Rate of energy in by}\\ \text{mass flow of humid air}\end{Bmatrix}-\begin{Bmatrix}\text{Rate of energy out by}\\ \text{mass flow of humid air}\end{Bmatrix}$$

$$-\begin{Bmatrix}\text{Rate of heat transfer}\\ \text{to solid phase}\end{Bmatrix}+\begin{Bmatrix}\text{Rate of energy in by mass}\\ \text{flow of evaporated moisture}\end{Bmatrix}$$

$$0 = G_a i_a\big|_{z=z} - G_a i_a\big|_{z=z+\Delta z} + \{-h_p(T_a - T_s) + R_d(\lambda_0 + C_v T_a)\}a_v S\Delta Z$$

Thus

$$G_a \frac{di_a}{dZ} = \{-h_p(T_a - T_s) - (\lambda_0 + C_v T_a)R_d\} a_v A \tag{4.7}$$

The enthalpy of humid air is defined as

$$i_a = (C_a + C_v H)T_a + \lambda_0 H$$

$$di_a = (C_a + C_v H)dT_a + (\lambda_0 + C_v T_a)dH .$$

Substitution into equation (4.7) gives

$$(C_a + C_v H)\frac{dT_a}{dZ} = -h_p(T_a - T_s)\frac{a_v A}{G_s} . \tag{4.8}$$

4.2.5 Solid particle movement

The velocity of solid particle along the dryer length can be calculated from the summation of forces acting on the solid particle.

$$\begin{Bmatrix} \text{mass of} \\ \text{particle} \end{Bmatrix} * \begin{Bmatrix} \text{acceleration} \\ \text{of particle} \end{Bmatrix} = \begin{Bmatrix} \text{drag force acting} \\ \text{on particle} \end{Bmatrix} - \begin{Bmatrix} \text{gravity force acting} \\ \text{on particle} \end{Bmatrix} + \begin{Bmatrix} \text{bouyant force acting} \\ \text{on particle} \end{Bmatrix}$$

$$\rho_s(1+W)V_p \frac{du_s}{dt} = \frac{1}{2}\frac{\pi d_p^2}{4}\rho_a C_D(u_a - u_s)^2 - V_p\rho_s(1+W)g + V_p\rho_a$$

If one assumes $\frac{\rho_a}{\rho_s} << 1$, it becomes

$$\frac{du_s}{dt} = \frac{3}{4}\frac{\rho_a}{d_p\rho_s(1+W)}C_D(u_a - u_s)^2 - g .$$

On utilizing the relation $u_s = \frac{dz}{dt}$, the equation becomes

$$u_s \frac{du_s}{dZ} = \frac{3}{4}\frac{\rho_a}{d_p \rho_s (1+W)} C_D (u_g - u_s)^2 - g. \tag{4.9}$$

4.3 Complementary equations

4.3.1 Rate of drying

Equations (4.2), (4.4), (4.6) and (4.8) describe the rate of change of the moisture content, humidity, and solid and air temperatures along the length of a pneumatic conveying dryer. However, the model equations require an indispensable complementary equation, the rate of drying, R_d. As mentioned that the present model consists of two competing drying mechanisms. When moisture content exists on or close to the particle surface, the film mass transfer rate dominates on the drying rate in this surface evaporation period. Otherwise, the drying rate in the internal moisture diffusion controlled period is dominated by the rate of internal moisture diffusion.

4.3.1.1 Drying rate in surface evaporation period

In the surface evaporation period, the moisture on the solid surface is removed. The drying rate is dominated by film mass transfer. Thus, the drying rate equation is defined as follows:

$$R_{ds} = k_H * (H_{sat} - H) \tag{4.10}$$

Where k_H is estimated from equation (4.23)

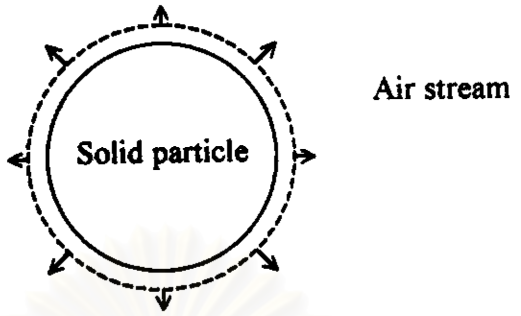

Figure 4.2 Diagram of film mass transfer

4.3.1.2 Drying rate in the internal moisture diffusion controlled period

In the internal moisture diffusion controlled period, the diffusion of moisture within the solid particle is the mechanism that governs the drying rate because the moisture at solid surface has already been removed and the solid surface has dried out. Therefore, the drying rate must be calculated from the rate of mass transfer to the solid surface. Moisture balance within the solid particle, as shown in Figure 4.3, is taken to derive the rate equation.

$$\begin{Bmatrix}\text{Rate of accumulation} \\ \text{of moisture}\end{Bmatrix} = \begin{Bmatrix}\text{Rate of moisture} \\ \text{in by diffusion}\end{Bmatrix} + \begin{Bmatrix}\text{Rate of moisture} \\ \text{out by diffusion}\end{Bmatrix}$$

$$4\pi r^2 \Delta r \frac{\partial c}{\partial t} = 4\pi r^2 J_r\Big|_{r=r} - 4\pi r^2 J_r\Big|_{r=r+\Delta r}$$

Thus

$$\frac{\partial c}{\partial t} = -\frac{1}{r^2}\frac{\partial (r^2 J)}{\partial r}.$$

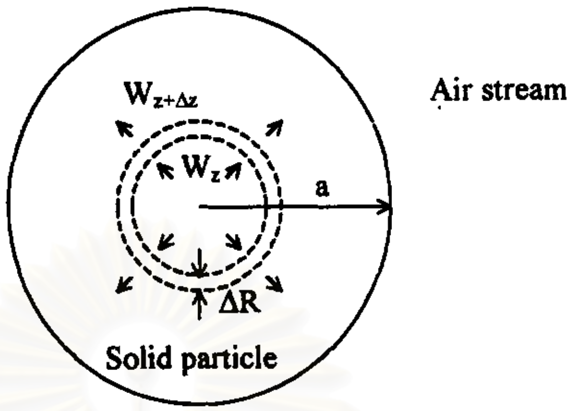

Figure 4.3 Diagram of moisture diffusion within solid

The mass flux, J_r, is given by Fick's law of diffusion as follows:

$$J_r = -D_m \frac{\partial c}{\partial r}$$

Then, the diffusion equation of moisture within a sphere becomes

$$\frac{\partial c}{\partial t} = \frac{D_m}{r^2} \frac{\partial \left(r^2 \frac{\partial c}{\partial r} \right)}{\partial r}$$

and

$$\frac{\partial c}{\partial t} = D_m \left(\frac{\partial^2 c}{\partial r^2} + \frac{2}{r} \frac{\partial c}{\partial r} \right).$$

The above equation can be rewritten by substitution W for c.

$$\frac{\partial W}{\partial t} = D_m \left(\frac{\partial^2 W}{\partial r^2} + \frac{2}{r} \frac{\partial W}{\partial r} \right) \quad (4.11)$$

The initial and boundary conditions are

$$c = c_0 \quad \text{for} \quad 0 \le r \le a, \quad t = 0, \quad (4.12)$$

$$R_{dd} = -D_m \frac{\partial c}{\partial r} = k(c - c_{eq}) \quad \text{at} \quad r = a, \quad t > 0 \tag{4.13}$$

$$\frac{\partial c}{\partial r} = 0 \qquad \text{at} \quad r = 0, \ t > 0. \tag{4.14}$$

From equation (4.3), rearrange by using the relation $\frac{dz}{dt} = u_s$, the rate of change in the humidity of ambient air is

$$\frac{dH}{dt} = \left(\frac{a_v A u_s}{G_a}\right) R_{dd} = \left(\frac{3m}{a\rho_s}\right) R_{dd} = \left[\frac{3m}{a\rho_s}\right] k(c - c_{eq}).$$

The initial and boundary conditions can be written in terms of the moisture content as

$$W = W_0 \quad \text{in} \quad 0 \le r \le a, \quad \text{and} \quad H = H_0; \quad t = 0,$$

$$-D_m \left(\frac{\partial W}{\partial r}\right)_{r=a} = k(W|_{r=a} - W_{eq}) = \left(\frac{a}{3m}\right)\frac{dH}{dt}, \qquad t > 0$$

$$\frac{\partial W}{\partial r} = 0 \qquad \text{at} \quad r = 0, \quad t > 0.$$

By using equation (4.1), the initial and boundary conditions are rewritten as

$$W = W_0 \quad \text{in} \quad 0 \le r \le a, \quad \text{and} \quad W_{eq} = W_{eq,0}; \quad t = 0, \tag{4.15}$$

$$-D_m \left(\frac{\partial W}{\partial r}\right)_{r=a} = k(W|_{r=a} - W_{eq}), \qquad t > 0 \tag{4.16}$$

$$\left(\frac{\partial W}{\partial r}\right)_{r=0} = 0, \qquad t > 0. \tag{4.17}$$

The analytical solution of equation (4.11) with the initial and boundary conditions, equations (4.15), (4.16) and (4.17), is presented by S. Matsumoto and D.C.T. Pei (1984b). By Laplace transformation the drying rate is

$$R_{dd} = \left\{ 2M^2 \sum_{n=1}^{\infty} \frac{\xi_n^2 \exp - \left[\xi_n^2 \left(\frac{D_m t}{a^2} \right) \right]}{Q_n} \right\} \left[\frac{D_m \rho_s (W_0 - W_{eq,0})}{a} \right] \tag{4.18}$$

where

$$Q_n = \left(\frac{M}{B} \right)^2 \xi_n^4 + M \left(M - \frac{M}{B} - \frac{2}{B} \right) \xi_n^2 + 3M + 1, \tag{4.19}$$

ξ_n are the positive roots of

$$\tan\xi = \xi \left\{ 1 - \frac{M}{B} \xi^2 \right\} \Big/ \left\{ 1 - M \left(\frac{1}{B} - 1 \right) \xi^2 \right\}, \tag{4.20}$$

$$B = \frac{ka}{D_m}, \quad \text{and} \quad M = \frac{1}{3m\alpha}. \tag{4.21}$$

4.3.2 Heat and mass transfer correlations

Well-known correlations of heat and mass transfer for an individual spherical particle have been proposed by W.E. Ranz and W.R. Marchall (1952). The correlations are

$$Nu = 2 + 0.6 Re^{1/2} Pr^{1/3} \tag{4.22}$$

$$\text{and} \quad Sh = 2 + 0.6 Re^{1/2} Sc^{1/3}. \tag{4.23}$$

However, the heat and mass transfer coefficients estimated from the above correlations tend to be overpredicted. A correction factor used to adjust the experimental and predicted values of the heat and mass transfer coefficients has been reported in the book by R. Toei (1986). The correction factor compensates for the agglomeration of wet particles during drying and is shown as a function of the particle size diameter in Figure 4.4.

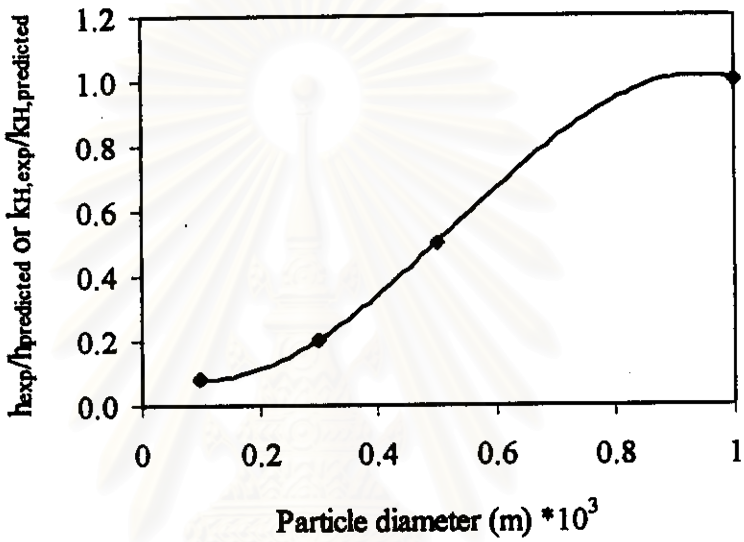

Figure 4.4 Heat and mass transfer coefficients correction factor as a function of particle size diameter

The equation obtained by curve-fitting of the correction factor in Figure 4.4 is

$$F = -3.34*10^9 d_p^3 + 5.3*10^6 d_p^2 - 1.1*10^3 d_p + 0.144. \qquad (4.24)$$

This equation is for the particle diameter of 0.1-1 mm. For the particle larger than 1 mm, the correction factor is 1.

4.4 General Model

A general pneumatic conveying drying model is obtained by combining the above two transport phenomena models of drying with the equations of change in the drying variables, i.e. moisture content, humidity, and solid and air temperatures. Since there are two competing models that describe the drying behavior, a criterion for the switching point between the two models is necessary.

Intuitively, the actual drying rate must be equal to the whichever is lesser between the rates predicted by the two competing model. Let R_{ds} and R_{dd} denote the rates predicted at a distance Z from the dryer inlet according to equations (4.10) and (4.18), respectively.

1. If $R_{ds} > R_{dd}$ at $Z = 0$, then the surface evaporation period does not exist and the actual drying rate is controlled by the rate of internal moisture diffusion from the beginning.
2. If $R_{ds} > R_{dd}$ at $Z = 0$, then the surface evaporation rate determines the actual drying rate in the vicinity of the dryer inlet.
3. As the drying material proceeds step by step along the dryer length ($\Delta Z = 1*10^{-4}$ m being the typical stepsize), the local value of R_{ds} tends to decrease at a slower pace than that of R_{dd}. If $R_{ds} < R_{dd}$ throughout the entire dryer length, then only surface evaporation controls the actual drying rate.
4. If $R_{ds} > R_{dd}$ at some point in the dryer length, then a switching to another dominant model occurs and the actual drying rate is determined thereafter by the rate of internal moisture diffusion (R_{dd})

Since it takes much time to evaluate and calculate the summation terms in equation (4.18), the drying rate from the internal moisture diffusion controlled model, (R_{dd}) is not estimated at every stepsize but only at every 1 cm of the drying length in order to save computational time.

4.5 Simulation technique

4.5.1 Input data

The data which are required in the simulation are listed as follows:

1. Dryer configuration: dryer diameter and dryer length.
2. Physical properties: mean particle size, true density of solid, specific heats of dry solid, water and water vapor and viscosity of air.
3. Dryer inlet conditions: air and solid temperatures, air humidity, solid moisture content, and mass flow rate of air (dry air) and solid (dry solid).
4. Model parameters: internal moisture diffusion coefficient, intrinsic equilibrium moisture content of solid, slope of the curve between the equilibrium moisture content and humidity.

It should be noted that in the program specific heats of dry solid, water and water vapor and viscosity of air have been given as function of temperature, pressure and humidity of air.

4.5.2 Numerical integration

In the solution of the complex nonlinear model, the fourth-order Runge-Kutta method is used to simultaneously integrate the set of ordinary differential equations. In the surface evaporation period, equation (4.10) is integrate simultaneously with the equations of change, i.e. equations (4.2), (4.4), (4.6), (4.8), and the equation of solid movement, equation (4.9). In the internal moisture diffusion controlled period, the drying rate of this period is calculated by summing the series up to a last term which is less than 0.01 % of the summation. The set of the drying rate equations in this period is used instead of the surface evaporation equation and integrated simultaneously with equations (4.2), (4.4), (4.6), (4.8) and (4.9). Because the drying time is the original independent variable of this drying rate equation, the term dZ/u_s is used to relate the stepsize of the drying length to the drying time. The positive roots of equation (4.20), ξ_n, are found by the bisection method with relative errors less than 0.01 %.

The step size used in the simulation is defined as $1*10^{-4}$ m of the drying length. In addition, numerical integration of the model using $5*10^{-5}$ m of the drying length as stepsize has been carried out to check the integration error due to the step size. The differences in the moisture content, humidity, and air and solid temperatures between the two step sizes are calculated in terms of the relative errors. As long as the relative errors throughout the entire dryer length are less than 0.1 %, the simulation result are acceptable. However, if anyone of the relative errors between the two step sizes is more than 0.1 %, the integration of the model will be restarted from the dryer inlet using one-tenth of both the older stepsizes.

4.6 A algorithm of the pneumatic conveying dryer model

A simplified algorithm of the present comprehensive model is listed below. Figure 4.5 illustrates the simplified flow chart of the model.

1. Input all the data mentioned in section 4.4.1.
2. Integrate the equations of change for one step size using the surface evaporation model, including finding the drying rate, R_{ds}, from the surfae evaporation model.
3. Estimate the drying rate, R_{dd}, from the internal moisture diffusion controlled model.
4. Compare R_{ds} and R_{dd}.

    4.1 If $R_{ds} < R_{dd}$, follow the following steps. Otherwise go to 4.2.

    4.1.1 Write a result to file

    4.1.2 Check whether the present length is less than the total dryer length?

    - If the answer is 'no', exit the program.
    - If the answer is 'yes', go back to step 2.

    4.2 The model switches to the internal moisture diffusion controlled model. Restart at the last step.
5. Integrate the equations of change for one step size using the internal moisture diffusion controlled model.
6. Write the results to file

7. Check whether the integrated length is less than the total dryer length?

   7.1 If the answer is 'no', go to step 5.

   7.2 If the answer is 'yes', exit the program.

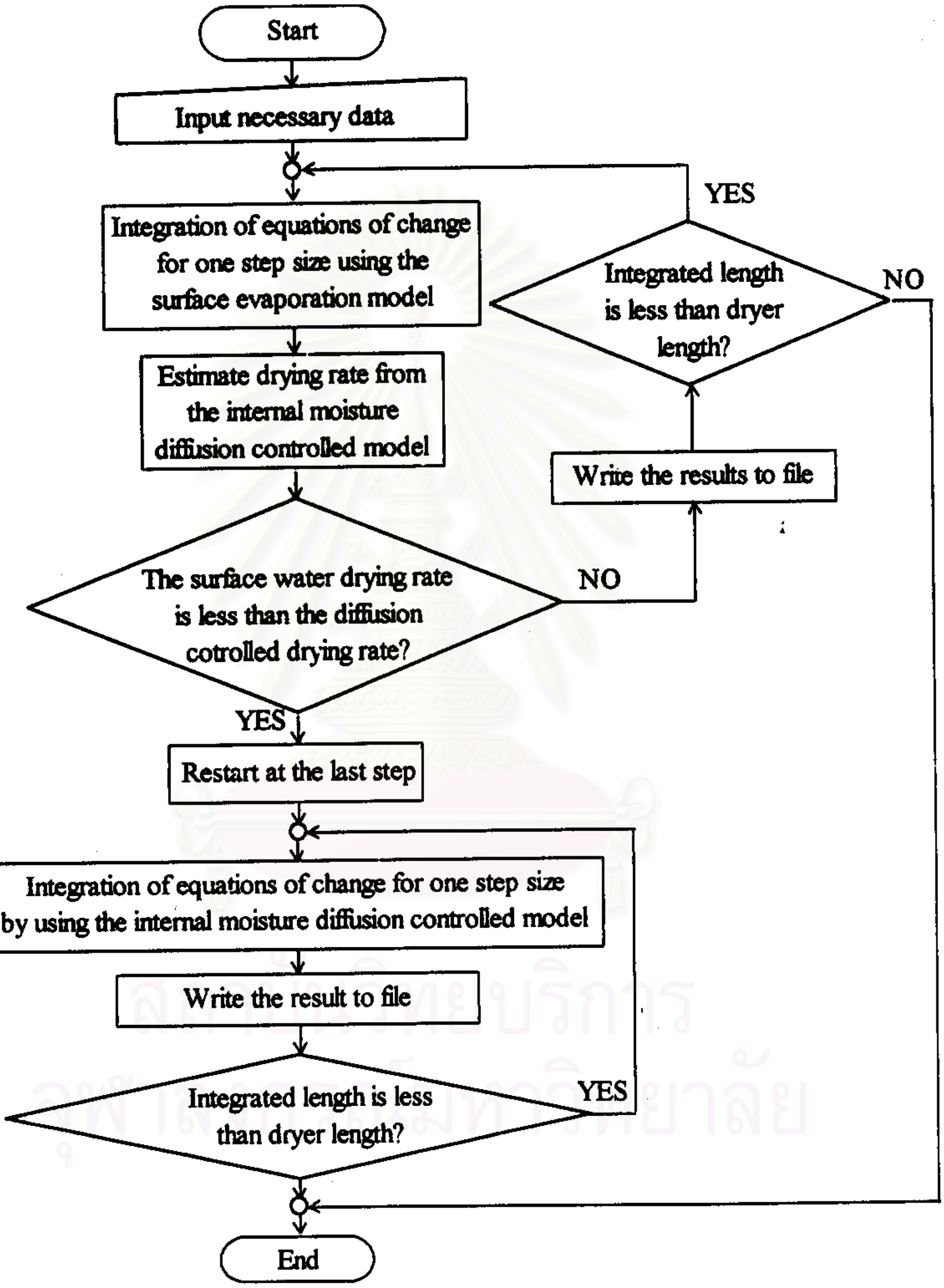

Figure 4.5 Simplified flow chart of the present model