CHAPTER 3

MATHEMATICAL MODELING

3.1 Mathematical Model

To understand and expect the performance of desiccant dehumidifier wheels for given operating conditions, lots of work on simulation need to be carried out. Such work requires methods that allow rapid and accurate evaluation of the investigating results. Many mathematical models on the desiccant dehumidifier wheels (cyclic and non-cyclic) have been proposed in the past decades. One of the pitfalls in the earlier mathematical models was the coefficient of mass transfer which does not consider the non-stationary of the processed air. Also, most of the proposed models were created based on the sensible heat and ignored the latent heat and this was a big reason of mismatching between the estimated values by these models and the experimental results. In the mathematical model of the current investigation, both of latent and sensible heats were considered. Besides, the mass transfer coefficient is augmented with a new proposed parameter. This parameter is an optimized function of the speed of processed air flow and its mass flow rate inside the channels of the stationary desiccant wheel as will be explained in details later.

As the dehumidification/regeneration process is a coupled mass and heat transfer between the moist air and the desiccant beds, the current model which is described in details in the next section depends on the two the principles of conservations (mass conservation and energy conservation).

3.2 Physical Description and Coordinate System

For simplicity and consistency with the below listed assumptions, the channel is assumed to be of cylindrical shape shown in Figure 3.1. This figure shows two cross sectional views of desiccant wheel channel which is shaped from the desiccant wheel wall, desiccant substrate material layer and the air stream channel.

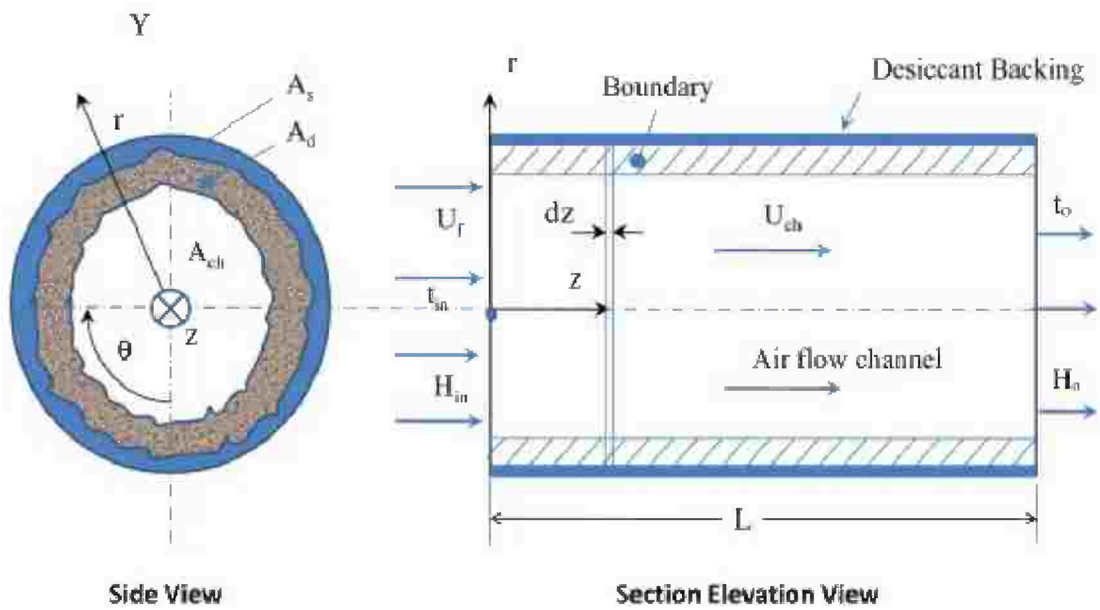

Figure 3.1 Physical Descriptions and Coordinate System of the Problem

In Figure 3.1, the axis "z" is along the desiccant wheel thickness, while the radius "r" is perpendicular to the air flow. The nomenclatures listed on the figure are as follows;

- U_f refers to the velocity of the processed air at the face of desiccant wheel.
- U_{ch} refers to the velocity of the processed air inside the channel of the desiccant wheel.
- H_{in} refers to the humidity ratio of the air entering the desiccant
- t_i is the temperature of the air flowing into the desiccant wheel
- t_o is the temperature of the air flowing out of the desiccant wheel
- H_o refers to the humidity ratio of the air getting out of the channel
- A_s refers to the cross section area of the substrate material
- A_d refers to the cross section area of the desiccant material
- A_{ch} refers to the cross section area of the channel, where the air flows.
- dz is the length of the incremental element of the desiccant channel through which the energy and mass balance equations are applied

The desiccant wheel described by the model is stationary as the dehumidified air is passing through till it gets saturated, then a regeneration process takes place. Thus the current model is describing non-cyclic dehumidification process as discussed in chapter 2. The current model describes the performance of the desiccant wheel after the decay of the unsteady variation period following the desiccant regeneration process.

3.3 Mathematical Model Assumptions

For the purpose of simplification, the following assumptions are made along desiccant channel

- One dimension approach is applied.
- Heat conduction and diffusion flux are neglected.
- Effect of centrifugal force is neglected as the desiccant wheel is considered stationary.
- No leakage takes place between dehumidification and regeneration sections.
- No pressure loss along the wheel thickness.
- Desiccant is uniformly distributed in the matrix. The desiccant passage is considered homogenous.
- The properties of air stream are assumed to be uniform.

3.4 Mass and Energy Balance Equations

The two governing equations of the studied model are the equation of mass conservation and the equation of the conservation of energy. The conservation of mass equation which represents the mass of water to be transferred between the processed air and the desiccant bed is written down as

$$G_{ch}\left(\frac{\partial H}{\partial z}\right)+\epsilon_d\rho_d\zeta\left(\frac{\partial w}{\partial \tau}\right)+\rho_a\left(\frac{\partial H}{\partial \tau}\right)=0 \tag{3.1}$$

Where;

$$G_{ch}=\frac{\dot{m}_a}{A_{ch}}$$

$\dot{m}_a$ is the air mass flow rate per desiccant channel area

and $\epsilon_d=\frac{A_d}{A_{ch}}$

ρ_d is the desiccant density

ζ represents the filling factor. This factor defines the ratio of the actual desiccant material volume to the apparent geometrical volume. According to Reference [24], ζ is 0.72.

The terms of the above equation describe the water exchanged by the moist air passing along the incremental element (dz) and the adjacent desiccant. This exchange takes place during the incremental time (dτ). This incremental time $d\tau = dz/U_{ch}$. The first term in the above equation "$G_{ch}\left(\frac{\partial H}{\partial z}\right)$" represents the water exchanged by the moist air passing through the element dz as shown in Figure 3.1. while the moist air flows along the incremental element dz, the change in water content in the desiccant bed during the incremental time dτ is represented by the second term “$\epsilon_d \rho_d \zeta \left(\frac{\partial w}{\partial \tau}\right)$”. The third term “$\rho_a \left(\frac{\partial H}{\partial \tau}\right)$” is the unsteady variation in air water content of the moist air with time.

The general form of energy balance for the passage element is

$$G_{ch}\left(\frac{\partial i_a}{\partial z}\right) + \epsilon_d \rho_d \zeta \left(\frac{\partial i_d}{\partial \tau}\right) + \rho_a \left(\frac{\partial i_a}{\partial \tau}\right) + q_z = 0 \tag{3.2}$$

The first term “$G_{ch}\left(\frac{\partial i_a}{\partial z}\right)$”in the above equation represents the change in the energy of the moist air as the air flows along the incremental element dz of the desiccant wheel. The second term “$\epsilon_d \rho_d \zeta \left(\frac{\partial i_d}{\partial \tau}\right)$” expresses the change in the energy of the desiccant bed along the incremental element dz during the incremental time dτ. The third term “$\rho_a \left(\frac{\partial i_a}{\partial \tau}\right)$” represents the unsteady variation in the energy of the moist air with time. The last term represents the rate of specific energy transfer through the boundary.

The governing equations are used to describe the desiccant performance after the diminishing of the unsteady variation (mass and energy) period. This period lasts for several minutes after the regeneration process. Thus the modified form of the conservation of mass equation after truncating the third term which represents the unsteady variation in air water content, will be

$$G_{ch}\left(\frac{dH}{dz}\right) + \epsilon_d \rho_d \, \zeta \left(\frac{dW}{d\tau}\right) = 0 \tag{3.3}$$

Then
$$G_{ch}\left(\frac{dH}{dz}\right) = -\epsilon_d \rho_d \, \zeta \left(\frac{dW}{d\tau}\right) \tag{3.4}$$

The left hand side of the above equation can be represented as

$$G_{ch}\left(\frac{dH}{dz}\right) = K_m f_c \left(H_{eq} - H\right) \tag{3.5}$$

$$\left(\frac{dH}{dz}\right) = \frac{K_m f_c}{G_{ch}}\left(H_{eq} - H\right) \tag{3.6}$$

Where;

$$f_c = \frac{4\sigma}{D_h}$$

K_m represents the coefficient of mass transfer between the processed air and the adjacent desiccant bed. This coefficient stands for diffusion within the adsorbent material and from its surface to the air flow.

H_{eq} is the Humidity ratio of the hypothetical layer of air next to the desiccant subjected area as shown in Figure 3.2.

σ Represents the contact ratio between the processed air and the adjacent desiccant bed

D_h is the hydraulic diameter (D_h = 4 A_{ch}/wetted perimeter of desiccant channel)

The R.H.S of Equation 3.4 can also be written as

$$-\epsilon_d \rho_d \, \zeta \left(\frac{dW}{d\tau}\right) = K_m f_c (H_{eq} - H) \tag{3.7}$$

$$\left(\frac{dW}{d\tau}\right) = \frac{K_m f_c}{\epsilon_d \rho_d \, \zeta} (H - H_{eq}) \tag{3.8}$$

Similarly; the third term in Equation 3.2 will be neglected as it represents the unsteady variation in the energy exchange between the processed air and the desiccant. Thus the modified form of this equation will be:

$$G_{ch} \left(\frac{\partial i_a}{\partial z}\right) + \epsilon_d \rho_d \zeta \left(\frac{\partial i_d}{\partial \tau}\right) + q_z = 0 \tag{3.9}$$

$$\epsilon_d \rho_d \zeta \left(\frac{\partial i_d}{\partial \tau}\right) = -G_{ch} \left(\frac{\partial i_a}{\partial z}\right) - q_z \tag{3.10}$$

Recall that the rate of heat transfer through the boundary "q_z" can be written as

$$q_z = Q_{ads} \left(\frac{\partial H}{\partial z}\right) \tag{3.11}$$

The heat of adsorption "Q_{ads}" is the sum of the heat of wetting and the latent heat of vaporization of water as shown below

$$Q_{ads} = h_w + L_T \tag{3.12}$$

Where;

h_w is the heat of wetting, i.e. the heat to be released by the desiccant material when it gets wet (J/Kg).

L_T is the latent heat of water vaporization. In other words, it the heat released when the water is adsorbed by the desiccant material (J/Kg).

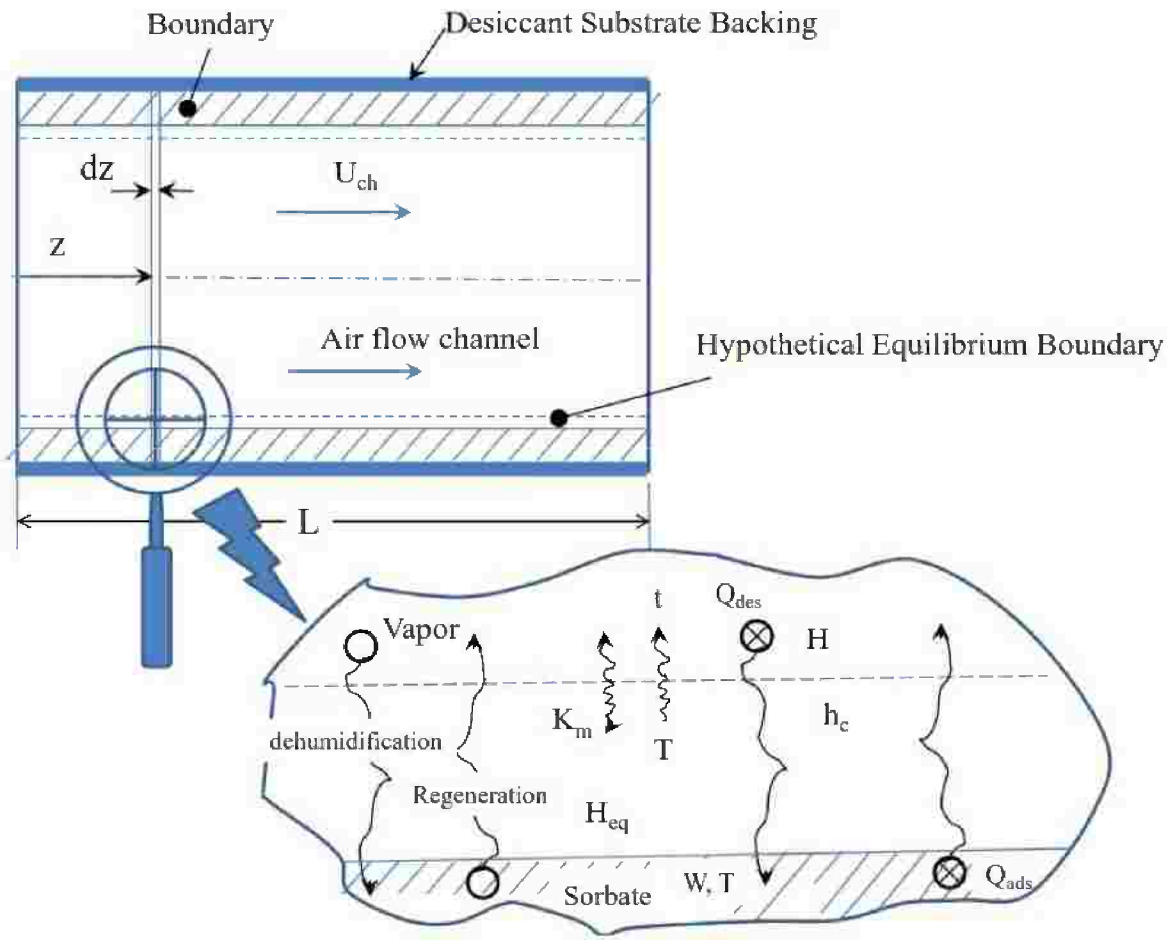

Figure 3.2 Zoomed in View of Hypothetical Layer of Air Next to Desiccant Bed

The analogy between the heat and mass transfer is obvious as the similarity between Equation 3.7 and the following equation is clear, where

$$G_{ch}\left(\frac{\partial i_a}{\partial z}\right) = h_c f_c (T - t) \tag{3.13}$$

Where;

h_c is the convective heat transfer coefficient which equals 44.6 W/m^2.K, Reference [9].

T is the temperature of the hypothetical layer shown in Figure 3.2.

t is the temperature of the dehumidified air.

i_a is the enthalpy of the moist air, where

$$i_a = C_a\, t \tag{3.14}$$

C_a is the mean specific heat of the moist air, which equals

$$C_a = C_{a,d} + C_{w,v}\, H \tag{3.15}$$

$C_{a,d}$ is the specific heat of the dry air

$C_{w,v}$ is the specific heat of the water vapor

Substituting Equation 3.15 into 3.14, we get the following

$$i_a = C_{a,d}\, t + C_{w,v}\, H\, t \tag{3.16}$$

Notice that the first term in the above equation represents the enthalpy of the dry air (the sensible heat). The second term represents the enthalpy of the evaporated water (the latent heat). Substituting with 3.14 into Equation 3.13 and performing some mathematical manipulations, we end up with the following equation.

$$\left(\frac{dt}{dz}\right) = \frac{h_c f_c}{G_{ch} C_a}(T - t) + \frac{K_m f_c C_{W,v}}{G_{ch} C_a} t\left(H - H_{eq}\right) \tag{3.17}$$

The following equation shows the relation between the specific enthalpy of desiccant and its temperature.

$$i_d = C_{b,m} T \tag{3.18}$$

and
$$C_{b,m} = (C_{d,d} + C_{w,L} W + \frac{\rho_s \epsilon_s}{\rho_d \epsilon_d} C_s) \tag{3.19}$$

Where;

$C_{b,m}$ is the mean specific heat of desiccant bed

$C_{d,d}$ is the specific heat of dry desiccant

$C_{W,L}$ is the specific heat of water liquid

C_s is the specific heat of substrate material

ρ_s is the density of the substrate material

$\epsilon_s = \frac{A_s}{A_{ch}}$

Then;

$$i_d = (C_{d,d} + C_{w,L} W + \frac{\rho_s \epsilon_s}{\rho_d \epsilon_d} C_s) T \tag{3.20}$$

Substituting with equations 3.11, 3.13, and 3.18 back into equation 3.10 and we get the following

$$\epsilon_d \rho_d \zeta \frac{\partial}{\partial \tau}\left(C_{b,m} T\right) = -h_c f_c (T - t) - Q_{ads}\left(\frac{\partial H}{\partial z}\right) \tag{3.21}$$

After performing the derivative in the L.H.S. of the above equation and some mathematical manipulation, we end up with

$$\frac{dT}{d\tau} = \frac{-h_c f_c}{\epsilon_d \rho_d \zeta C_{b,m}}(T - t) - \frac{C_{w,L}}{C_{b,m}} T \frac{\partial W}{\partial \tau} - \frac{Q_{ads}}{\epsilon_d \rho_d \zeta C_{b,m}}\left(\frac{\partial H}{\partial z}\right) \tag{3.22}$$

Using equations 3.6 and 3.8 in the above equation, the equation will have the following form

$$\frac{dT}{d\tau} = \frac{-h_c f_c}{\epsilon_d \rho_d \zeta C_{b,m}}(T - t) - \frac{K_m f_c C_{w,L}}{\epsilon_d \rho_d \, \zeta C_{b,m}} T\left(H - H_{eq}\right) - \frac{K_m f_c Q_{ads}}{G_{ch} \epsilon_d \rho_d \zeta C_{b,m}}\left(H_{eq} - H\right) \tag{3.23}$$

or

$$\frac{dT}{d\tau} = \frac{K_m f_c Q_{ads}}{G_{ch} \epsilon_d \rho_d \zeta C_{b,m}}\left(H - H_{eq}\right) - \frac{h_c f_c}{\epsilon_d \rho_d \zeta C_{b,m}}(T - t) - \frac{K_m f_c C_{w,L}}{\epsilon_d \rho_d \, \zeta C_{b,m}} T\left(H - H_{eq}\right) \tag{3.24}$$

As one can see; the dehumidification process can be mathematically modeled by a set of four ordinary first degree differential equations (Equations 3.6, 3.8, 3.17 and 3.24). These equations are coupled and require two boundary and two initial conditions to be solved. The incremental distance is related to the incremental time through the speed of moist air stream inside the desiccant wheel channels $d\tau = dz / U_{ch}$. For simplicity the following parameters (K_i's, where i=1:7) are used, where

$$K_1 = \frac{K_m f_c}{G_{ch}} \tag{3.25}$$

$$K_2 = \frac{K_m f_c}{\epsilon_d \rho_d \, \zeta} \tag{3.26}$$

$$K_3 = \frac{h_c f_c}{G_{ch} C_a} \tag{3.27}$$

$$K_4 = \frac{K_m f_c C_{W,v}}{G_{ch} C_a} \tag{3.28}$$

$$K_5 = \frac{K_m f_c Q_{ads}}{G_{ch} \epsilon_d \rho_d \zeta C_{b,m}} \tag{3.29}$$

$$K_6 = \frac{h_c f_c}{\epsilon_d \rho_d \zeta C_{b,m}} \tag{3.30}$$

$$K_7 = \frac{K_m f_c C_{w,L}}{\epsilon_d \rho_d \, \zeta C_{b,m}} \tag{3.31}$$

Thus; the governing equations in their short form are listed down as follow

$$\frac{dH}{dz} = K_1(H_{eq} - H) \tag{3.32}$$

$$\left(\frac{dW}{d\tau}\right) = K_2(H - H_{eq}) \tag{3.33}$$

$$\left(\frac{dt}{dz}\right) = K_3(T - t) + K_4 t(H - H_{eq}) \tag{3.34}$$

$$\frac{dT}{d\tau} = K_5(H - H_{eq}) - K_6(T - t) - K_7 T(H - H_{eq}) \tag{3.35}$$

3.5 Numerical Technique

The governing equations of the coupled mass and heat transfer are casted into state form as listed down in Equations 3.29 to 3.32. The Runge-Kutta 4th order method is used to implement the integration process. This technique is a robust numerical integration methodology which is effectively used to solve highly coupled ordinary/partially differential equations. This method was first developed by the German mathematicians C.D.T. Runge and M.W. Kutta in the latter half of the nineteenth century [43]. Notice that, an nth-order Runge-Kutta method requires n evaluations of this function per step. It can easily be appreciated that as n is increased a point is quickly reached beyond which any benefits associated with the increased accuracy of a higher order method more than offset by the computational "cost" are involved in the necessary additional evaluation of the function per step. In most situations of interest a fourth-order Runge-Kutta integration method, where n = 4, represents an appropriate compromise between the competing requirements of a low truncation error per step and a low computational cost per step.

To reach to the general form of the 4th order Runge-Kutta, we start with the Taylor expansion of a general first order differential equation $dy/dx = f(x, y)$. At the end, we reach the following equation, where the dependent variable at step "i+1" y_{i+1} can be evaluated if its value at the previous step y_i is known beside the selected incremental value of the dependent variable x.

$$y_{i+1} = y_i + \frac{dy}{dx}\Big|_{x_i, y_i}(x_{i+1} - x_i) + \frac{1}{2!}\frac{d^2y}{dx^2}\Big|_{x_i, y_i}(x_{i+1} - x_i)^2 + \frac{1}{3!}\frac{d^3y}{dx^3}\Big|_{x_i, y_i}(x_{i+1} - x_i) + \frac{1}{4!}\frac{d^4y}{dx^4}\Big|_{x_i, y_i}(x_{i+1} - x_i)^4 \quad (3.36)$$

Or

$$y_{i+1} = y_i + f(x_i, y_i)h + \frac{1}{2!} f^{'}(x_i, y_i)h^2 + \frac{1}{3!} f^{''}(x_i, y_i)h^3 + \frac{1}{4!} f^{'''}(x_i, y_i)h^4 \quad (3.37)$$

Where;

$$h = x_{i+1} - x_i$$

The short form of Runge-Kutta is

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h \quad (3.38)$$

$$k_1 = f(x_i, y_i) \quad (3.39a)$$

$$k_2 = f\left(x_i + \frac{h}{2}, y_i + k_1\frac{h}{2}\right) \quad (3.39b)$$

$$k_3 = f\left(x_i + \frac{h}{2}, y_i + k_2\frac{h}{2}\right) \quad (3.39c)$$

$$k_4 = f(x_i + h, y_i + k_3h) \quad (3.39d)$$

In the current study, the increment dz in the coupled differential Equations 3.32 to 3.35 listed above is replaced with dτ. This change helps out in creating the functions f_i's which represent the first derivative of each of the variables (*H, W, t, T*) with the time. As our mathematical model is composed of four differential equations, the general form of the first derivative of any of the four variables is

$$\frac{dy_j}{d\tau} = f_j(y_1, y_2, ..., y_n),\ j = 1:n \quad (3.40)$$

Where; n represents the number of variables.

In the current model, the variables are defined as

- y_1 is the air humidity ratio "*H*"
- y_2 is the water content in desiccant "*W*"
- y_3 is the dry bulb temperature of the air "*t*"
- y_4 is the temperature of the desiccant "*T*"

The independent variable x in the current case is the time τ which is implicitly existing in the f_j's functions. The suitable incremental time is iteratively selected such that the computation process will converge quickly with acceptable errors between the predicted values of the four variables and those experimentally measured. The results of four experiments conducted by A. Abdou [19] are employed for enhancing the proposed model, while the fifth experiment is used for validation purpose. The variables recorded in the experiment during the unsteady variation of the variables are truncated and we considered those of the steady variations. These results are listed in appendix A. The initial and boundary values are the variables recorded at the beginning of the steady variation stage. These values are listed down in Table 3.1. The results of the numerical solution, the augmentation parameters and the discussions are discussed in details in the next chapter.

Table 3.1 The Initial and Boundary Conditions of the Four Differential Equations

Experiment No. / Initial Value	(1)	(2)	(3)	(4)	(5)
H **(kg/kg)**	0.0096	0.0088	0.0091	0.0094	0.0098
W **(kg/kg)**	0.173614	0.1453 12	0.1542345	0.172141	0.1645873
t **(°C)**	26.9	28.5	28	26.7	28.1
T **(°C)**	26.9	28.5	28	26.7	28.1