5.1. INTRODUCTION TO MODELLING

Mathematical model represents all the important features of the system for the purpose of deriving the mathematical equations governing behavior of the system. This chapter describes simple mathematical models for the preliminary design of an air dehumidification and regeneration process occurring in a structured packing used in liquid desiccant cooling system. Considering a simple control volumes of dehumidifier and regenerator, mass and energy balance equations for air and desiccant solution have been obtained for both the components of liquid desiccant system. These equations are non-linear coupled first order differential equations and have to be solved simultaneously. Analytically closed form of solution of these equations is not possible. Thus these equations are solved numerically by dividing the absorber/regenerator into a large number of steps. For the given inlet information at inlet of step (solution, air temperature, mass flow rates, air humidity, solution concentration), the outlet conditions will be obtained assuming constant properties and heat & mass transfer coefficients within that step. Step by step calculations is carried out from top to bottom of the absorber/regenerator with appropriate step size depending upon the required accuracy.

The governing mass and energy balance equations have been used for the simulation of the absorber and regenerator using Warner technique. FORTRAN 77 computer language has been used for coding of the simulation. Performance measures of dehumidifier in terms of dehumidification of air in the absorber and evaporation of water in the regenerator have been studied for both main components.

5.2. MODELING OF ABSORBER

Schematic diagram of an air dehumidification system with the liquid desiccant is given in figure 5.1. A honeycomb celdek packing is used in dehumidifier in the
present work. Strong desiccant solution flows in downward direction through celdek packing and air flows in upward direction through the packing.

Figure 5.1 Simplified schematic diagram of the absorber

A small element of thickness dX at distance X from the top of the absorber as shown in figure 5.2 is considered for deriving the mass and energy balance equation. ω_a and H_a are the specific humidity and specific enthalpy of the air respectively and \( \dot{m}_s \), C_s and H_s are the mass flow rate, desiccant concentration and specific enthalpy respectively of the desiccant considered at top of the element. ω_a+dω_a, H_a+dH_a, \( \dot{m}_s+d\dot{m}_s \), C_s+dC_s and H_s+dH_s are the corresponding properties at bottom of the element, which is after thickness dX from top of the element. The counter flow of the air and desiccant solution is also shown in the element.

Applying the fundamental mass and energy balance across the element, governing differential equations have been obtained for the air and desiccant solution with following assumptions:

1. The system is operating in a steady state mode.
2. Only moisture is transferred between the air and the desiccant.
3. Desiccant-air contact area is taken equal to packing area.
4. The thickness of the desiccant falling film is very small.
5. The absorber/regenerator is divided into large number of steps to simulate it. The properties of the air and desiccant are assumed to be constant within the step.
6. During absorption of moisture of the air in the absorber the latent heat of condensation is transferred to the desiccant film and in case of regenerator, the latent heat is taken from the desiccant film.

![Figure 5.2 Control volume of the absorber](image)

**5.2.1. Mass Balance Equation for Moisture in Air**

Moisture present in the air leaving the control volume = Moisture present in the air entering the control volume - moisture relieved by the air due to mass transfer from air to liquid

\[
\dot{m}_a \omega_a = \dot{m}_a (\omega_a + d\omega_a) - K \dot{P}_a dX (\omega_a - \omega_{eq})
\]

\[
\frac{d\omega_a}{dX} = K \dot{P}_a (\omega_a - \omega_{eq}) \tag{5.1}
\]
5.2.2. Mass Balance Equation for Water in Solution

Mass of water in liquid desiccant leaving the control volume = Mass of water in liquid desiccant entering the control volume + Mass of water removed from the air due to mass transfer to desiccant solution

\[(\dot{m}_w + d\dot{m}_w)(1 - C_w + dC_w) = \dot{m}_w (1 - C_w) + KP_a dX (\omega_a - \omega_{eq})\]

\[\dot{m}_w (1 - C_w) + \dot{m}_w dC_w + d\dot{m}_w (1 - C_w) + d\dot{m}_w dC_w = \dot{m}_w (1 - C_w) + KP_a dX (\omega_a - \omega_{eq})\]

Neglecting second order derivatives, we have

\[\dot{m}_w dC_w + d\dot{m}_w (1 - C_w) = KP_a dX (\omega_a - \omega_{eq})\]

\[\frac{d\dot{m}_w (1 - C_w)}{dX} = KP_a dX (\omega_a - \omega_{eq}) \quad (5.2)\]

5.2.3. Energy Balance Equation for Air

Total enthalpy of the air leaving the control volume = Total enthalpy of the air entering the control volume + increase in energy of the air due to mass transfer from liquid desiccant to air + increase in enthalpy of the air due to heat transfer from liquid desiccant to air

\[\dot{m}_a \quad H_a = \dot{m}_a \quad (H_a + dH_a) + H_{fg} KP_a dX (\omega_{eq} - \omega_a) + U_{as} P_a dX (T_a - T_a)\]

\[\dot{m}_a \quad dH_a = H_{fg} KP_a dX (\omega_a - \omega_{eq}) + U_{as} P_a dX (T_a - T_s)\]

\[\dot{m}_a \quad (C_{p_a} dT_a + d\omega_a H_{fg}) = H_{fg} KP_a dX (\omega_a - \omega_{eq}) + U_{as} P_a dX (T_a - T_s)\]

\[\dot{m}_a \quad (C_{p_m} dT_a) + \dot{m}_a dW_a H_{fg} = H_{fg} KP_a dX (\omega_a - \omega_{eq}) + U_{as} P_a dX (T_a - T_s)\]

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Neglecting higher derivative, we have

\[ \dot{m}_a C_{pm} \frac{dT_a}{dX} = U_a s_\alpha P_a (T_a - T_s) \]  

(5.3)

### 5.2.4. Energy Balance Equation for Desiccant

Total enthalpy of the liquid desiccant solution leaving the control volume =

Total enthalpy of the liquid desiccant solution entering the control volume + increase in energy of the liquid desiccant solution due to mass transfer from the air to liquid desiccant + increase in energy of the liquid desiccant solution due to heat transfer from air to liquid desiccant

\[
(\dot{m}_s + d\dot{m}_s)(H_s + dH_s) = \dot{m}_s H_s + H_{f,g} P_a dX (\omega_a - \omega_{eq}) + U_a s_\alpha dX (T_a - T_s)
\]

Neglecting second order derivatives, we have

\[
\dot{m}_s \frac{dH_s + d\dot{m}_s H_s}{dX} = H_{f,g} K P_a dX (\omega_a - \omega_{eq}) + U_a s_\alpha dX (T_a - T_s)
\]

\[
\frac{d(\dot{m}_s H_s)}{dX} = H_{f,g} K P_a (\omega_a - \omega_{eq}) + U_a s_\alpha P_a (T_a - T_s)
\]

(5.4)

Where \( \omega_{eq} \) is moisture contents of air in equilibrium with water vapour pressure \( (P_{eq}) \) of desiccant solution at the given concentration and temperature as given below.

\[
\omega_{eq} = 0.62 \frac{P_{eq}}{P_{atm} - P_{eq}}
\]

(5.5)

The equations are non-linear coupled first order differential equations and have to be solved simultaneously.
5.3. MODELING OF REGENERATOR

In regenerator, the desiccant solution is heated and it gets regenerated by releasing its moisture to the air. Schematic diagram of the regenerator with liquid desiccant is shown in figure 5.3. A honeycombCeldek packing has been used in the regenerator in present work. Weak desiccant solution flows in downward direction and air flows in upward direction through the packing.

![Simplified schematic diagram of the regenerator](image)

**Figure 5.3** Simplified schematic diagram of the regenerator

A small element of thickness dX at distance X from the top of the regenerator as shown in figure 5.4 is considered for deriving the mass and energy balance equation. Mass and energy balance equations for the regeneration process are derived considering the assumptions similar to the dehumidification process.
5.3.1. Mass Balance Equation for Moisture in Air

Moisture present in the air leaving the control volume = Moisture present in the air entering the control volume + moisture added to the air due to mass transfer from liquid desiccant to air

\( \dot{m}_a \omega_a = \dot{m}_a \left( \omega_a + d\omega_a \right) + K P_a dX \left( \omega_{eq} - \omega_a \right) \)

\( \dot{m}_a \frac{d\omega_a}{dX} = K P_a \left( \omega_{eq} - \omega_a \right) \) \hspace{1cm} (5.6)

5.3.2. Mass Balance Equation for Water in Solution

Mass of water in liquid desiccant leaving the control volume = Mass of water in liquid desiccant entering the control volume - Mass of water removed from the solution due to mass transfer from desiccant solution to the air

\( (\dot{m}_a + d\dot{m}_s)(1 - C_s + dC_s) = \dot{m}_s (1 - C_s) - K P_a dX \left( \omega_{eq} - \omega_s \right) \)
Neglecting second order derivatives, we have

\[ \dot{m}_s (1 - C_s) + \dot{m}_s dC_s + d\dot{m}_s (1 - C_s) + d\dot{m}_s dC_s = \dot{m}_s (1 - C_s) + KP_a dX (\omega_{eq} - \omega_a) \]

5.3.3. Energy Balance Equation for Air

Total enthalpy of the air leaving the control volume = Total enthalpy of the air entering the control volume + increase in energy of the air due to mass transfer from liquid solution to air + increase in enthalpy of the air due to heat transfer from liquid solution to air

\[ \dot{m}_a \ H_a = \dot{m}_a (H_a + dH_a) + H_{fa} KP_a dX (\omega_a - \omega_{eq}) + U_{as} P_a dX (T_a - T_s) \]
\[ \dot{m}_a dH_a = H_{fa} KP_a dX (\omega_{eq} - \omega_a) + U_{as} P_a dX (T_a - T_s) \]
\[ \dot{m}_a (C_{pm} dT_a + d\omega_a H_{fa}) = H_{fa} KP_a dX (\omega_{eq} - \omega_a) + U_{as} P_a dX (T_s - T_a) \]
\[ \dot{m}_a (C_{pm} dT_a) + \dot{m}_a dW_a H_{fg} = H_{fg} KP_a dX (\omega_{eq} - \omega_a) + U_{as} P_a dX (T_s - T_a) \]
\[ \dot{m}_a C_{pm} \frac{dT_a}{dX} = U_{as} P_a (T_s - T_a) \] (5.8)

5.3.4. Energy Balance Equation for Desiccant

Total enthalpy of the liquid desiccant solution leaving the control volume = Total enthalpy of the liquid desiccant solution entering the control volume - decrease in energy of the liquid desiccant solution due to mass transfer from the liquid
desiccant to air - decrease in energy of the liquid desiccant solution due to heat transfer from liquid desiccant to air

\[
(\dot{m}_s + d\dot{m}_s)(H_s + dH_s) = \dot{m}_s H_s - H_f g K P_a dX (\omega_a - \omega_{eq}) - U_{as} P_a dX (T_a - T_s)
\]

\[
\dot{m}_s H_s + \dot{m}_s dH_s + d\dot{m}_s H_s + d\dot{m}_s dH_s = \dot{m}_s H_s + H_f g K P_a dX (\omega_{eq} - \omega_a) + U_{as} P_a dX (T_a - T_s)
\]

\[
\dot{m}_s dH_s + d\dot{m}_s H_s = H_f g K P_a dX (\omega_{eq} - \omega_a) + U_{as} P_a dX (T_s - T_a)
\]

\[
\frac{d(\dot{m}_s H_s)}{dX} = H_f g K P_a (\omega_{eq} - \omega_a) + U_{as} P_a (T_s - T_a)
\]

\[ (5.9) \]

5.4. SIMULATION PROCEDURE

A detailed analysis of actual operation of the absorber and the regenerator has been done to study the corresponding outlet and performance parameters. The absorber/regenerator is divided into \( n \) number of steps each and at each step finite difference method is applied to solve the governing differential equations of the mass and energy balance for air and desiccant solution. Various needed parameters of the interest are temperatures of air and solution, specific humidity and concentration of solution at the bottom of each step. Direction of flow of the air and solution is counter flow in both the main components. Adiabatic conditions have been assumed for both the main components. This detailed simulation has been carried out at one typical set of inlet conditions of air and solution from experimental observations.

The inlet data required for the simulation are the geometrical data of the absorber and the regenerator, mass flow rate and inlet temperature of solution, mass flow rate and the inlet conditions of air. In view of the counter flowing fluids in the absorber and the regenerator, values of number of variables have to be assumed to start the simulation procedure. Followings variables are required in the simulation of the absorber and regenerator:
(1) Mass flow rate of the air in the absorber/regenerator ($\dot{m}_a$)
(2) Dry bulb temperature of air at inlet of absorber/regenerator (DBT$_i$)
(3) Wet bulb temperature of air at inlet of absorber/regenerator (WBT$_i$)
(4) Mass flow rate of desiccant solution in the absorber/regenerator ($\dot{m}_s$)
(5) Temperature of solution at inlet of the absorber/regenerator (T$_{si}$)
(6) Concentration of desiccant solution at inlet of the absorber/regenerator (C$_{si}$)
(7) Dry bulb temperature of air leaving the absorber/regenerator (DBT$_o$)
(8) Specific humidity of air leaving the absorber/regenerator ($\omega_o$)
(9) Length of the absorber/regenerator (L)
(10) Number of steps from top to bottom of the absorber/regenerator (n)

Iterations are done in n number of steps for entire length from top to bottom of the absorber/regenerator. Although desiccant inlet parameters are known at top of absorber and air inlet parameters are known at bottom of the absorber/regenerator. So the input data required for the first element of thickness dX at top of the absorber/regenerator which is top of the first element is known partially, which are temperature, flow rate and concentration of the desiccant solution. Guess values of the unknown input data; dry bulb temperature and specific humidity of the air provided for calculations at the first element. Fourth order Runge-Kutta method has been applied to solve the governing differential equations for the element and output data corresponding to input data is obtained at bottom of the element. This way output data at bottom of the first element will be input data at top of the second element.

Then calculations for second step are done and proceed to bottom of the absorber/regenerator with onwards step by step calculations. This way the output data is obtained at bottom of the absorber/regenerator, which provides specific humidity and dry bulb temperature to compare with known values from inlet condition of the air. The residuals are used by the technique to improve the guess values for next iteration again from top to bottom of the absorber/regenerator. This way, with number of iterations bring residuals of comparison of specific humidity and dry bulb temperature to a minimum value, hence true output variables are attained by the simulation.
Graphical representations in figures 5.5-5.11 show the gradual change in the process parameters of the air and desiccant solution after convergence with minimum residuals.

5.5. SIMULATION OF ABSORBER

For the case of absorber, typical experimental data selected for the study are $\dot{m}_a = 0.024 \text{ kg/s}$, DBT$_i = 37.3^\circ\text{C}$, WBT$_i = 27.3^\circ\text{C}$, $m_{si} = 0.056 \text{ kg/s}$, T$_{si} = 34.5^\circ\text{C}$, $C_{si} = 36.42\%$. The predicted values of various parameters have been plotted in figures 5.5 - 5.7 from top to bottom, with X = 0 representing the top of the absorber.

Predicted variation of specific humidity along the length of absorber is presented in the figure 5.5. The specific humidity of the air is decreasing from bottom to top of the absorber which caused due to release of moisture from air toward desiccant because of vapour pressure difference between the air and desiccant solution.

![Graph](image)

**Figure 5.5** Variation of specific humidity along length from top to bottom of the absorber
Figure 5.6 represents the variation of predicted temperature of air and desiccant solution with respect to the length of absorber. Temperature of solution is increased when it passes from top to bottom of the absorber. Increase in temperature of desiccant solution is due to release of condensation heat during dehumidification of air. Figure 5.7 shows the variation of the concentration of desiccant along the length of the absorber. Concentration of desiccant solution continues to decrease during dehumidification as it passes from top to bottom of the absorber due to transfer of moisture from air to desiccant solution.

Figure 5.6 Variation of temperature of solution along length from top to bottom of the absorber
5.6. SIMULATION OF REGENERATOR

Simulations have also been carried out for the regenerator by dividing its length into $n=100$ equal steps. Again for purpose of simulation, typical experimental data have been selected ($\dot{m}_a = 0.0359 \text{ kg/s}$, DBT$_i = 40.5.6^\circ\text{C}$, WBT$_i = 31.7^\circ\text{C}$, $\dot{m}_{si} = 0.07 \text{ kg/s}$, $T_{si} = 45.5^\circ\text{C}$, $C_{si} = 35.25\%$). The predicted values of various important parameters along the lengths of the regenerator are plotted in figures 5.8 – 5.10 to understand the phenomenon occurring in the regenerator. Predicted variation in the specific humidity along the length of regenerator is shown in the figure 5.8. The specific humidity of the air is increasing from top to which is due to transfer of moisture from water present in desiccant solution to the air.
Figure 5.8 Variation of specific humidity along the length from top to bottom of the regenerator

Figure 5.9 Variation of temperature of the air along the length from top to bottom of the regenerator
Figure 5.10 Variation of temperature of desiccant solution along the length from top to bottom of the regenerator

Figure 5.11 Variation of desiccant concentration along the length from top to bottom of the regenerator
Figures 5.9 represents the variation of predicted temperature of the air along the length of the regenerator. It has been observed from the graph that temperature of air is increased during regeneration process when air is passed from bottom to top of the regenerator. Increase in temperature of the air is due to the heat transfer from the solution. Figure 5.10 explains the variations of solution temperature along length of the regenerator. Temperature of solution is decreased when it passes from top to bottom in the regenerator. Figure 5.11 presents the effect of concentration of desiccant along the length of the regenerator. Concentration of desiccant solution is increasing from top to bottom of the regenerator due to release of moisture from desiccant solution to the air.

5.7. COMPARISON OF PREDICTED AND EXPERIMENTAL DATA

The data required as input for the simulation program is taken from the experimental observations and the predicted values have been compared with the experimental results.

Figures 5.12 to 5.18 present the deviations between predicted and experimental results of the different important parameters for the absorber. The maximum deviations are found to be within ±15%. The deviation of experimental and predicted results of inlet specific humidity, outlet specific humidity and change in specific humidity in the absorber are found to be -1%, +7% to – 5% and + 20% to -15% respectively as represented by figures 5.12-5.14. It is observed from figure 5.15 that deviation of the temperature of the air lies within +10%. Figure 5.17 shows that deviation of predicted and experimental moisture removal rate is found within the range of +15% to -12%. Maximum deviation of 4% for the desiccant concentration at the outlet of absorber is found between predicted and experimental values as shown by figure 5.18.

The deviations of predicted values with experimental results of inlet and outlet specific humidity and change in specific humidity are presented in figures 5.19 to 5.21. ±15% deviation of experimental and predicted results of outlet specific humidity and change in specific humidity is observed from the graphs. It is observed from
figure 5.22 that predicted outlet temperature of the air is smaller by 3-4°C than the experimental values and its deviation range lies within -10%.

It has been observed that predicted outlet solution temperature values are deviated by +13.6% with the experimental results as shown by figure 5.23. Figure 5.24 shows that deviation of predicted and experimental evaporation rate is found within the range of ±8%. The predicted values of the desiccant concentration at outlet of the regenerator are deviated within the range of +1% to -5% with respect to experimental results as shown by figure 5.25.

![Figure 5.12](image.png)

**Figure 5.12** Experimental and predicted values of inlet specific humidity \((\omega_{ai})\) in the absorber
Figure 5.13 Experimental and predicted values of outlet specific humidity ($\omega_{ao}$) in the absorber.

Figure 5.14 Experimental and predicted values of change in specific humidity (d$\omega$) in the absorber.
Figure 5.15 Experimental and predicted values of temperature of air at outlet of the absorber

Figure 5.16 Experimental and predicted values of temperature of solution at outlet of the absorber
Figure 5.17 Experimental and predicted values of moisture removal rate (MRR) in the absorber

Figure 5.18 Experimental and predicted values of concentration of solution at outlet of the absorber
Figure 5.19 Experimental and predicted values of specific humidity ($\omega_{ai}$) at inlet of the regenerator

Figure 5.20 Experimental and predicted values of specific humidity at outlet of the regenerator
Figure 5.21 Experimental and predicted values of change in specific humidity in the regenerator

Figure 5.22 Experimental and predicted values of temperature of air at outlet of the regenerator
Figure 5.23 Experimental and predicted values of temperature of solution at outlet of the regenerator

Figure 5.24 Experimental and predicted values of evaporation rate in the regenerator
Figure 5.25 Experimental and predicted values of concentration of desiccant solution at outlet of the regenerator