CHAPTER 3

MODELING FOR DESIGN AND SIMULATION OF HYDROCHLORIC VAPOR PACKED ABSORBER.

3.1.   Hydrochloric Acid Storage System.

Hydrochloric acid storage system as shown in Figure 3.1, consists of a hydrochloric acid storage tank which is connected with a hydrochloric vapor packed absorber. Hydrochloric acid continuously vaporizes due to its high vapor pressure property at ambient temperature and the vapor is continuously vented through vent pipe to maintain tank pressure at safety condition at atmospheric pressure. The vapor flows through the vent pipe into packed absorber which is operated by continuous flow of water through packed column. Absorber vent gas is emitted at hydrochloric vapor content less than environmental impact level of 200 mg/Nm^3 or 122 ppm. Absorbed water which is at weak acid condition flows to waste water treatment unit before it is discharged to plant effluent.

3.2. Derivation of Mathematical Modeling for Design of Packed Absorber for Hydrochloric Vapor Absorption.

In order to set up mathematical model for packed absorber design, the model is separated into two parts i.e., prediction model for vaporization rate from storage tank and model of packed absorber. Model to prediction of vaporization rate from storage tank is set by assuming that only hydrochloric vapor and water vapor are in gas phase over solution of hydrochloric acid. Hydrochloric and water in hydrochloric acid is continuously vaporized in steady-state condition and heat for vaporization is transferred from solar and surrounding to storage tank.

The composition of gas phase can be calculated using assumption that the composition in vapor mixture is the composition in a saturated condition. Mole fraction in gas phase can be calculated in term of saturated vapor pressure over hydrochloric acid. By assumption that gas phase behavior is ideal gas, ideal gas law for gas mixture is applied to calculate mole fraction in gas phase. Mole fraction of water in gas is

$$w = \frac{p_{H2O}}{P} \qquad (3-1)$$

and mole fraction of hydrochloric in gas is

$$y = \frac{p_{HCl}}{P}$$
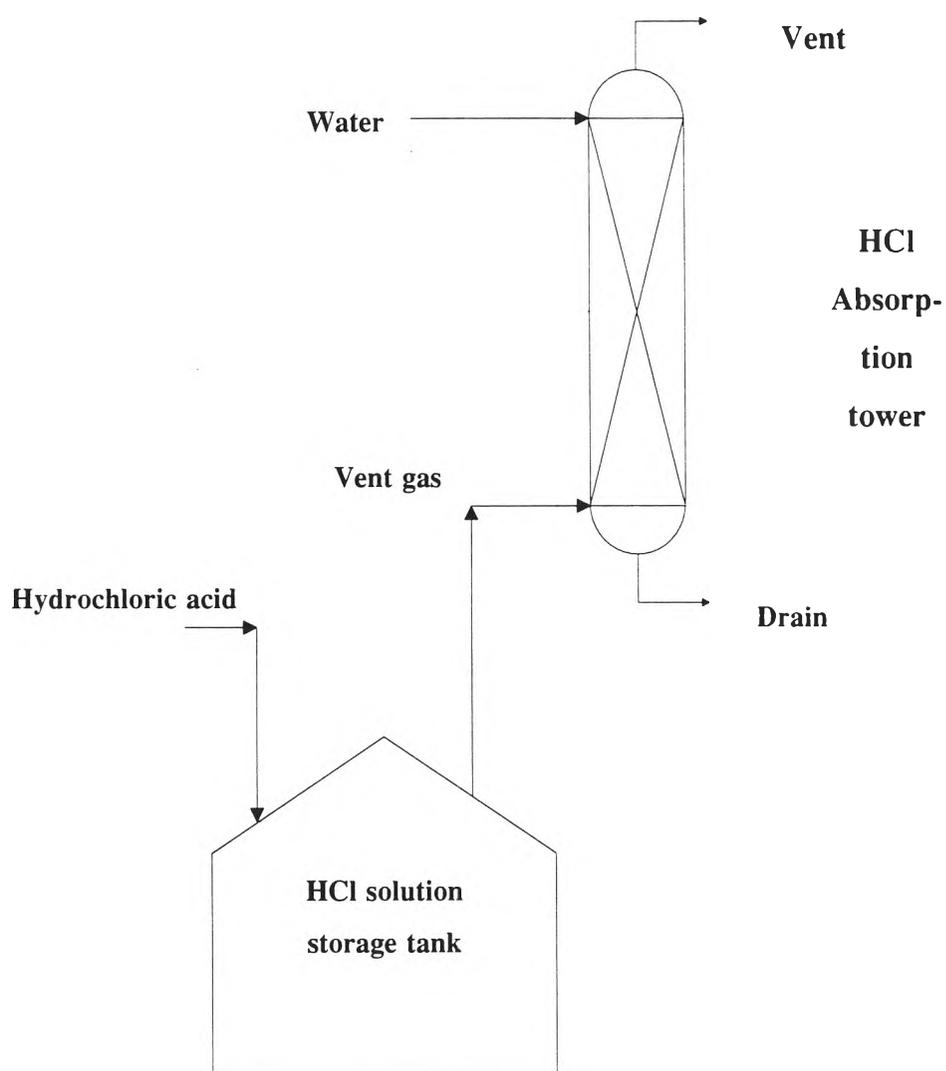
Figure 3.1 Hydrochloric acid storage system.

Vapor pressure over hydrochloric in storage tank and vapor pressure estimation can be calculated by used equation (A-10) and (A-11).

$$log_{10}p_{HCl} = A+(B/T) .(101325/760) \qquad Pa$$

$$log_{10}p_{H2O}= A+(B/T) .(101325/760) \qquad Pa$$

$$P = p_{HCl} + p_{H2O} \qquad Pa$$

The amount of gas phase flowed from storage to packed absorber can be calculated by assumption that hydrochloric and water are vaporized by heat which is transferred from solar radiation and heat from surrounding to storage tank. From hydrochloric storage tank energy balance equation (2-39), gas mixture of hydrochloric and water is vaporized at saturated composition is calculated by given equation

$$G_s = \frac{\left\{ \left[\left(\frac{Q}{A}\right)_{sun} \alpha_{sun} A \right] + \alpha_{sur} \theta \left[T_s^4 - T^4 \right] A \right\} \times 10^{-3}}{\lambda_y y + \lambda_w w}$$

$$G_s = \frac{\left[\left(\frac{Q}{A}\right)_{sun} \alpha_{sun} + \theta \alpha_{sur} \left[T_s^4 - T^4 \right] \right] A \times 10^{-3}}{\lambda_y y + \lambda_w w} \qquad (kgmol/ s) \qquad (3-3)$$

Result from equation (3-3) is a molecular flux for mixture of hydrochloric and water which vaporize to packed absorber at total cross section area of storage tank. Vapor continuously vaporizes from hydrochloric acid surface in storage tank through the vent pipe to packed absorber, the molecular flow rate at inlet of packed absorber is

$$G_0 = \left(\frac{G_s}{A}\right) \qquad kgmol/m^2 s \qquad (3-4)$$

Where A = cross section area of packed column = $\pi (D/2)^2$, m^2

D = pack column diameter, m

G_s = molecular flow rate of gas vaporized from storage tank, kgmol/s

G_0 = molecular flow rate of gas vaporized at inlet of packed column, kgmol/m^2 s

Second model of packed absorber is set by separate packed absorber to N stages at height 0.01 m. per stages, each stages is called n-th model. The condition of inlet gas and outlet liquid of packed absorber are calculated for use to be input value of the n-th cell model in packed absorber mathematical modeling by overall mass and energy balance calculation.

Overall mass and energy balance equations from transfer between phase in hydrochloric vapor packed absorber at n-th cell model are

1. Hydrochloric mass transfer to liquid phase (N_{An})
2. Mass transfer from liquid phase to gas phase (N_{wn})
3. Heat of solution (Heat of hydrochloric dissolved in water) (q_{An})
4. Heat transfer from gas phase to liquid phase (q_{Gn})
5. Heat of water vaporization (q_{wn})

Composition in gas phase from assumption are summarized in Table 3.1

Table 3.1 Composition in gas and liquid phase.

	Position in packed absorber	
	inlet (0)	outlet (n+1)
Gas phase composition	water, hydrochloric	water
Liquid phase composition	water	water, hydrochloric

Overall mass balance

$$G_0 + L_0 \quad = \quad G_{n+1} + L_{n+1} \qquad (3\text{-}5)$$

Hydrochloric mass balance

$$G_0 y_0 + L_{n+1} x_{n+1} \quad = \quad G_{n+1} y_{n+1} + L_0 x_0 \qquad (3\text{-}6)$$

by assumption that all hydrochloric vapor is absorbed by water (zero emission to atmosphere) and pure water is an absorbent;

x_{n+1} and y_{n+1} $\quad = \quad$ 0 equation (3-6) is reduced to

$$G_0 y_0 \quad = \quad L_0 x_0 \qquad (3\text{-}7)$$

Water mass balance

$$G_0(1-y_0) + L_{n+1}(1-x_{n+1}) = G_{n+1}(1-y_{n+1}) + L_0(1-x_0) \tag{3-8}$$

Overall energy balance

$$c_{PG,0}G_0 t_{G0} + c_{PL,n+1}L_{n+1}t_{Ln+1} = c_{PG,n+1}G_{n+1} t_{Gn+1} + c_{PL,0}L_0 t_{L0} \tag{3-9}$$

Gas phase energy balance

$$c_{PG,0}G_0 t_{G0} = c_{PG,n}G_{n+1} t_{Gn+1} + \Sigma q_{Gn} \tag{3-10}$$

Liquid phase energy balance

$$c_{PL,0}L_0 t_{L0} = c_{PL,n+1}L_{n+1} t_{Ln+1} + \Sigma q_{L,n} \tag{3-11}$$

Total amount of hydrochloric transfer to liquid phase (ΣN_{An}) is calculated by equation (2-39).

$$\Sigma N_{An} = \frac{G_0(y_0 - y_{n+1})}{(1 - y_{n+1})} - \frac{\Sigma N_{Wn}(y_{n+1})}{(1 - y_{n+1})}$$

From assumption that hydrochloric vapor is not emitted to atmosphere ; $y_{n+1} = 0$

Flow rate of inlet liquid phase and outlet liquid phase can be calculated from inlet liquid phase molar flow rate $\quad L_{n+1} = L_t \cdot \left(\dfrac{18}{3600}\right) \quad$ kgmol/m^{2}s $\tag{3-12}$

where L_t = inlet water flow rate (m^3/h) which calculate from assigned limited pH by equation.

$$pH = (-1)\log_{10}\left(\left(\frac{\sum N_{An} \cdot 3600}{L_t \cdot 1000}\right) + 10^{-7}\right) \tag{3-13}$$

outlet liquid phase molar flow rate $\quad L_0 = L_{n+1} + \Sigma N_{An} - \Sigma N_{wn} \quad$ kgmol/m^{2}s

Outlet liquid phase temperature (t_{L0}) can be calculated from liquid phase energy balance equation.

$$t_{L0} = \left[\frac{\left(c_{PL,n+1}L_{n+1}t_{Ln+1}\right) + \sum q_{L,n}}{c_{PL,0}L_0}\right] \tag{3-14}$$

Volumetric heat transfer coefficient can be calculated by overall gas phase energy balance (3-10) by assumption that heat transfer rate from gas phase to liquid phase is constant rate in every cell models of packed absorber.

$$\Sigma q_{Gn} = C_{PG,0} \, G_0 t_{G0} - C_{pG,n} G_n t_{Gn} \tag{3-14}$$

and $\quad \Sigma q_{Gn} \quad = \quad h_G a \, (t_{G0} - t_{Ln})(ht) \qquad \text{w/m}^2 \tag{3-15}$

where $\quad ht \quad = \quad$ height of packed column , m

$\quad t_{Ln} \quad = \quad$ inlet liquid temperature , °C (K)

$$h_G a \quad = \quad \frac{\Sigma q_{Gn}}{(t_{Go} - t_{Ln})(ht)} \qquad \text{w/m}^3\text{K} \tag{3-16}$$

$h_G a$ is assumed that constant along packed column height and is used for calculation of equation (2-20).

Hydrochloric acid vapor/liquid equilibrium relation.

From study of hydrochloric vapor absorption which is described in chapter 2, experimental results indicate concentration of hydrochloric in gas phase which equilibrium with concentration of hydrochloric acid at weak acid condition was zero; $y_{Sn} = 0$. This assumption is used in n-th cell modeling.

n-th model modeling

After required variables and properties data are calculated in previous steps, packed column model for n-th cell calculation which is described in chapter 2. is used in this sequence. The n-th cell model is assigned that height of n-th cell was 0.01 m. The calculation is commenced at first cell of packed column by input variables:

$G_0 \quad = \quad$ gas molar flow rate at inlet of first cell.

$L_0 \quad = \quad$ liquid molar flow rate at outlet of first cell.

$t_{G0} \quad = \quad$ inlet gas temperature at inlet of first cell

$t_{L0} \quad = \quad$ outlet liquid temperature at outlet of first cell

$y_0 \quad = \quad$ mole fraction of hydrochloric in gas phase flows to first cell

$w_0 \quad = \quad$ mole fraction of water in gas phase flows to first cell

From input variables n-th model calculation are calculated in following steps.

1. Gas phase and liquid phase physical properties for using in calculation at condition of n-th cell can be calculated by equations and data in Appendix A.

Inlet gas properties is calculated by assumed that gas phase inlet temperature is equal hydrochloric acid temperature. From equation (A-1) and data in Table A.1, inlet gas viscosity (μ_v) is

$$\mu_V = y\mu_{HCl} (36.5)^{0.5} + w \, \mu_{H2O}(18)^{0.5}$$

Inlet gas density (ρ_V) is calculated by equation (A-5)

$$\rho_V = \left(\frac{1}{RT}\right) (M_{HCl}y_{HCl} + M_{H2O}y_{H2O}) \, (y_{HCl}P + y_{H2O}P)$$

$$\rho_V = \left(\frac{P}{RT}\right) (M_{HCl}y_{HCl} + M_{H2O}y_{H2O})$$

where P = 1 atm

R = 0.082 m^3 . atm / kmol . K

$$\rho_V = 1 / (0.082T) . (36.5y + 18w) \qquad kg/m^3$$

gas phase heat capacity is calculated by equation (A-14)

$$c_{P,G} = y(6.7+0.000084 \, T) + w(8.22+0.00015 \, t + 0.00000134 \, T^2) \quad (kcal/kg\text{-}mol \, K)$$

liquid phase heat capacity is calculated by equation (A-15)

$$c_{P,L} = (0.0007x^2 - 0.0342x + 0.9991) . (4.18) . (18) \, (KJ/kmol \, k)$$

2. Water transfer to gas phase rate is neglected by assumption that absorbed water is not vaporized in every cells of packed column, water evaporation rate per cell is

$$N_{wn} \quad = \quad 0 \qquad kmol/m^2 s \qquad\qquad (3\text{-}17)$$

3. Hydrochloric mass transfer rate (gas to liquid); N_{an} can be calculated from equation (2-16)

$$N_{An} = k_G a_w(y_n - y_{Sn}) \, \Delta Z$$

y_{sn} in equation (2-16) is zero and k_G; gas phase mass transfer coefficient is calculated by equation (2-45) and a_W; surface area of wetted packing is calculated by equation (2-46).

$$\frac{k_G RT}{a_v D_{HCl - H2O} P} = C_1 \left(\frac{G_{V}}{a_v \mu_v}\right)^{0.7} \left(\frac{\mu_v}{\rho_v D_{HCl - H2O}}\right)^{1/3} (a_v D_P)^{-2.0}$$

$$\frac{a_w}{a_v} = 1 - \exp\left(-1.45\left(\frac{\sigma_c}{\sigma}\right)^{0.75}\left(\frac{G_L}{a_v \mu_v}\right)^{0.1}\left(\frac{G_L^2 a_v}{\rho_L^2 g}\right)^{-0.05}\left(\frac{G_L^2}{\rho_L \sigma a_v}\right)^{0.2}\right)$$

gas phase diffusion coefficients can be calculated by equation (A-7)

$$D_{HCl\text{-}H2O} = 1.101747733 \times 10^{-9}\left(\frac{T^{1.75}}{P}\right) \quad m^2/s$$

result of calculation for N_{An} is substituted in equation (2-8) at the next step.

4. Mass balance gas phase, n-th cell can be calculated from equation (2-8)

$$G_{n+1} + N_{wn} = G_n + N_{An}$$

result was G_n which is used in the next cell model.

5. Hydrochloric mass balance gas phase, n-th cell can be calculated from equation (2-9)

$$y_{n-1} G_{n-1} = y_n G_n + N_{An}$$

result was y_n which is used in the next cell model.

6. Water mole fraction in gas phase at n-th cell can be calculated from equation

$$w_n = (1-y_n)$$

result was w_n which is used in the next cell model.

7. Mass balance liquid phase, n-th cell can be calculated from equation (2-11)

$$L_{n+1} N_{An} = L_n + N_{wn}$$

result was L_{n+1} which is used in the next step.

8. Hydrochloric mass balance liquid phase, n-th cell can be calculated from equation (2-12)

$$x_{n+1} L_{n+1} + N_{An} = x_n L_n$$

result was x_{n+1} which is used in the next step.

9. Heat effect in n-th cell can be calculated from equation (2-18), (2-19) and (2-20)

Heat of hydrochloric dilution in water $\quad q_{An} = \lambda_A N_{An}$

Heat of water evaporation $\quad q_{Wn} = \lambda_W N_{Wn} = 0$

Heat transfer from gas to liquid $\quad q_{Gn} = h_G a(t_{Gn} - t_{Ln})\Delta Z$

Calculation results from equation (2-18), (2-19) and (2-20) is used in equation (2-15)

Overall enthalpy balance

$$q_{Ln} = q_{An} + q_{Gn} - q_{Wn}$$

q_{Gw} and q_{Ln} are used in calculation for temperature of gas and liquid of the next cell.

10. Temperature of gas and liquid in the next cell can be calculated by following equation,

Gas phase temperature in the next cell can be calculated by equation (2-13)

Heat balance gas phase for n-th cell

$$C_{PG}t_{Gn-1}G_{n-1} = C_{PG}t_{Gn}G_n + q_{Gn}$$

Liquid phase temperature in the next cell can be calculated by equation (2-14)

Heat balance liquid phase for n-th cell is

$$C_{PL}t_{Ln+1}L_{n+1} + q_{Ln} = C_{PL}t_{Ln}L_n$$

11. Sum of hydrochloric dissolved in water at n-th cell and height of column at n-th cell can be calculated by equations

$$\sum_{i=0}^{n} N_A = N_{A1} + N_{A2} + \ldots\ldots\ldots\ldots N_{An} \tag{3-17}$$

and $\qquad h_n = n(0.01)$

12. Amount of hydrochloric dissolved in outlet water can be calculated by equation

$$X = \frac{\sum N_A \cdot 36.5}{L_0 \cdot 18} \qquad \text{\% by weight} \tag{3-18}$$

13. Concentration of hydrochloric in vent gas can be calculated by equation

$$Y = \frac{y_n \cdot 36.5 \cdot 1000000}{22.4} \qquad \text{mg/Nm}^3 \tag{3-19}$$

14. n-th cell model is continuously calculated from step1 to step 13 until hydrochloric vapor is totally absorbed.

3.3 Mathematical Model for Design of Packed Absorber.

General mathematical model for design of packed absorber is the model which consists all calculation procedure which are described in item 3.1. Model is separated into two parts i.e. part of model for prediction vaporization rate from hydrochloric acid storage tank and part of model for packed absorber. Fixed variables are assigned for calculation as following, packed absorber diameter is 0.9 m. and is not lower than eight times of packing size (minimum absorber diameter which is not effected to liquid distribution (9)), height of absorber is 0.3048 m., limited pH of outlet water and water flow rate to absorber is 0.01 m^3/h

At first model for prediction of vaporization rate from hydrochloric acid storage tank is used, calculation results is gas flow rate to packed absorber which is used by model for packed absorber. The n-th cell model calculation in the model for packed absorber is continuously calculated until calculations are converge. Height of absorber at the final n-th is compared with assigned height of packed absorber. If height of absorber at n-th cell is higher than assigned height packed absorber, trial for the new packed absorber height is commenced by increasing 0.01m. from exist value and recalculate following procedure of packed column design at overall energy balance step by fixed diameter of absorber. The trial calculation for height of packed absorber column is continuously calculated until height of n-th cell is lower than assigned height of absorber. For packed column diameter which is assigned beginning value at 1.0 m., the calculation for proving that water flows through packed column is not flooding is calculated by equation to estimate maximum allowed inlet gas phase velocity(14).

$$V = 0.9\sqrt{\frac{1}{\rho_v}} \tag{3-20}$$

If inlet gas phase velocity is lower than a limit, diameter is decreased by 0.01 m. from existing value and then recalculate at step of calculation for the molar flow rate at inlet of packed column. The trial calculation for diameter of packed absorber is continuously calculated until the criteria of diameter is reached.

Mathematical model for design of packed absorber can be reduced to design in case of fixed packed absorber diameter. Design procedure for packed absorber design in case of fixed packed absorber diameter is applied from the general mathematical model for design of packed absorber by reducing calculation for absorber diameter step. Mathematical model for design of

packed absorber can be reduced to design in case of fixed water flow rate is applied from mathematical modeling of packed absorber design from the general design model by reducing calculation for water flow rate step.

3.4 Mathematical Model for Simulation of Packed Absorber.

Model for simulation of packed absorber is separated into two cases i.e. model for simulation of packed absorber of hydrochloric acid storage tank and modeling for simulation packed absorber without hydrochloric acid storage tank. Mathematical model for simulation of packed absorber in case of packed absorber is connected with hydrochloric acid storage tank is applied from general mathematical modeling of packed absorber design by fixing absorber diameter, reducing calculation for water flow rate step and reducing calculation for height of absorber step.

Mathematical model for simulation of packed absorber in case of simulation of only packed absorber without hydrochloric acid storage tank is applied from modeling for simulation of packed absorber of hydrochloric acid storage tank by reducing model for prediction vaporization rate from storage tank.

3.5 Packed Absorber Design Programming.

Models for design and simulation which are described in items 3.3 and 3.4 are programmed to be packed absorber design program in C language(details of source code are presented in Appendix E) for convenient and correct calculation which consists of 5 modules as shown in Figure 3.2. and detail of modules are

1.   Module for design of new packed absorber for hydrochloric acid storage tank which calculation results consist packed column height, packed and absorbed water flow rate for limited pH of outlet water.

Object of new packed absorber design module is for sizing new packed absorber which requires data of hydrochloric acid in tank as concentration and temperature, storage tank size and operating condition, selected packing data (such as type, size, material, surface tension and specific surface), limited pH of outlet water, inlet water data as temperature, absorptivity for low temperature radiation of tank external surface, solar absorptivity of tank external surface and solar radiation to tank surface.

After program read all input data, calculation process as is described in general model for design packed absorber are continued with trial and error as shown in Figure 3.3 until module criteria is met. Height of absorber from calculation is added safety factor by plus calculation result with 1.5, 1.5 is recommend safety factor for adiabatic absorption (5). Absorber diameter is limited by flooding of water and minimum value at 8 times of packing size to ensured that liquid distribution in packed column is not effected(9).

2.   Module for design of new packed absorber for hydrochloric acid storage tank which calculation results consist packed column height, packed and absorbed water flow rate for limited pH of outlet water at fixed diameter of absorber.

Object of new packed absorber design module is for sizing new packed absorber which requires data of hydrochloric acid in tank as concentration and temperature, storage tank size and operating condition, selected packing data (such as type, size, material, surface tension and specific surface), limited pH of outlet water, inlet water data as temperature, absorptivity for low temperature radiation of tank external surface, solar absorptivity of tank external surface and solar radiation to tank surface.

After program read all input data, calculation process as is described in model for design packed absorber in case of fixed packed absorber diameter are continued with trial and error as shown in Figure 3.4 until module criteria is met. Height of absorber from calculation is added safety factor by plus calculation result with 1.5, 1.5 is recommend safety factor for adiabatic absorption (5).

3.   Module new packed absorber for hydrochloric acid storage tank which calculation results consist packed column height and outlet pH at fixed packed column diameter and absorbed water flow rate.

Object of new packed absorber design module is for sizing new packed absorber which requires data of hydrochloric acid in tank as concentration and temperature, storage tank size and operating condition, selected packing data (such as type, size, material, surface tension and specific surface), limited pH of outlet water, inlet water temperature, absorptivity for low temperature radiation of tank external surface, solar absorptivity of tank external surface and solar radiation to tank surface.

After program read all input data, calculation process as is described in mathematical model for design of packed absorber in case of fixed water flow rate are continued with trial and error as shown in Figure 3.5 until module criteria is met. Height of absorber from calculation is added safety factor by plus calculation result with 1.5, 1.5 is recommend safety factor for adiabatic absorption (5). Absorber diameter is limited by flooding of water and packing size to ensured that liquid distribution in packed column is not effected (9).

4. Module for simulation of packed absorber in case of packed absorber is connected with hydrochloric acid storage tank.

Object of packed absorber testing module is for operating test of exist packed absorber which requires data of hydrochloric acid in tank as concentration and temperature, storage tank size and operating condition, height and diameter of packed column, packing data (such as type ,size, material, surface tension and specific surface), inlet water temperature, absorptivity for low temperature radiation of tank external surface, solar absorptivity of tank external surface and solar radiation to tank surface

After program read all input data, calculation process as is described in model for simulation of packed absorber of hydrochloric acid storage tank are continued with trial and error as shown in Figure 3.6 until module criteria is met.

5. Module for packed absorber simulation in case of packed absorber is not connected with hydrochloric acid storage tank.

Object of packed absorber testing module is for operating test of exist packed absorber which requires data of inlet gas phase properties (as flow rate, composition, temperature, viscosity and density) , height and diameter of packed column, packing data (such as type, size, material, surface tension and specific surface) and inlet water data as temperature and flow rate.

After program read all input data, calculation process as is described in model for simulation packed absorber without hydrochloric acid storage tank are continued with trial and error as shown in Figure 3.7 until module criteria is met.

3.6 Program Using Guide

Computer program for design packed absorber of hydrochloric acid storage tank is DOS platform program, the program using guide are described in Appendix C.

Start

Main menu select

1.Packed absorber design; "case A."

2.Packed absorber design

with fixed water flow rate; "case B"

2.Packed absorber design

with fixed absober diameter; "case C"

3.Existing packed absorber simulation;"case D"

(unknown inlet gas phase condition)

4.Existing packed absorber simulation;"case E"

(known inlet gas phase condition)

| Model of packed absorber design detail in case A | Model of packed absorber design detail in case B | Model of packed absorber design detail in case C | Model of packed absorber simulation detail in case D | Model of packed absorber simulation detail in case E |

Figure 3.2 Main program flow chart

```
                    ┌─────────────┐
                    │    Start    │
                    └─────────────┘
                           │
                           ▼
```

Read input data

1.Hydrchloric acid concentration.

2.Hydrochloric acid temperature.

3.Packing data; size, type, material, specific surface, surface tension.

4.Inlet water temperature.

5.Limited pH of outlet water.

6.Absorptivity. Solar absorptivity, Solar radiation

7. Storage tank surface area

Inlet gas phase condition calculation

1.Saturated HCl vapor pressure.

2.Saturated H2O vapor pressure.

3.Saturated vapor pressure over solution.

4.HCl mole fraction in gas phase.

5.H2O mole fraction in gas phase.

Specified packed column size

◄—ht = ht+0.01—►   1.Column diameter (dia); begin at 0.9m.   ◄—dia = dia+0.01—►

2.Column height (ht); begin at 0.3048m.

Calculation

1.Packed column inlet gas phase flow rate estimation.

2.Inlet water flow rate from limited pH

Figure 3.3 Case A flow chart

Oveall mass and heat transfer calculation

1. Overall mass balance;for calculate total HCl
   transfer from gasphase to liquid phase.
2. Overall liquid phase heat balance;for estimate
   packed column outlet water temperature.
3. Overall gas phase heat balance;for estimate
   total heat transfer from gas phase to liquid
   phase

n-th cell calculation ; begin at n = 0

1. Gas phase density estimation.
2. Gas phase viscosity estimation.
3. Diffusion coefficient for gas phase.
4. Gas phase specific heat capacity.
5. Liquid phase specific heat capacity.
6. Liquid phase surface tension.
7. Gas phase mass transfer coefficient.
8. HCl transfer from gas to liquid phase.
9. H2O transfer from liquid to gas phase.
10. Cell outlet gas phase flowrate.
11. Cell inlet liquid phase flowrate.
12. Heat of HCl dilution in liquid phase.
13. Heat of H2O evaporation to gas phase.
14. Cell inlet liquid phase temperature.
16. Cell outlet gas phase temperature.
17. HCl and H2O mole fraction in gas phase.
18. Height pf packed column at n-th cell.
19. Sum of HCl dissolved in liquid at n-th cell.

$n = n+1$

Sum of HCl dissolved in
liquid lower than total HCl transfer
to liquid phase

—Yes—

Figure 3.3 (cont.)

Figure 3.3 (cont.)

Start

Read input data

1.Hydrpchloric acid concentration.

2.Hydrochloric acid temperature.

3.Packing data; size, type, material,

specific surface, surface tension.

4.Inlet water temperature.

5.Inlet water flow rate

6.Absorptivity. Solar absorptivity, Solar radiation

7. Storage tank surface area

Inlet gas phase condition calculation

1.Saturated HCl vapor pressure.

2.Saturated H2O vapor pressure.

3.Saturated vapor pressure over solution.

4.HCl mole fraction in gas phase.

5.H2O mole fraction in gas phase.

Specified packed column size

←─ht = ht+0.01─→   1.Column diameter; begin at dia = 0.9m   ←─dia = dia+0.01─→

2.Column height (ht); begin at 0.3048m.

Calculation

1.Packed column inlet gas phase flow rate estimation.

Figure 3.4 Case B flow chart

Oveall mass and heat transfer calculation

1.Overall mass balance;for calculate total HCl
transfer from gasphase to liquid phase.

2.Overall liquid phase heat balance;for estimate
packed column outlet water temperature.

3.Overall gas phase heat balance;for estimate total
heat transfer from gas phase to liquid phase

n-th cell calculation ; begin at n = 0

1.Gas phase density estimation.

2.Gas phase viscosity estimation.

3.Diffusion coefficient for gas phase.

4.Gas phase specific heat capacity.

5.Liquid phase specific heat capacity.

6.Liquid phase surface tension.

7.Gas phase mass transfer coefficient.

8.HCl transfer from gas to liquid phase.

9.H2O transfer from liquid to gas phase.

10.Cell outlet gas phase flowrate.

11.Cell inlet liquid phase flowrate.

12.Heat of HCl dilution in liquid phase.

13.Heat of H2O evaporation to gas phase.

14.Cell inlet liquid phase temperature.

16.Cell outlet gas phase temperature.

17.HCl and H2O mole fraction in gas phase.

18.Height pf packed column at n-th cell.

19.Sum of HCl dissolved in liquid at n-th cell.

$\leftarrow n = n+1 \rightarrow$

Sum of HCl dissolved in
liquid lower than total HCl transfer
to liquid phase

—Yes—▶

Figure 3.4 (cont.)

No

Height of packed column at
n-th cell higher than specified
packed column height

Yes

No

Water flood in absorber and
water flow is channeling

No

Yes

Print calculation results

Figure 3.4 (cont.)

```
                    ┌─────────────────┐
                    │     Start       │
                    └─────────────────┘
                             │
                             ▼
```

Read input data

1.Hydrpchloric acid concentration.

2.Hydrochloric acid temperature.

3.Packing data; size, type, material,

specific surface, surface tension.

4.Inlet water temperature.

5.Limited pH of outlet water.

6.Absorptivity, Solar absorptivity, Solar radiation

7. Storage tank surface area

8. Packed column diameter.

Inlet gas phase condition calculation

1.Saturated HCl vapor pressure.

2.Saturated H2O vapor pressure.

3.Saturated vapor pressure over solution.

4.HCl mole fraction in gas phase.

5.H2O mole fraction in gas phase.

Specified packed column size

ht = ht+0.01   Column height (ht) ; begin at 0.3048m.

Calculation

1.Packed column inlet gas phase flow rate estimation.

2.Inlet water flow rate from limited pH

Figure 3.5 Case C flow chart

Oveall mass and heat transfer calculation

1. Overall mass balance;for calculate total HCl transfer from gasphase to liquid phase.

2. Overall liquid phase heat balance;for estimate packed column outlet water temperature.

3. Overall gas phase heat balance;for estimate total heat transfer from gas phase to liquid phase

n-th cell calculation ; begin at n = 0

1. Gas phase density estimation.

2. Gas phase viscosity estimation.

3. Diffusion coefficient for gas phase.

4. Gas phase specific heat capacity.

5. Liquid phase specific heat capacity.

6. Liquid phase surface tension.

7. Gas phase mass transfer coefficient.

8. HCl transfer from gas to liquid phase.

9. H2O transfer from liquid to gas phase.

10. Cell outlet gas phase flowrate.

11. Cell inlet liquid phase flowrate.

12. Heat of HCl dilution in liquid phase.

13. Heat of H2O evaporation to gas phase.

14. Cell inlet liquid phase temperature.

16. Cell outlet gas phase temperature.

17. HCl and H2O mole fraction in gas phase.

18. Height pf packed column at n-th cell.

19. Sum of HCl dissolved in liquid at n-th cell.

← n = n+1 →

Sum of HCl dissolved in liquid lower than total HCl transfer to liquid phase

—Yes—▶

Figure 3.5 (cont.)

Figure 3.5 (cont.)

```
        ╭─────────────╮
        │   Start      )
        ╰─────────────╯
              │
              ▼
```

Read input data

1.Hydrpchloric acid concentration.

2.Hydrpchloric acid temperature.

3.Packing data: size, type, material,

specific surface, surface tension.

4.Inlet water data; temperature, flow rate.

5.Packed column height and diameter.

6.Absorptivity, solar absorptivity, solar radiation

7.Storage tank surface

Inlet gas phase condition calculation

1.Saturated HCl vapor pressure.

2.Saturated H2O vapor pressure.

3.Saturated vapor pressure over solution.

4.HCl mole fraction in gas phase.

5.H2O mole fraction in gas phase.

6.Gas phase density.

7.Gas phase viscosity.

Calculation

Packed column inlet gas phase flow rate estimation.

Oveall mass and heat transfer calculation

1.Overall mass balance;for calculate total HCl

transfer from gasphase to liquid phase.

2.Overall liquid phase heat balance;for estimate

packed column outlet water temperature.

3.Overall gas phase heat balance;for estimate

total heat transfer from gas phase to liquid

phase

Figure 3.6 Case D flow chart

n-th cell calculation ; begin at n = 0

1.Gas phase density estimation.

2.Gas phase viscosity estimation.

3.Diffusion coefficient for gas phase.

4.Gas phase specific heat capacity.

5.Liquid phase specific heat capacity.

6.Liquid phase surface tension.

7.Gas phase mass transfer coefficient.

8.HCl transfer from gas to liquid phase.

9.H_2O transfer from liquid to gas phase.

10.Cell outlet gas phase flowrate.

11.Cell inlet liquid phase flowrate.

12.Heat of HCl dilution in liquid phase.

13.Heat of H_2O evaporation to gas phase.

14.Cell inlet liquid phase temperature.

16.Cell outlet gas phase temperature.

17.HCl and H_2O mole fraction in gas phase.

18.Height pf packed column at n-th cell.

19.Sum of HCl dissolved in liquid at n-th cell.

n = n+1

Height of packed column at n-th cell lower than specified packed column height

Yes

No

Print calculation results

Figure 3.6 (cont.)

```
                    ╭─────────────╮
                    │    Start     )
                    ╰─────────────╯
                          │
                          ▼
  ┌──────────────────────────────────────────────────┐
  │                Read input data                     │
  │            1.Inlet gas phase flowrate.             │
  │           2.Inlet gas phase temperature.           │
  │            3.Inlet gas phase density.              │
  │      4.HCl and H2O composition in gas phase.       │
  │         5.Packing data; size, type, material,      │
  │          specific surface, surface tension.        │
  │      6.Inlet water data: temperature, flow rate    │
  │       7.Packed column height and diameter.         │
  └──────────────────────────────────────────────────┘
                          │
                          ▼
  ┌──────────────────────────────────────────────────┐
  │  Oveall mass and heat transfer calculation         │
  │   1.Overall mass balance;for calculate total HCl   │
  │      transfer from gasphase to liquid phase.       │
  │   2.Overall liquid phase heat balance;for estimate │
  │      packed column outlet water temperature.       │
  │   3.Overall gas phase heat balance;for estimate    │
  │    total heat transfer from gas phase to liquid    │
  │                      phase                         │
  └──────────────────────────────────────────────────┘
                          │
                          ▼
```

Figure 3.7 Case E flow chart

n-th cell calculation ; begin at n = 0

1.Gas phase density estimation.

2.Gas phase viscosity estimation.

3.Diffusion coefficient for gas phase.

4.Gas phase specific heat capacity.

5.Liquid phase specific heat capacity.

6.Liquid phase surface tension.

7.Gas phase mass transfer coefficient.

8.HCl transfer from gas to liquid phase.

9.H2O transfer from liquid to gas phase.

10.Cell outlet gas phase flowrate.

11.Cell inlet liquid phase flowrate.

12.Heat of HCl dilution in liquid phase.

13.Heat of H2O evaporation to gas phase.

14.Cell inlet liquid phase temperature.

16.Cell outlet gas phase temperature.

17.HCl and H2O mole fraction in gas phase.

18.Height pf packed column at n-th cell.

19.Sum of HCl dissolved in liquid at n-th cell.

n = n+1

Height of packed column at n-th cell lower than specified packed column height

Yes

No

Print calculation results

Figure 3.7 (cont.)