# CHAPTER 5

# RESULTS AND DISCUSSIONS

Mathematical model in packed absorber design program is separated into two parts. The first part was the model for prediction of vaporization rate from hydrochloric acid storage tank and the second part was the model of packed absorber. From experimental results in Chapter 4, results are used as program input data to verify program accuracy.

## 5.1 Model for Prediction of Vaporization Rate Accuracy Verification.

Modeling for predict vaporization rate accuracy is verified by comparison of experimental results with program calculation results. Experimental results on exposure of hydrochloric acid in plastic bottles to air are presented in Tables 4.1 and 4.2. The results indicate that vaporization rate of outdoor condition is higher than vaporization rate of indoor condition. For indoor exposure, the experimental results indicate that hydrochloric and water are vaporized by diffusion to air because temperature difference of solution in bottles and surrounding is not high enough to cause major heat transfer from surrounding to hydrochloric in the bottles. For outdoor exposure, hydrochloric and water are vaporized by diffusion and by energy transfer from sorrounding. The net vaporization rate by energy transfer from sorrounding of outdoor exposure is calculated by deduct heat for diffusing vaporization from total heat for vaporization. Heat for diffusing vaporization for outdoor exposure is assummed that equal heat for diffusing vaporization for indoor exposure. Required input data of program were experimental results in Tables 4.1 and 4.2 and solar radiation data from Meteorological department, solar radiation data are presented in Table D.2. Program calculation results by model for packed absorber simulation (Simulation for packed absorber of hydrochloric acid storage tank as described in Chapter 3: modeling case D) are present in Tables 5.3 and 5.4. Results of the experiment on existing packed absorber in plant site is also used to verified program accuracy, gas vaporization rate is calculated from experimental result is shown in Table 5.6. Operating conditions of a surge tank in Table 4.5 are used as input data of program, program calculation results by model case D with varied solar radiation to tank are presented in Table 5.7

From calculation results of experiment in Tables 5.1 and 5.2 indicate that vaporized rate is lower than program calculated results in Tables 5.3 and 5.4. Table 5.5 presents solar radiation value from trial and error to obtain calculation results which is equal net heat transfer from surrounding in experiment as show in Table 5.1. Calculation results indicate that solar radiation required to vaporize is lower than average solar radiation data from Meteorological department. Vaporization rate in experiment with existing packed absorber which is shown in Table 5.6 are also lower than program calculated results in Table 5.7. The main cause of deviation is the correct solar radiation is not available and the exact radiation heat transfer properties as solar absorptivity and low temperature absorptivity are also not available. Solar radiation value in Table 5.3 is average value in the past four year at the day time in the month of experiment. Solar radiation value in Table 5.4 is 10 percentages of solar radiation in Table 5.3 by assumption that 90 percentages of solar radiation is reflected at building material.

Absorptivity data is average value for paint, exact absorptivity for polypropylene plastic bottle is not available. In Table 5.7, program calculation results is shown in various value which depend on solar radiation because storage tank is installed in first floor of hydrochloric acid synthesis unit, the solar radiation is not directly radiation to tank, the exact solar radiation to tank is difficulty to predict.

Results comparison of the experiment results and results of program indicate that limited of modeling using is accuracy of input data for calculation, especially for solar radiation and absorptivity. For the new packed absorber design of outdoor hydrochloric acid storage tank, selection of solar radiation data should be the average solar radiation at midday. For the new packed absorber design of indoor hydrochloric acid storage tank, selection of solar radiation data should be proportional with the average solar radiation at midday. The appropriate apsorptivity value may be estimated by using absorptivity value of roof or paint of building material. For example, if storage tank is installed in building where is painted by simple white color, average absorptivity for solar radiation of white paint is 0.1, absorbed solar radiation of building is estimated that about 10 percentages of average solar radiation at midday.

Table 5.1 Calculation for estimated vaporization rate from hydrochloric solution at outdoor condition

| weight before exposure (g) | weight after exposure (g) | total vaporized (g) | exposure time (hr) | vaporization rate (kg/S) | estimated HCl mole ratio in gas | estimated H2O mole ratio in gas | vaporization rate (kgmole/S) | heat for vaporized (kJ/S) | net heat from solar radiation (kJ/S) |
|---|---|---|---|---|---|---|---|---|---|
| 382.26 | 379.01 | 3.25 | 1 | 9.0278E-07 | 0.925 | 0.075 | 2.5711E-08 | 0.000463 | 5.5548E-05 |
| 410.09 | 404.9 | 5.19 | 2 | 7.2083E-07 | 0.925 | 0.075 | 2.0529E-08 | 0.00037 | 0.000183736 |
| 402.31 | 395.29 | 7.02 | 3 | 6.5E-07 | 0.925 | 0.075 | 1.8512E-08 | 0.000333 | 0.0001543 |
| 390.42 | 383.25 | 7.17 | 4 | 4.9792E-07 | 0.925 | 0.075 | 1.4181E-08 | 0.000255 | 0.000116081 |
| 374.6 | 355.12 | 19.48 | 5 | 1.0822E-06 | 0.925 | 0.075 | 3.0822E-08 | 0.000555 | 0.000409061 |
| | | | | | | Average | 2.1951E-08 | 0.000395 | 0.000183745 |

Table 5.2 Calculation for estimated vaporization rate from hydrochloric solution at indoor condition

| weight before exposure (g) | weight after exposure (g) | total vaporized (g) | exposed time (hr) | vaporization rate (kg/S) | estimated HCl mole ratio in gas | estimated H2O mole ratio in gas | vaporization rate (kgmole/S) | heat for vaporized (kJ/S) |
|---|---|---|---|---|---|---|---|---|
| 399.68 | 396.82 | 2.86 | 1 | 7.9444E-07 | 0.925 | 0.075 | 2.2626E-08 | 0.000407 |
| 364.32 | 361.71 | 2.61 | 2 | 3.625E-07 | 0.925 | 0.075 | 1.0324E-08 | 0.000186 |
| 390.85 | 387.08 | 3.77 | 3 | 3.4907E-07 | 0.925 | 0.075 | 9.9416E-09 | 0.000179 |
| 399.99 | 396.08 | 3.91 | 4 | 2.7153E-07 | 0.925 | 0.075 | 7.7331E-09 | 0.000139 |
| 368.77 | 363.65 | 5.12 | 5 | 2.8444E-07 | 0.925 | 0.075 | 8.1009E-09 | 0.000146 |
| | | | | | | Average | 1.1745E-08 | 0.000211 |

Table 5.3 Program simulated results for comparison with experiment results in table 4.1 (outdoor exposure of hydrochloric acid)

| total bottle surface area (m2) | solar radiation (W/m2) | solution temperature (C) | surrounding temperature (C) | heat from radiation (kJ/S) | heat emitted to surrounding (kJ/S) | heat for vaporization (kJ/S) | estimated HCl mole ratio in gas | estimated H2O mole ratio in gas | vaporization rate (kgmol/s) |
|---|---|---|---|---|---|---|---|---|---|
| 0.02 | 786 | 38 | 30 | 0.001572 | 0.000947616 | 0.000624384 | 0.925 | 0.075 | 3.468E-08 |
| 0.02 | 786 | 40 | 31 | 0.001572 | 0.001081809 | 0.000490191 | 0.925 | 0.075 | 2.7227E-08 |
| 0.02 | 786 | 41 | 33 | 0.001572 | 0.000975651 | 0.000596349 | 0.925 | 0.075 | 3.3123E-08 |
| 0.02 | 786 | 40 | 35 | 0.001572 | 0.000612673 | 0.000959327 | 0.925 | 0.075 | 5.3284E-08 |
| 0.02 | 786 | 42 | 35 | 0.001572 | 0.000866106 | 0.000705894 | 0.925 | 0.075 | 3.9208E-08 |
| | | | | | | | | Average | 3.7504E-08 |

Remark

1. Solar absorptivity of plastic bottles is estimated at 0.1.

2. Absorptivity for low temperature radiation of plastic bottles is estimated at 0.9.

3. Mole fraction in gas phase were calculated from saturated vapor pressure of hydrochloric acid at concentration as 35% by weight and at 35 C

4. Solar radiation was average value at 9.00 A.M. to 3.35 P.M. in April of 1993-1997

Table 5.4 Program simulated results for comparison with experiment results in table 4.2 (indoor exposure of hydrochloric acid)

| total bottle surface area (m2) | solar radiation (W/m2) | solution temperature (C) | surrounding temperature (C) | heat from radiation (kJ/S) | heat emitted to surrounding (kJ/S) | heat for vaporization (kJ/S) | estimated HCl mole ratio in gas | estimated H2O mole ratio in gas | vaporization rate (kgmol/s) |
|---|---|---|---|---|---|---|---|---|---|
| 0.02 | 78.6 | 30 | 30 | 0.0001572 | 0 | 0.0001572 | 0.925 | 0.075 | 8.7314E-09 |
| 0.02 | 78.6 | 31 | 31 | 0.0001572 | 0 | 0.0001572 | 0.925 | 0.075 | 8.7314E-09 |
| 0.02 | 78.6 | 33 | 33 | 0.0001572 | 0 | 0.0001572 | 0.925 | 0.075 | 8.7314E-09 |
| 0.02 | 78.6 | 34 | 35 | 0.0001572 | -0.000119012 | 0.000276212 | 0.925 | 0.075 | 1.5342E-08 |
| 0.02 | 78.6 | 34 | 35 | 0.0001572 | -0.000119012 | 0.000276212 | 0.925 | 0.075 | 1.5342E-08 |
| | | | | | | | | Average | 1.1376E-08 |

Remark 1. Solar absorptivity of plastic bottles is estimated at 0.1.

2. Absorptivity for low temperature radiation of plastic bottles is estimated at 0.9.

3. Mole fraction in gas phase were calculated from saturated vapor pressure of hydrochloric acid at concentration as 35% by weight and at 35 C.

4. Solar radiation to tank is equal 10% of total radiation at outdoor condition by assumption that 10% of solar radiation is absorbed by building and transfer to bottles at steady-state condition.

Table 5.5 Program simulated results for comparison with calculation results in table 5.1 (outdoor exposure of hydrochloric acid)

| total bottle surface area (m2) | solar radiation (W/m2) | solution temperature (C) | surrounding temperature (C) | heat from radiation (kJ/S) | heat emitted to surrounding (kJ/S) | heat for vaporization (kJ/S) | estimated HCl mole ratio in gas | estimated H2O mole ratio in gas | vaporization rate (kgmol/s) |
|---|---|---|---|---|---|---|---|---|---|
| 0.02 | 501.5 | 38 | 30 | 0.001003 | 0.000947616 | 5.53838E-05 | 0.925 | 0.075 | 3.0762E-09 |
| 0.02 | 632.5 | 40 | 31 | 0.001265 | 0.001081809 | 0.000183191 | 0.925 | 0.075 | 1.0175E-08 |
| 0.02 | 565 | 41 | 33 | 0.00113 | 0.000975651 | 0.000154349 | 0.925 | 0.075 | 8.5731E-09 |
| 0.02 | 364.5 | 40 | 35 | 0.000729 | 0.000612673 | 0.000116327 | 0.925 | 0.075 | 6.4612E-09 |
| 0.02 | 638 | 42 | 35 | 0.001276 | 0.000866106 | 0.000409894 | 0.925 | 0.075 | 2.2767E-08 |
| | | | | | | | | Average | 1.021E-08 |

Remark

1. Solar absorptivity of plastic bottles is estimated at 0.1.

2. Absorptivity for low temperature radiation of plastic bottles is estimated at 0.9.

3. Mole fraction in gas phase were calculated from saturated vapor pressure of hydrochloric acid at concentration as 35% by weight and at 35 C

4. Solar radiation are results of trial and error to obtain heat for vaporization equal net heat transfer from solar radiation in Table 5.1.

Table 5.6 Calculation for vaporization rate from experimental results in Table4.5

| Hydrochloric acid | | Absorbed water | | vaporization | Total vaporization | Packed absorber | Heat for |
|---|---|---|---|---|---|---|---|
| concentration (% by wt) | temperature (C) | flow rate (kg/hr) | HCl dissolved (% by wt) | rate of HCl (kgmol/S) | rate (kgmol/S) | inlet flow rate (kgmol/m2 S) | vaporization (kJ/S) |
| 35 | 34.5 | 35 | 1.75 | 4.66134E-06 | 5.03929E-06 | 0.00016661 | 0.09072716 |
| 35.3 | 34 | 70 | 0.87 | 4.6347E-06 | 5.01049E-06 | 0.000165658 | 0.09020872 |
| 35.2 | 33 | 89 | 0.96 | 6.50228E-06 | 7.0295E-06 | 0.000232411 | 0.12655883 |
| 35.2 | 34 | 125 | 0.22 | 2.09285E-06 | 2.26254E-06 | 7.48047E-05 | 0.04073464 |
| 35.4 | 34 | 143 | 0.85 | 9.25038E-06 | 1.00004E-05 | 0.000330637 | 0.18004712 |
| 35.2 | 34 | 218 | 0.41 | 6.80213E-06 | 7.35366E-06 | 0.000243129 | 0.13239499 |
| 35.4 | 34 | 324 | 0.14 | 3.45205E-06 | 3.73195E-06 | 0.000123387 | 0.06718994 |
| 35.3 | 33.5 | 502 | 0.16 | 6.11263E-06 | 6.60825E-06 | 0.000218484 | 0.11897478 |
| | | | | Average | 5.87951E-06 | 0.00019439 | 0.10585452 |

Remark 1.Diameter of packed absorber was 0.204 m.

Table 5.7 Program simulated results by using input data from experimental results in Table 4.5

| surrounding temperature (C) | total tank surface (m2) | solar radiation (W/m2) | hydrochloric acid | | heat from radiation (kJ/S) | heat emitted to surrounding (kJ/S) | heat for vaporization (kJ/S) | estimated HCl mole ratio in gas | estimated H2O mole ratio in gas | vaporization rate (kgmol/s) | vaporization rate (kgmol/ m2 S) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | concentration (%by weight) | temperature (C) | | | | | | | |
| 32 | 16 | 200 | 35 | 35 | 0.32 | 0.282857637 | 0.037142363 | 0.925 | 0.075 | 2.063E-06 | 6.30923E-05 |
| 32 | 16 | 250 | 35 | 35 | 0.4 | 0.282857637 | 0.117142363 | 0.925 | 0.075 | 6.5065E-06 | 0.000198985 |
| 32 | 16 | 450 | 35 | 35 | 0.72 | 0.282857637 | 0.437142363 | 0.925 | 0.075 | 2.428E-05 | 0.000742557 |
| 32 | 16 | 600 | 35 | 35 | 0.96 | 0.282857637 | 0.677142363 | 0.925 | 0.075 | 3.7611E-05 | 0.001150235 |
| 32 | 16 | 771.3 | 35 | 35 | 1.23408 | 0.282857637 | 0.951222363 | 0.925 | 0.075 | 5.2834E-05 | 0.001615804 |
| | | | | | | Average | 0.443958363 | | | 2.4659E-05 | 0.000754135 |

Remark

1. Solar absorptivity of storage tank surface is estimated at 0.1.
2. Absorptivity for low temperature radiation of storage tank surface is estimated at 0.9.
3. Mole fraction in gas phase were calculated from saturated vapor pressure of hydrochloric acid at 35% by weight concentration and at35 C, this condition were average condition in experiment.
4. Diameter of packed absorber was 0.204 m.

## 5.2 Calculation for Prediction of Composition in Gas Accuracy Verification.

Experimental results in Table 4.3 indicate that only hydrochloric vaporized from hydrochloric acid. Hydrochloric composition from material balance calculation of experimental results is the confirmation of correction in asumption in the calculation for prediction of composition in gas. At ambeint temperature, hydrochloric composition at saturated condition with comercial hydrochloric acid product (35% by weight concentration) is nearly 1.0.

## 5.3 Packed Absorber Modeling Accuracy Verification

Modeling for packed absorber accuracy is verified by using results of experiment in item 4.3 in Chapter 4 as program input data, selected program is module case E (Packed absorber simulation with inlet gas data), results of program calculation is compared with experimental results. From Table 5.5, the average inlet gas flow rate is used by conversion to 0.473 $Nm^3/h$. Inlet gas phase temperature is assumed that equal hydrochloric acid temperature.

Mole fraction of hydrochloric and water in inlet gas phase are calculated by assumption that gas vaporize in saturated condition and are calculated from hydrochloric acid condition at concentration was 35 % by weight and temperature was 35 °C. Inlet gas density and viscosity are calculated from mole fraction and temperature of gas. Results of program simulation are present in Appendix D and are summarized in Table 5.8

Table 5.8 Program simulated results by using data from experiment in item 4.3 of Chapter 4

For hydrochloric solution storage tank packed absorber

Packed column height 1.5m, diameter .204m, packing type 5/8 inches polypropylene pall rings.

Input data is experimental data from Table 4.6

| Input data | | | | Calculation Results | | | |
|---|---|---|---|---|---|---|---|
| Solution in tank | | Absorbed water | | Outlet Water | | | vent gas |
| temperature (°C) | concentration (%wt) | flow rate ($m^3/h$) | inlet temperature (°C) | outlet pH | hydrochloric in outlet water (% wt) | temperature (°C) | hydrochloric composition ($mg/m^3$) |
| 35 | 35 | 0.035 | 35 | 0.26 | 2.02 | 42.96 | 2438.54 |
| 35 | 35 | 0.07 | 35 | 0.56 | 1.02 | 38.89 | 89.64 |
| 35 | 35 | 0.089 | 35 | 0.66 | 0.80 | 38.01 | 22.24 |
| 35 | 35 | 0.125 | 35 | 0.81 | 0.57 | 37.08 | 2.38 |
| 35 | 35 | 0.143 | 35 | 0.86 | 0.50 | 36.79 | 0.89 |
| 35 | 35 | 0.218 | 35 | 1.05 | 0.33 | 36.10 | 0.03 |
| 35 | 35 | 0.324 | 35 | 1.22 | 0.22 | 35.67 | 0.00 |
| 35 | 35 | 0.502 | 35.5 | 1.41 | 0.14 | 35.35 | 0.00 |

Remark

1. Inlet gas flow rate = 0.474 $Nm^3/h$
2. Mole fraction of hydrochloric in inlet gas = 0.925
3. Mole fraction of water in inlet gas = 0.075
4. Inlet gas density = 1.39 $kg/m^3$
5. Inlet gas viscosity = 0.000149 (kg/m s)

Packed absorber simulation results by using input data at the same value of results of the experiment as described in item 4.3 indicate that assumption and mathematical model in program has some deviation from real condition by comparison in three items.

5.3.1 pH of outlet water and hydrochloric dissolved in outlet water.

Experimental results in Table 4.5 indicate that concentration of hydrochloric dissolved in water are varied with water flow rate but does not depend on water flow rate only. At higher inlet water temperature at flow rate 502 kg/h, temperature 35.5 °C, hydrochloric dissolved in water analyzed result is higher than at water flow rate 324 kg/h, inlet temperature 35 °C, the cause may be from hydrochloric vaporization rate is not constant through experimental period. For analyzed result at absorbed water flow rate 125 kg/h hydrochloric dissolved much differ from other flow rate, the cause may be from error in analysing.

Simulation results indicate that concentration of hydrochloric dissolved in water are varied with variety of water flow rate at smooth trend because modeling is assumed that gas vaporizes at constant rate from hydrochloric acid storage tank which the tank is in steady-state condition. Hydrochloric content in outlet water from experiment differ from program calculated result because water in experiment was not pure water (pH = 7.0) but in modeling water is assigned as pure water.

5.3.2 Absorber outlet water temperature.

Experimental results in Table 4.5 indicted that outlet water temperature are varied with flow rate and depen on inlet water temperature. The results show that the heat of hydrochloric dissolved in water (heat of solution) is the significance heat effect in hydrochloric vapor absorption especially at low water flow rate operation.

Simulation results of program simulated are summarized in Table 5.7 indicate that outlet temperature from calculation are nearly experimental result. Cause of some difference is outlet water temperature in modeling is depend on accuracy of liquid phase heat capacity prediction and amount of hydrochloric dissolved in water. At high water flow rate, calculation results are less difference from experiment because specific heat capacity prediction result of liquid phase (weak acid) was nearly pure water.

5.3.3 Hydrochloric vapor in vent gas of packed absorber

Experimental results in Table 4.6 indicate that hydrochloric vapor is not emitted with vent gas from absorber but simulation results in Table 5.8 shown that absorber can not absorbed total hydrochloric vapor at low absorbed water flow rate operation. Simulation results indicate that mathematical model for predict volumetric mass transfer coefficient give calculation result lower than real condition.

### 5.4 Design Program Testing Result

Packed absorber design program accuracy is verified by use input data from maximum operating condition of existing packed absorber (unit description in Table 4.4) to compare design result with size of existing packed absorber. Design program is tested in case of packed absorber design with fixed absorber diameter, program designed results are shown in Figure D.1 and D.2 in Appendix D. Result of design program are presented in Table 5.9.

Table 5.9 Comparison program design result with existing absorber

| Result | Existing absorber (detail in Table 4.2) | Result of design program at limited pH = 1.5 | Result of design program at limited pH = 2.0 |
|---|---|---|---|
| Height (m) | 1.5 | 1.48 | 0.81 |
| Diameter (m) | 0.204 | 0.204 | 0.204 |
| Water flow rate ($m^3$/h) | 0.1-0.5 | 2.64 | 8.35 |

The results of design program which design packed absorber for maximum operating condition of hydrochloric storage tank in plant site indicate difference from size and design water flow rate of existing packed absorber. The diference depend on selection of solar radiation and absorptivity to use as program input data for gas vaporized to absorber prediction modeling in program.. In Table 5.9 solar radiation and absorptivity value for design program input are average data, solar radiation is assigned at 800 W/$m^2$, absorptivity for solar radiation is 0.1, absorptivity for low temperature radiation is 0.9.