

/(ABSORPTION OF AMMONIA INTO WATER/

by

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## I. Introduction

Ammonia is a flammable and toxic material. Flammability limits of ammonia vapor in ambient air are 28% (rich) to 15% (lean) by volume [1]. The threshold limit value (TLV) that a worker can be exposed to for ammonia is 25 ppm by volume in air as established by the American Conference of Governmental Industrial Hygienists [2]. An ammonia release to the atmosphere first involves an explosive hazard when diluted to the flammability limits and continues to incur a health hazard to concentrations of 25 ppm.

The American National Standards Institute (ANSI)/American Society of Heating, Refrigerating, and Air-Conditioning Engineers (ASHRAE) Standard 15-1978 [3] suggests that a vessel of water may serve as a barrier preventing significant release of ammonia from refrigeration systems to the atmosphere. A ratio of one gallon of water for every pound of ammonia vented is recommended in the standard. A 1988 Building Officials and Code Administrators (BOCA) Code [4] included this recommendation as a requirement for larger ammonia refrigeration systems. Saye [5], on the other hand, has identified technical limitations on the procedure. Comprehensive tests evaluating this suggested practice have not been conducted and are the subject of this paper.

In the experiments discussed in this paper, ammonia was absorbed into water. Three absorption situations or cases were experimentally investigated where the quantity of

ammonia absorbed was measured. The desorption of ammonia from an ammonia-water mixture was also experimentally investigated. Two of the ammonia absorption cases involved ammonia vapor absorption into water, and the remaining case involved liquid ammonia absorption into water.

#### 1. Technical Background

Knowledge of the thermodynamic properties of ammonia, water and ammonia-water mixtures are essential to this project. Keenan and Keyes [6] established tables of pure water properties in 1936, and Haar and Gallagher [7] developed accurate tables of ammonia properties in 1978. For ammonia-water mixtures, Jennings and Shannon [8] in 1938 reviewed the then available experimental data and developed a table of saturated properties. Later, in 1964, Macriss et. al. [9] refined the mixture data with experiments in conjunction with data from the literature by Jennings and Shannon. Schulz [10] in 1971 derived separate equations of state for the vapor and liquid phases over the saturation temperature range of  $-100^{\circ}\text{F}$  ( $-73^{\circ}\text{C}$ ) to  $350^{\circ}\text{F}$  ( $177^{\circ}\text{C}$ ). Recently two investigators have developed equations of state for the ammonia-water system. El-Sayed and Tribus [11] reported a computational scheme predicting ammonia-water mixture properties appropriate for the temperature and pressure ranges of 1 psia (7 kPa) to 1600 psia (10.9 kPa) and  $-80^{\circ}\text{F}$  ( $-60^{\circ}\text{C}$ ) to  $930^{\circ}\text{F}$  ( $500^{\circ}\text{C}$ ). Finally Ziegler and Trepp [12] in 1984 developed an ammonia-water equation of state applicable to the pressure and temperature ranges of  $-45^{\circ}\text{F}$  ( $-43^{\circ}\text{C}$ ) to  $440^{\circ}\text{F}$  ( $227^{\circ}\text{C}$ ) and 3 psia (20 kPa) to 700



psia (5 MPa). Equilibrium values of mixture properties are graphed in an enthalpy-concentration chart by Threlkeld [13].

## 2. Technical Work Statement

The effectiveness of the ANSI/ASHRAE Standard 15-1978 was determined by two parallel efforts -- experiments and analysis. Three cases were tested:

Case 1: Ammonia vapor absorption into a partially filled vessel of water.

Case 2: Ammonia liquid absorption into a partially filled vessel of water.

Case 3: Ammonia vapor absorption into a water spray.

For each case, three ammonia-water ratios were tested:

Ratio 1: One-half pound of ammonia per gallon of water.

Ratio 2: One pound of ammonia per gallon of water.

Ratio 3: Two pounds of ammonia per gallon of water.

Each Case was analytically modeled to predict the water temperature history upon absorption of ammonia and the ammonia absorption rate.

Desorption of ammonia from the ammonia-water mixture was also evaluated. A long term test was conducted where the ammonia content of the liquid mixture was periodically measured.

## II. Experimental Equipment

### 1. Ammonia Supply and Receiver Vessel

Figure 1 is a schematic of the experimental apparatus used. The apparatus was set up in the Animal Science Farm Shop, metal machinery shed, North of the Kansas State University main campus.

The receiver vessel was a cylindrical tank four feet in diameter and 11 feet tall erected vertically. Inside at the bottom of the tank was a steel shroud 40 inches in diameter and 12 inches deep made of 20 gage sheet steel. The shroud, held above the bottom of the tank by PVC pipe sections, had 1/4 inch holes drilled in the bottom to facilitate drainage. The shroud contained a stainless steel mesh 5-6 inches thick supported by PVC pipe sections. The mesh was made of 16 layers of crimped 304 stainless steel woven fabric cloth obtained from the Stainless Steel Woven Fabric Cloth Co., Inglewood, California. The woven fabric cloth was a 1/4" x 1/4" screen made of 0.008 inch diameter wire. Because the layers of woven fabric cloth were corrugated, they were alternated to provide thickness. The layers were sandwiched between two 16 gage expanded steel screens. Steel wire was run through the mesh and screens to prevent movement of the layers, and the sandwich was cut into a cylindrical shape with a hole in the center for the ammonia supply line to pass through.

The ammonia supply line to the receiver tank was a two inch pipe of schedule 40 black steel running the length of the tank and through the stainless steel mesh. A four

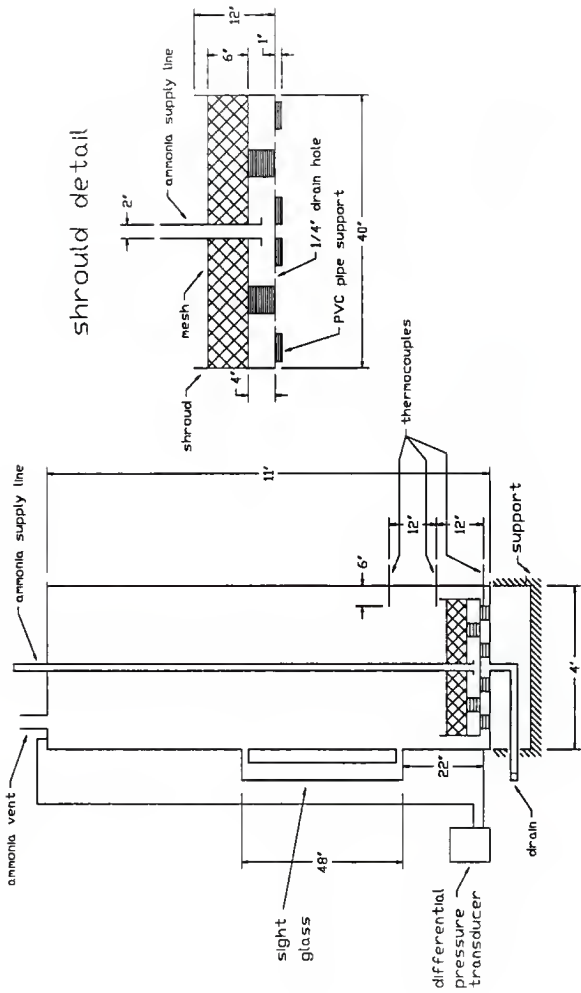


Figure 1: Test Apparatus Schematic.

inch PVC pipe vent was attached to the top of the tank and directed outside the building, and a drain/fill pipe was attached to the bottom of the tank.

Ammonia was supplied to the tank from a 1000 gallon agricultural ammonia tank rented from the Manhattan Farmers Co-op Association. Piping from the ammonia tank to the receiver tank apparatus is shown in Figures 2 and 3 for Cases 1 and 3 and Case 2 respectively. For Cases 1 and 2, the external ammonia supply line was made of schedule 40 black steel pipe two inches in diameter. To approach the desired ammonia flowrate of 40 lbm/min, it was necessary to open both vapor supply valves on the ammonia supply tank. The tank hoses from the ammonia supply valves were attached to a tee on the top of a cylindrical separator vessel six inches in diameter and 12 inches tall. The external ammonia supply line was also attached to the top of the separator. As a valve on the tee was opened, ammonia proceeded from the tee to within two inches of the bottom of the separator; where the liquid would fall to the bottom, and the vapor would escape into the ammonia supply line. For Case 2, the external supply line was made of schedule 40 black steel pipe 1/2 inch in diameter, and had a ball valve mounted in the line to control the liquid ammonia flow. A single hose from the ammonia tank liquid supply valve was connected to the inlet of the supply line.

The receiver vessel was charged with water through the bottom drain pipe for Cases 1 and 2. For Case 3, water was sprayed into the receiver through two water spray fog nozzles mounted in the top of the vessel as shown in Figure

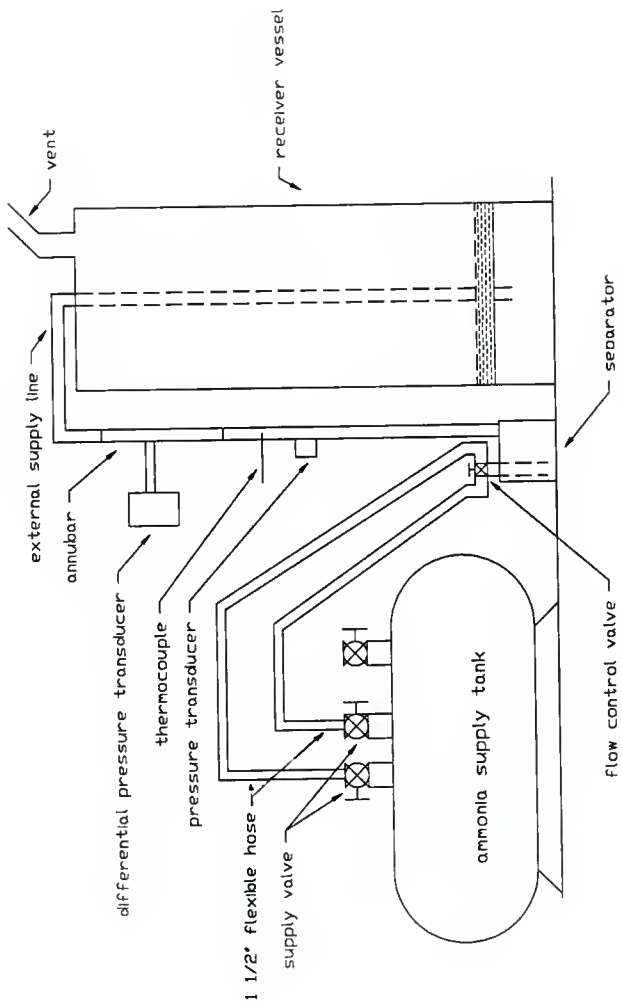


Figure 2: Piping Schematic Between Ammonia Tank and Receiver Tank Apparatus for Vaporous Ammonia Flow.

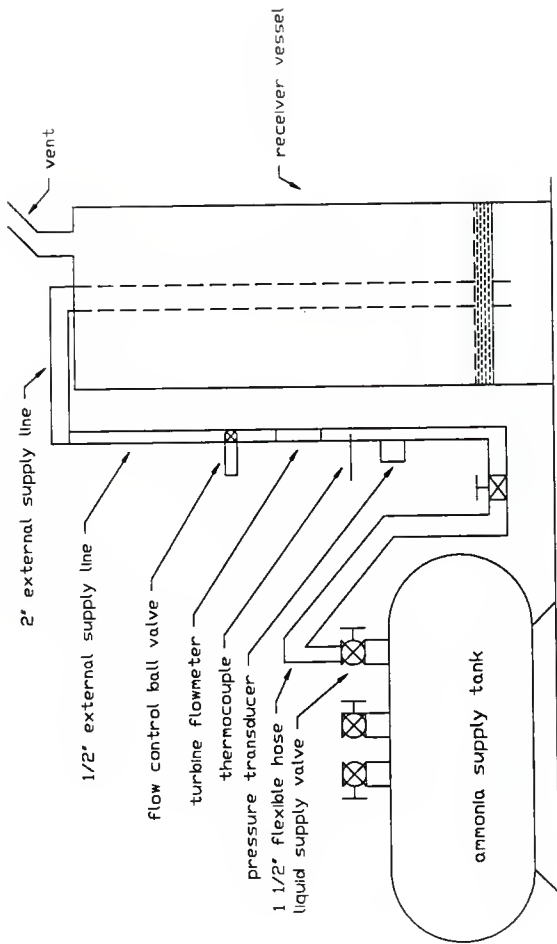


Figure 3: Piping Schematic Between Ammonia Tank and Receiver Tank Apparatus for Liquid Ammonia Flow.

4. The nozzles were the slot-jet type, Model No. 3/4-FF-4.8-SS obtained from Spraying Systems Co., Wheaton, Illinois, and provided a volume mean droplet size of 430  $\mu\text{m}$  at a rated flowrate of 4.8 gal/min (18.2 liters/min) at 40 psig (276 kPa) according to the manufacturer.

## 2. Instrumentation

Four Omega stainless steel sheathed copper-constantan thermocouples were used to measure the temperature of the liquid in the tank and the ammonia supply temperature. A Tobar differential pressure transducer was used to measure the pressure (weight) of the liquid in the tank. This was backed up by an Inferno sight glass mounted on the side of the vessel, through which the level of the fluid in the tank could be seen. A Setra pressure transducer was used to measure the ammonia supply pressure. The flowrate of the ammonia supply was measured by a Dieterich differential pressure transducer connected to a Dieterich annubar flow sensor for Cases 1 and 3, and a Hoffer turbine flowmeter for Case 2. All thermocouples were referenced to a large aluminum block in a thermally insulated box whose temperature was measured by two temperature sensitive solid-state current sources. Table 1 details the instrumentation used and the corresponding ranges. Measurement uncertainties are given in Appendix A. Appendix A also shows the thermocouple and temperature reference circuits.

Three thermocouples were inserted into the receiver vessel near the bottom of the tank below the shroud; 12

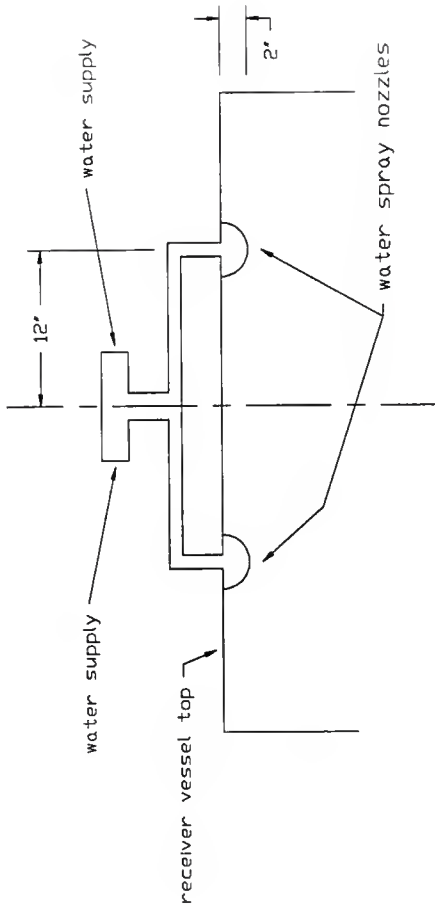


Figure 4: Diagram of Water Droplet Spray Nozzle Placement.



**Table 1  
Instrumentation**

Instrument	Company	Model No.	Serial No.	Range	Output
Type T Thermocouple	Omega Engineering, Inc. Stamford, Connecticut	TQIn-18G-24	--	-300 to 500° F	X5V
Amplifier	Omega Engineering, Inc. Stamford, Connecticut	OMNI-AMP	--	--	--
Differential Pressure Transducer	Tobar, Inc. Tempe, Arizona	75FM1120/ 33212,A2,D3	C8850029W	0-100iwg	1-5V
Amplifier	Tobar, Inc. Tempe, Arizona	75FM1120/ 33211,A1,D3	--	--	--
Sight Glass	Inferno Manufacturing Corp. Shreveport, Louisiana	4 ft, Borosilicate Sight Glass, Carbon Steel Shield			
Pressure Transducer	Setra Systems, Inc. Acton, Massachusetts	P/N 211621	--	0-250 psi	.1-5.1V
Differential Pressure Transducer	Dieterich Standard Boulder, Colorado	1151DP4E 12B1A2	1056436	0-133 iwg	1-5V
Annubar Flow Sensor	Dieterich Standard Boulder, Colorado	DNT-10, 2 inch, Sch 40, CP1S	236218.01.1	0-133 iwg	--
Turbine Flowmeter	Hoffer Flow Controls, Inc. Port Monmouth, New Jersey	HO(1/2)x(1/2)- 1.25-9.5-B-1M-NPT	24795	0-9.5 gal/min	0-5V
Frequency to Voltage Converter	Hoffer Flow Controls, Inc. Port Monmouth, New Jersey	ACC-28-5-1-1	24327	--	--

inches above the bottom of the tank, just above the shroud; and 24 inches above the bottom of the tank. To obtain a reasonable representation of the liquid temperature at each level, the thermocouples were inserted through the wall to a depth of six inches. The fourth thermocouple was inserted into the ammonia supply line external to the tank. The Tobar differential pressure transducer was connected by 1/2 inch flexible rubber hose to the top and bottom of the tank. The pressure transducer was mounted in the external ammonia supply line. For Cases 1 and 3, the annubar flow sensor was mounted in the external ammonia supply line and was attached to the Dieterich differential pressure transducer by 1/2 inch flexible rubber hose. For Case 2, the turbine flowmeter was mounted in the external ammonia supply line. The fourth thermocouple, pressure transducer, and flowmeter were all mounted upstream of the ball valve in the external ammonia supply line. This prevented flashing of the liquid ammonia to atmospheric pressure before the pressure, temperature and flow readings were taken.

### 3. Data Acquisition Equipment

A Zenith 150 computer (IBM compatible), Zenith Data Systems Corp., St. Joseph, Michigan, and a MetraByte Corporation, Taunton, Massachusetts, DAS-8 eight channel, 12 bit, high speed, A/D converter, and timer/counter board were used to record data during the experiments [14]. Each of the instruments had a maximum output of  $\pm 5$  V measured by the eight analog input channels on the DAS-8. Resolution of the voltage measurement was 0.00244 volts. A digital computer

program written in QuickBASIC [15] converted DAS-8 data to actual measured quantities and stored it on a floppy disk. The programs for Cases 1 and 3 and Case 2 are included in Appendix B.

#### 4. Data Reduction

Data recorded during the ammonia release was used to calculate the average temperature of the liquid and the concentration of ammonia in the liquid at each time step. When there were 200 gallons of liquid in the tank, temperature measurements were taken near the top, middle, and bottom of the liquid mixture. The average liquid temperature was obtained by averaging the measurements taken by each of the thermocouples in the tank. Uncertainty of the average temperature is calculated to be  $\pm 3.1^\circ\text{F}$  ( $\pm 1.7^\circ\text{C}$ ).

The mass of ammonia released during the Case 1 and 3 experiments is given by,

$$m_{\text{rel}} = \dot{m}_a \rho_{\text{amm}} \Delta t$$

where,

$m_{\text{rel}}$  = mass of ammonia released, lbm

$\dot{m}_a$  = average mass flowrate of ammonia, lbm/min

$\rho_{\text{amm}}$  = density of ammonia, lbm/ft<sup>3</sup>

$\Delta t$  = total time of ammonia release, minutes

Uncertainty in the mass of ammonia released for Cases 1 and 3 is less than  $\pm 3\%$ .

The mass of ammonia released during the Case 2 experiments is given by,

$$m_{\text{rel}} = \dot{V}_a K \rho_{\text{amm}} \Delta t$$

where,

$\dot{V}_a$  = volumetric flowrate of ammonia, gal/min

K = conversion factor from gallons to ft<sup>3</sup>

Uncertainty in the mass of ammonia released for Case 2 is less than ±3%.

The mass of liquid in the tank is given by,

$$M_i = \frac{P_i A_{\text{tank}} \rho_{\text{water}}}{12}$$

where,

$M_i$  = mass of liquid in the tank, lbm

$P_i$  = pressure transducer reading, iwg

$A_{\text{tank}}$  = cross sectional area of the tank, ft<sup>2</sup>

$\rho_{\text{water}}$  = density of water, lbm/ft<sup>3</sup>

Uncertainty of the mass of liquid in the tank is ±1.5%.

The mass of water at time step zero,  $M_o$ , is the mass of water in the tank before the ammonia flow. During the Case 1 and 2 experiments, the mass of ammonia in the tank and the concentration of ammonia in the liquid are given by,

$$M_{\text{ai}} = M_i - M_o$$

and

$$x_i = \frac{M_{ai}}{M_i}$$

where,

$M_o$  = mass of water initially in the tank, lbm

$M_{ai}$  = mass of ammonia in the tank, lbm

$x_i$  = concentration of ammonia in the liquid

The uncertainties of the mass of ammonia in the tank, and the concentration of ammonia in the liquid are  $\pm 2\%$  and  $\pm 7.5\%$  respectively.

During the Case 3 experiments, the total mass of water sprayed into the tank over a given time is given by,

$$M_{wi} = t_i \dot{V}_w K \rho_{water}$$

where,

$M_{wi}$  = total mass of water sprayed into tank, lbm

$t_i$  = time since start of ammonia flow, min

$\dot{V}_w$  = flowrate of water into the tank, gal/min

$K$  = conversion factor from gallons to  $ft^3$

$\rho_{water}$  = density of water,  $lbm/ft^3$

The flowrate of water was measured to be 7 gal/min for these experiments. Uncertainty of this water flowrate is  $\pm 7\%$ .

The mass of ammonia in the tank and the concentration of ammonia in the liquid are given by,

$$M_{ai} = M_i - M_{wi}$$

and

$$x_i = \frac{M_{ai}}{M_i}$$

where,

$M_{ai}$  = mass of ammonia in the tank, lbm

$x_i$  = concentration of ammonia in the liquid

The uncertainties of the mass of ammonia in the tank, and the concentration of ammonia in the liquid are  $\pm 3.3\%$  and  $\pm 3.6\%$  respectively.

### III. Test Procedures and Repeatability

All instrument output signals were sampled once every five seconds during the ammonia flow, and once every 30 minutes from 2 to 48 hours after the flow. Each Case was repeated 4-5 times at ammonia-water Ratio 1 (see page 3 for a summary of "Ratio" numbers and their meaning) to establish repeatability of the instruments and test procedures. It was assumed that the repeatability of the tests would be the same at Ratios 2 and 3 as at Ratio 1. Because the tests could not be repeated identically each time due to environmental factors outside experimental control, the ratios of the average temperature rise versus the mass of ammonia released ( $\Delta T_{ave}/m_{rel}$ ) and the rate of concentration rise versus the average flowrate ( $\Delta x/\Delta t/\dot{m}$ ) were used to compare the repeated tests.

#### 1. Case 1

Case 1 tests had ammonia flowrates of 10, 20, and 40 lbm/min corresponding to ammonia-water Ratios 1, 2, and 3 respectively, with each ammonia flow lasting for 10 minutes. The receiver vessel was charged with 200 gallons of water before the computer sampling program was started. Ten or more seconds after the program was started, to allow for determination of initial conditions, the valve connecting the ammonia tank hoses to the separator was opened, starting ammonia flow into the receiver vessel. The ammonia flowrate was monitored on the computer screen and adjusted manually

at the valve to obtain the desired flow. After 10 minutes, the ammonia flow was shut off at the valve. Five second sampling intervals were allowed to continue for approximately 200 seconds before the program was switched to the 30 minute sampling rate.

The test at ammonia-water Ratio 1 for Case 1 was repeated five times. Comparisons for the five tests are shown in Figures 5 and 6 and Table 2.

**Table 2**

<u>Case 1 Repeatability Comparison</u>		
Test No.	$\Delta T_{ave}/\dot{m}_{rel}$	$\Delta x/\Delta t/\dot{m}$
	(°F/lbm)	(%/lbm)
1	3.48	.0590
2	3.53	.0605
3	3.41	.0582
4	3.53	.0577
5	3.63	.0565

The average temperature rise versus mass of ammonia released was repeatable to within  $\pm 3.5\%$ , and the rate of concentration rise versus average flowrate was reproducible to within  $\pm 3.7\%$ .

## 2. Case 2

Case 2 tests had ammonia flowrates of 2, 4, and 8 gallons/min (roughly equivalent to 10, 20, and 40 lbm/min) corresponding to ammonia-water Ratios 1, 2, and 3



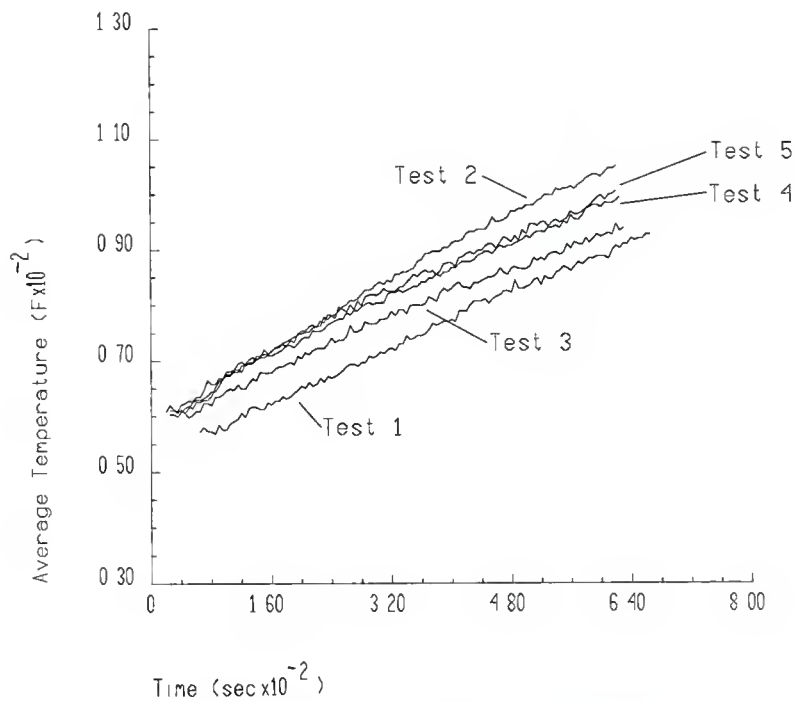


Figure 5: Variation of Liquid Average Temperature for Ammonia Vapor Absorption into Water Repeatability Tests.

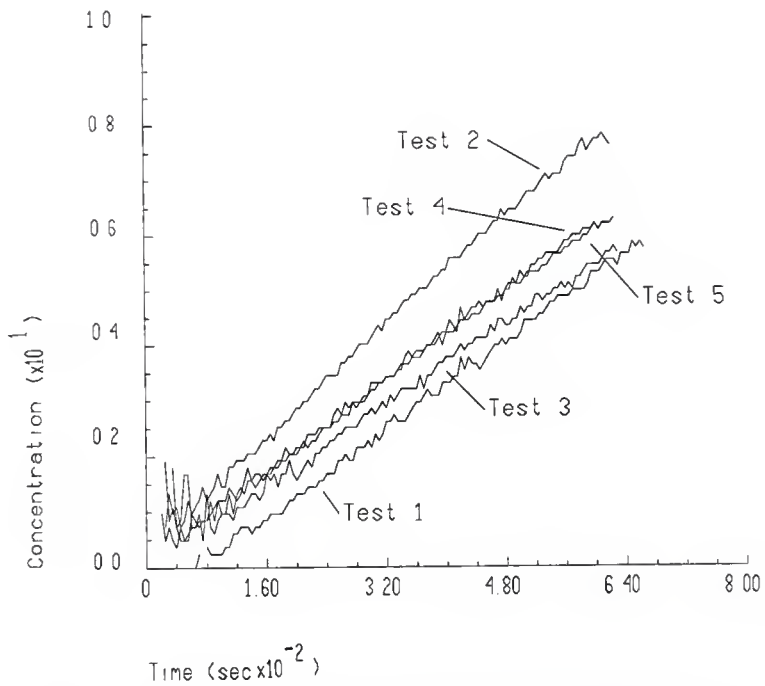


Figure 6: Variation of Concentration for Ammonia Vapor Absorption into Water Repeatability Tests.

respectively, with each ammonia flow lasting for 10 minutes. The tests were run identically to the Case 1 tests except that the valve used to regulate ammonia flow was in the external ammonia supply line downstream from the pressure transducer, thermocouple, and flowmeter. This prevented flashing of the ammonia to atmospheric pressure before the pressure, temperature, and flow readings were taken.

The test at ammonia-water Ratio 1 for Case 2 was repeated four times. Comparisons are shown for the four tests in Figures 7 and 8 and Table 3.

**Table 3**

<u>Case 2 Repeatability Comparison</u>		
Test No.	$\Delta T_{ave}/m_{rel}$	$\Delta x/\Delta t/\dot{m}$
	(°F/lbm)	(%/lbm)
1	.153	.0560
2	.133	.0574
3	.107	.0611
4	.099	.0521

The average temperature rise versus mass of ammonia released was repeatable to within 25%, and the rate of concentration rise versus average flowrate was reproducible to within 8%. The repeatability range of the average temperature rise versus mass of ammonia released for Case 2 was larger by a factor of 10 than for Case 1 because the values of average temperature rise versus mass of ammonia released were smaller by a factor of 10. The smaller values resulted

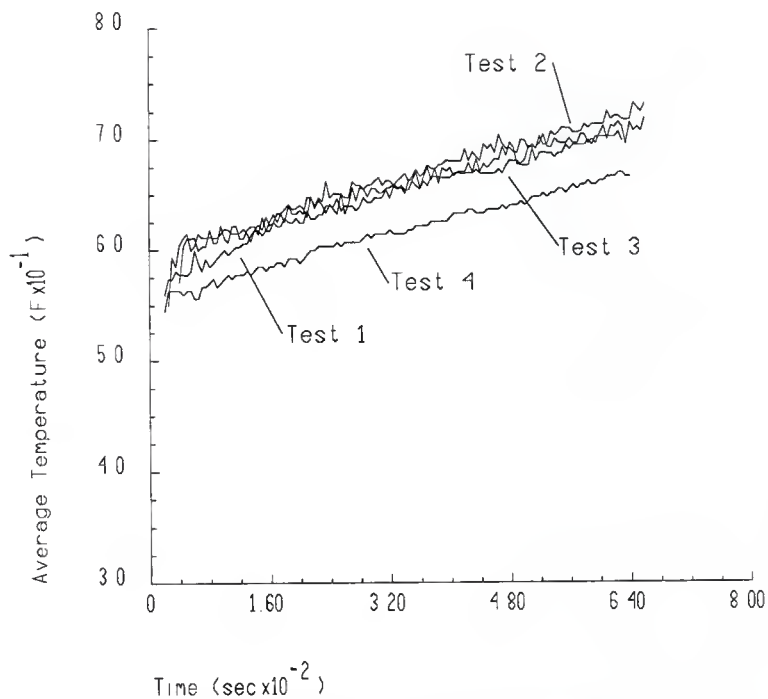


Figure 7: Variation of Liquid Average Temperature for Ammonia Liquid Absorption into Water Repeatability Tests.

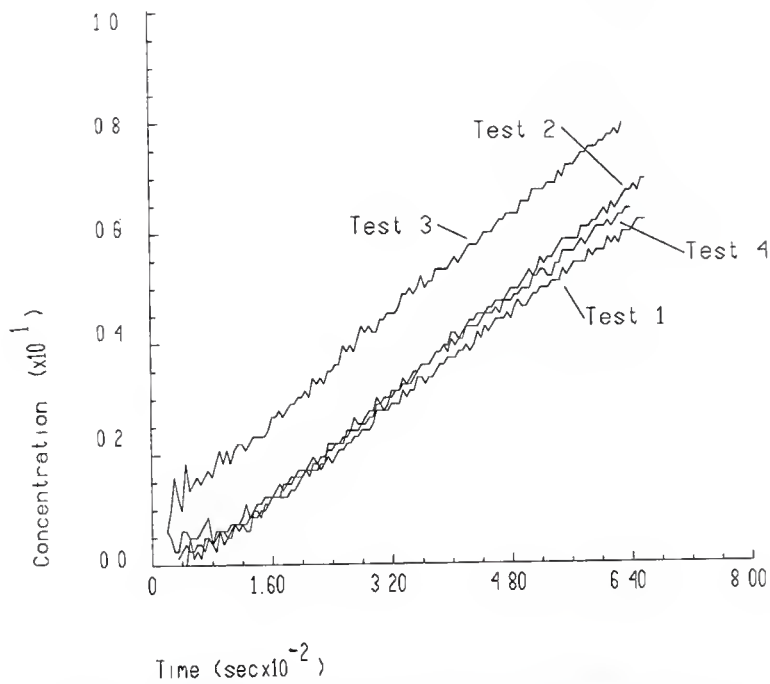


Figure 8: Variation of Concentration for Ammonia Liquid Absorption into Water Repeatability Tests.

because the temperature rise was not as large for Case 2 as for Case 1.

### 3. Case 3

Case 3 tests were run in a water spray of approximately 7 gal/min (26.5 liters/min) at 30 psi (207 kPa). Ammonia flowrates were 3.5, 7, and 14 lbm/min corresponding to ammonia-water Ratios 1, 2, and 3 respectively. Tests began with the receiver vessel empty. Water spray was initiated and the computer sampling program started. After 10 or more seconds to establish initial conditions, the ammonia flow was started by opening the valve connecting the ammonia tank hoses to the separator. Adjustments to the ammonia flow were made manually at the valve by monitoring the flowrate on the computer screen. The ammonia flow and then the water flow were shut off after the tank had filled to approximately 200 gallons as seen in the sight glass. Sampling was allowed to continue for approximately 200 seconds before the sampling program was switched to the 30 minute sampling rate.

The test at ammonia-water Ratio 1 for Case 3 was repeated five times. Comparisons are shown for the five tests in Figure 9 and Table 4. The average temperature rise versus mass of ammonia released was repeatable to within 14%. Note that in Figure 9, all of the curves follow the same pattern showing that identical processes were occurring during each test. The rate of concentration rise versus average flowrate was only repeatable to within 130%. A comparison plot of this data is not included.

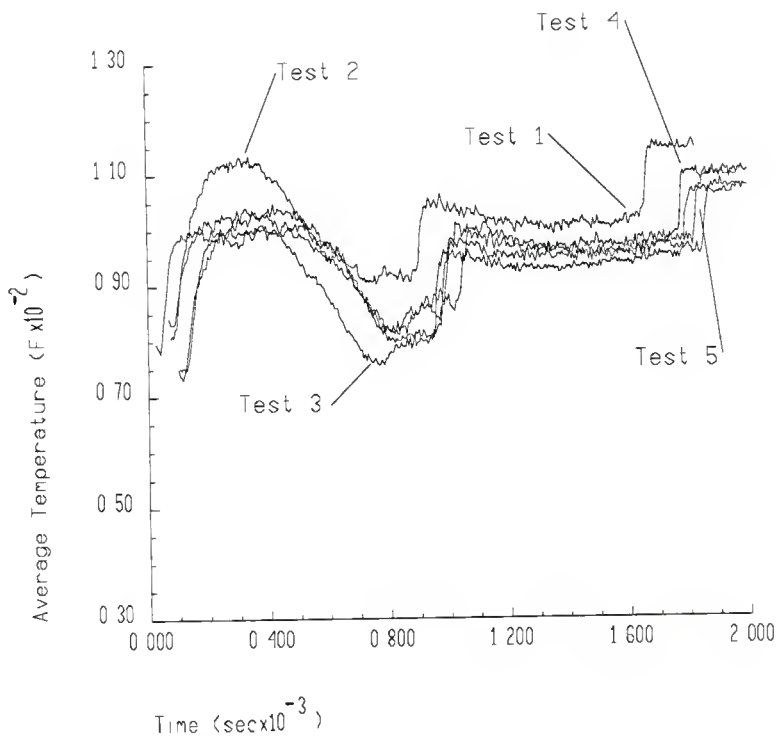


Figure 9: Variation of Liquid Average Temperature for Ammonia Vapor Absorption into Water Spray Repeatability Tests.

Table 4

<u>Case 3 Repeatability Comparison</u>		
Test No.	$\Delta T_{ave}/m_{rel}$	$\Delta x/\Delta t/\dot{m}$
	(°F/lbm)	(%/lbm)
1	8.52	.0340
2	7.24	.0170
3	7.52	.0093
4	8.79	.0124
5	6.68	.0077

#### 4. Desorption

Experiments were conducted to investigate the desorption of ammonia from an ammonia-water mixture. Twelve steel 55 gallon drums were used to simulate the receiver tank and an automotive heater hose approximately two feet long served as a vent. The inside diameter of the hose was 3/4 inch.

The drums were divided into two groups of six drums each -- one group to remain inside, unexposed to sunlight, and the other group outside, exposed to the sun. In each group, two drums served as experimental controls where only water was added. The remaining four drums of each group contained differing levels of ammonia concentration varying from 18% to 27%. Of course, the outside drums were exposed to weather conditions that prevailed over the duration of the test. The unexposed drums were located inside the metal



storage shed close to the receiver tank used in the absorption tests.

The exposure tests lasted 50 days, starting June 30, 1989 and continuing through August 19. This time duration is much longer than would have been possible with the receiver tank itself. Review of the long term sampling data from the receiver tank indicated negligible ammonia loss as the decrease in liquid mixture height in the tank was immeasurable even after several days. Therefore, the drum exposure tests were conducted to obtain reliable long term data.

The volume of ammonia-water mixture added to the drums was based on the conditions that existed in the receiver tank. The ratio of the volume occupied by the water to that of the total receiver tank volume was 0.194. For the drums this resulted in a liquid mixture volume of 10.6 gal (40.1 liters) or about 90 lbm (41 kg) of water. All the drums used in the exposure test were filled to this volume ratio.

#### IV. Results

Experimental results are first compared to saturation conditions projected by the equilibrium chart in Figure 10. Plots of the experimental results are given in Figures 11-37. Table 5 details which Figures correspond to which Cases and Ratios. Plots of other measurements taken during these experiments are given in Appendix C.

Table 5

<u>Figure Case and Ratio Designations</u>			
Case	1	2	3
<u>Ratio</u>			
1	11-13	14-16	17-19
2	20-22	23-25	26-28
3	29-31	32-34	35-37

All ammonia-water Ratios are compared at each Case to determine the effects of ammonia-water Ratio on ammonia absorption. All three Cases are then compared at each ammonia-water Ratio to determine the effects of absorption situation (Case) on ammonia absorption. Other phenomena observed during testing are then discussed followed by desorption test results.

The influence of the mesh geometry on the ammonia absorption is not known since the mesh configuration remained the same throughout all of the experiments in this research. Although the mesh may have been over- or under-designed, for the purposes of this research it was assumed

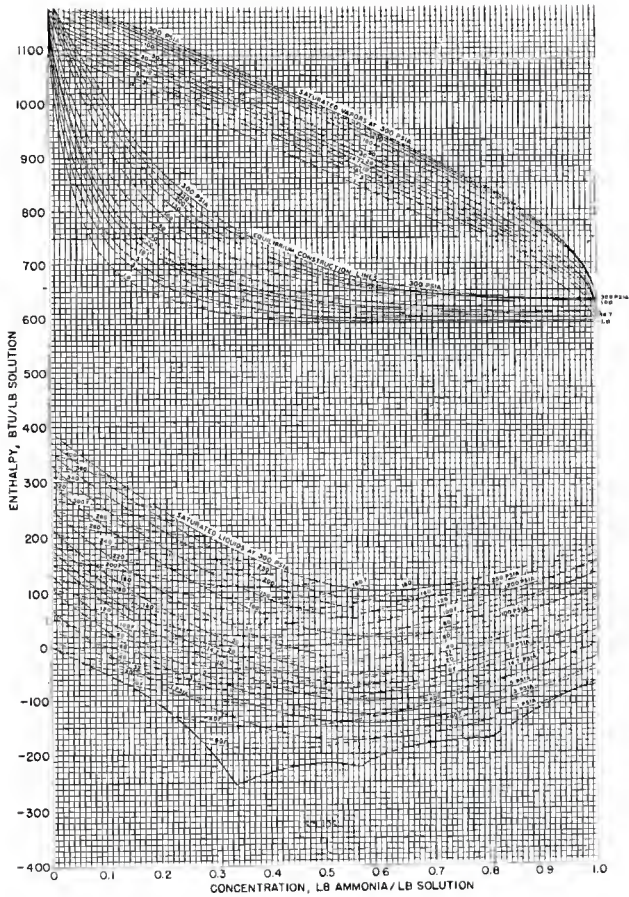


Figure 10: Ammonia-Water Mixture Equilibrium Chart.

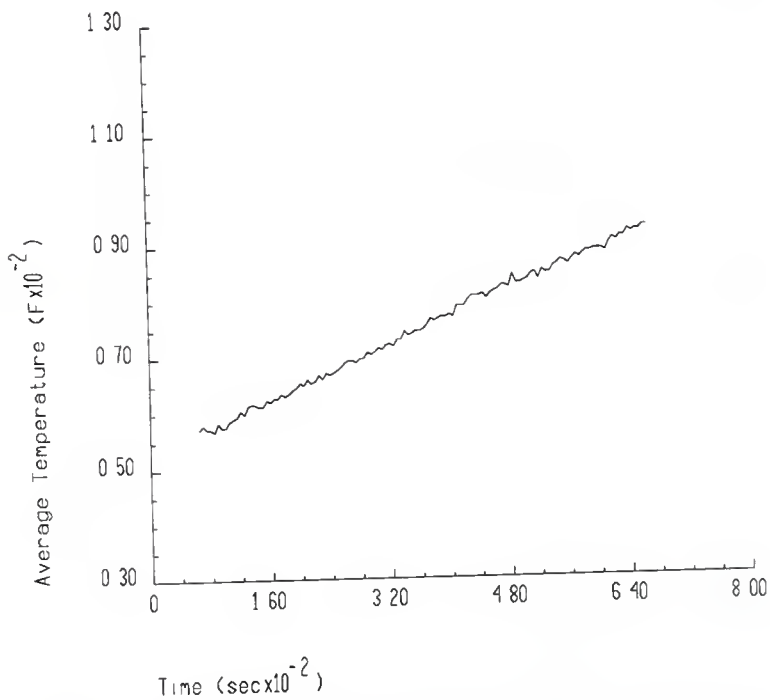


Figure 11: Variation of Average Temperature for Ammonia Vapor Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

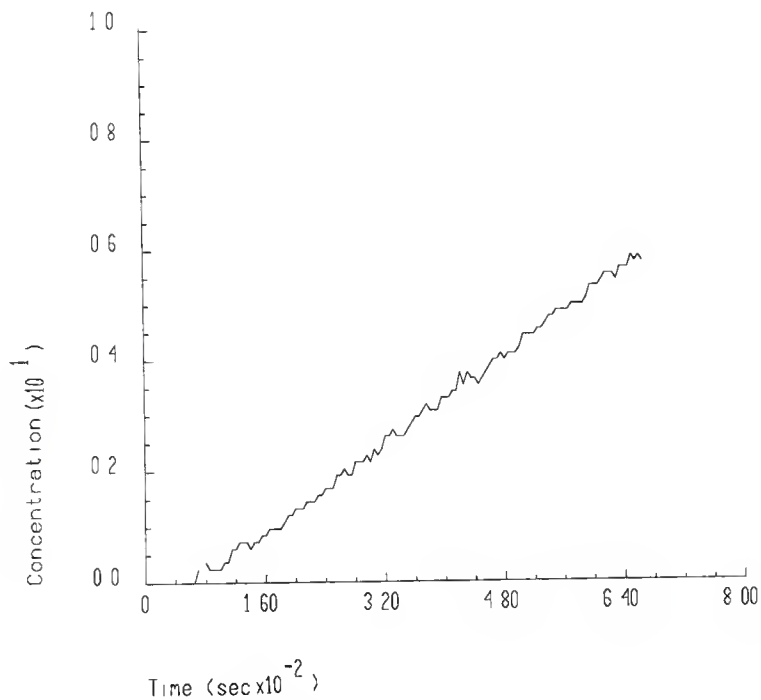


Figure 12: Variation of Concentration for Ammonia Vapor Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

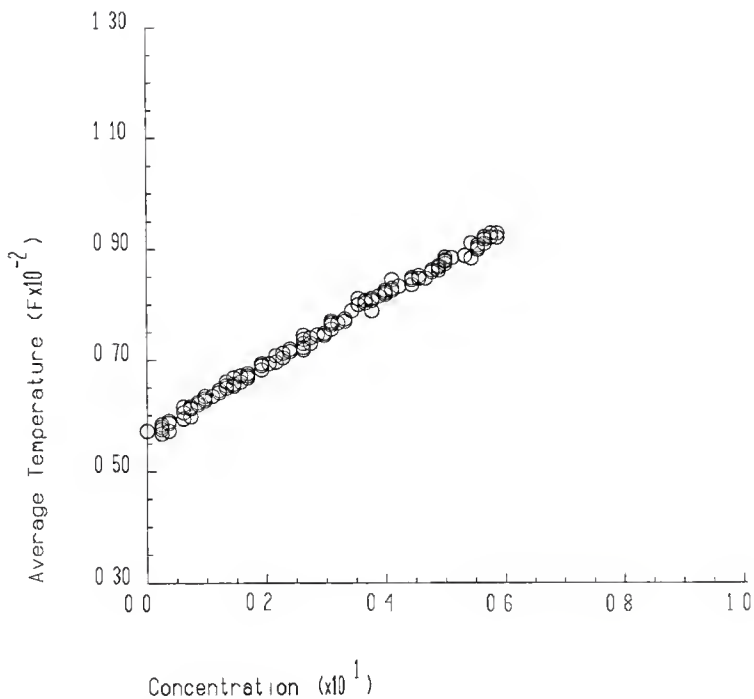


Figure 13: Concentration versus Average Temperature for Ammonia Vapor Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

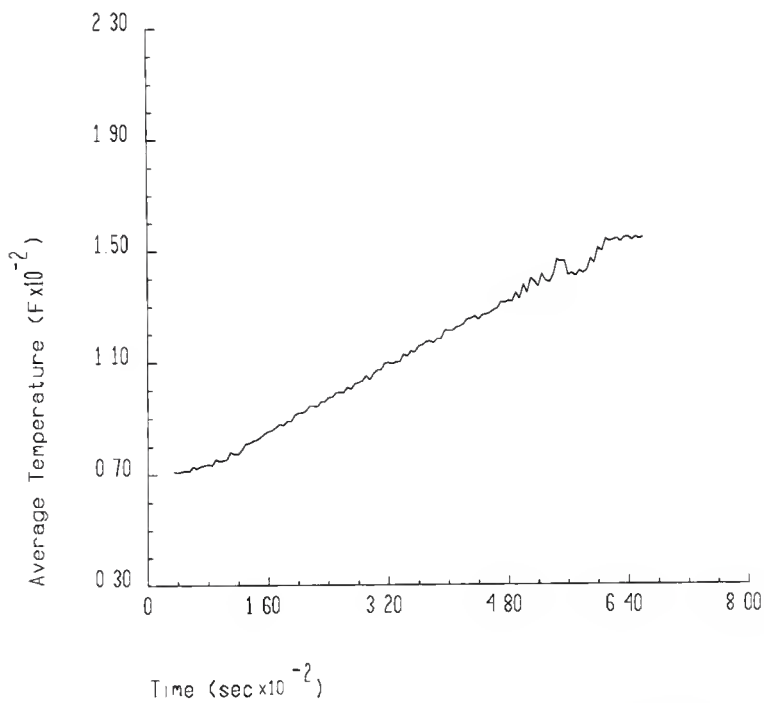


Figure 14: Variation of Average Temperature for Ammonia Vapor Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

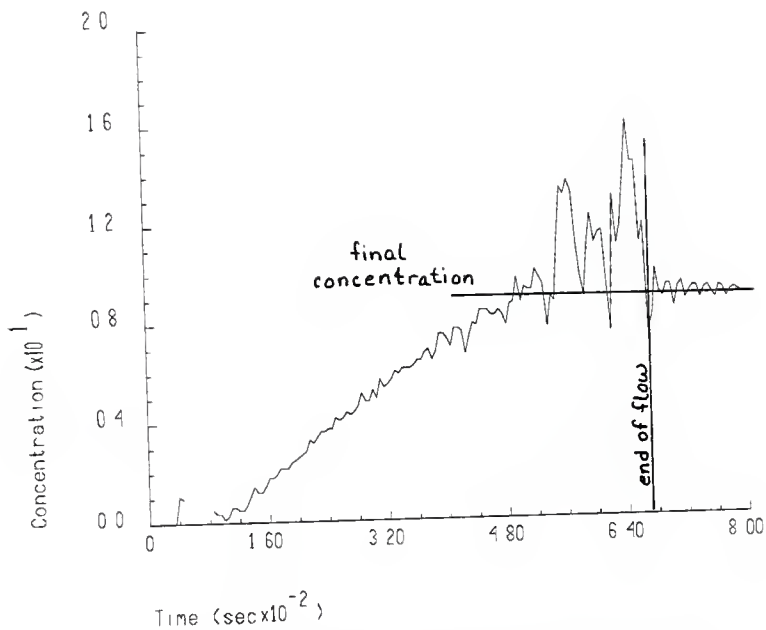


Figure 15: Variation of Concentration for Ammonia Vapor Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.



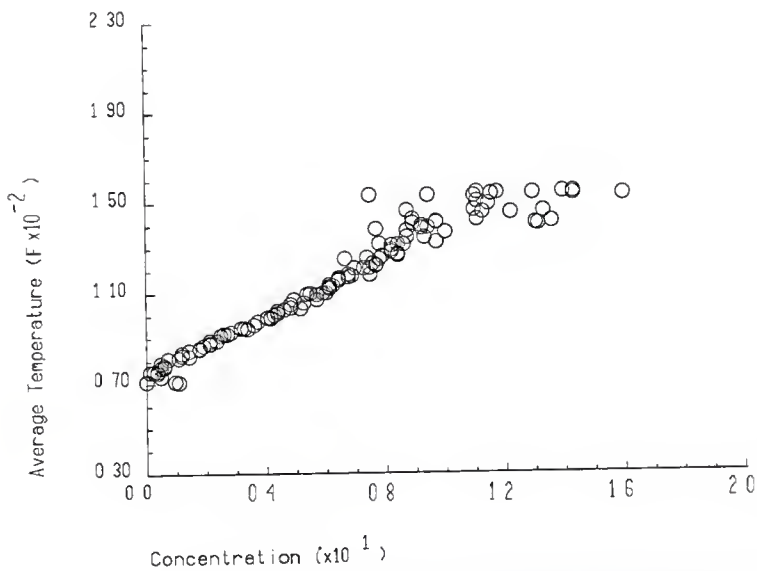


Figure 16: Concentration versus Average Temperature for Ammonia Vapor Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

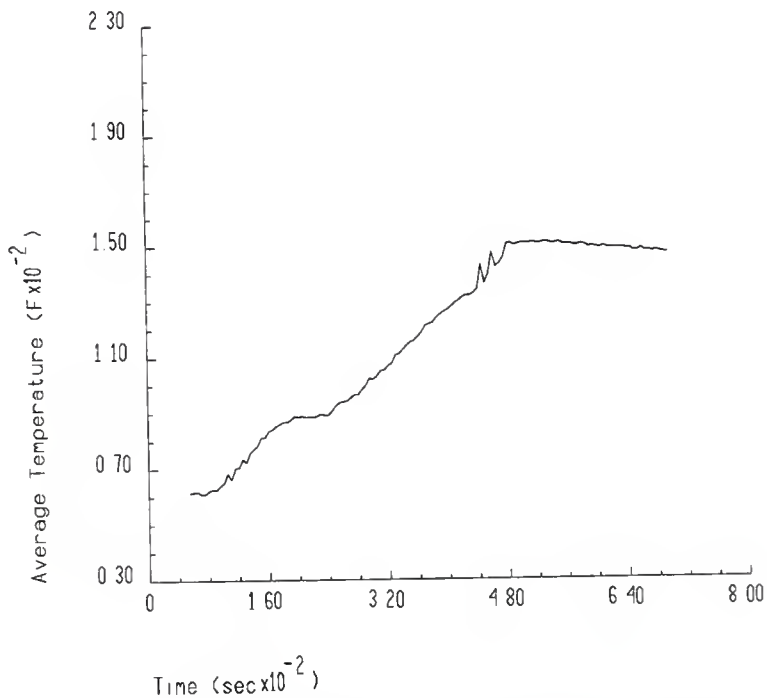


Figure 17: Variation of Average Temperature for Ammonia Vapor Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

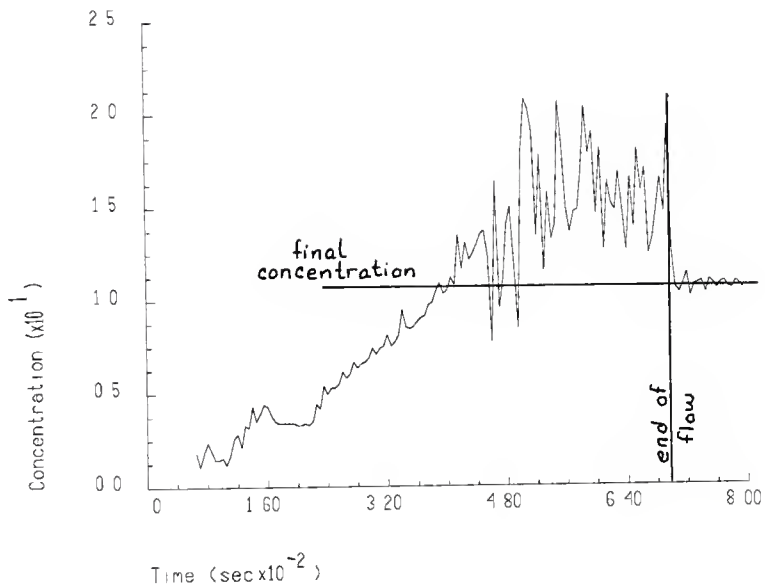


Figure 18: Variation of Concentration for Ammonia Vapor Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

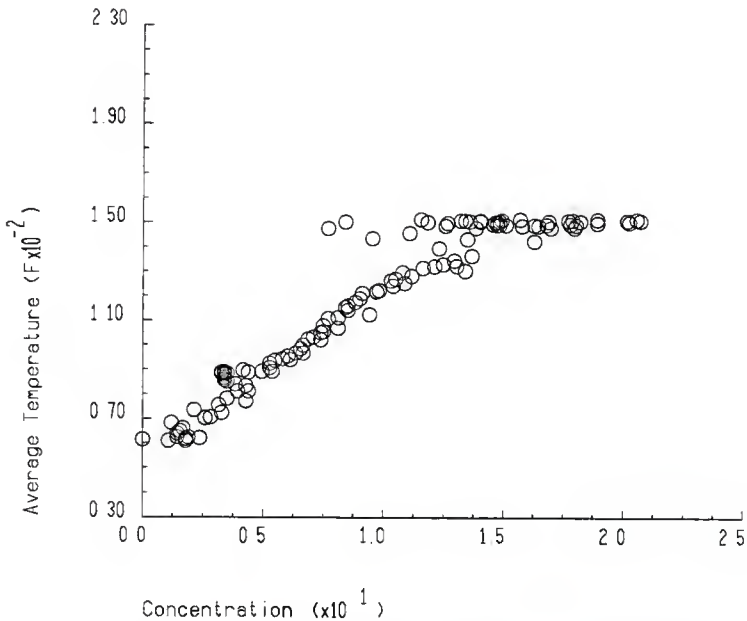


Figure 19: Concentration versus Average Temperature for Ammonia Vapor Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

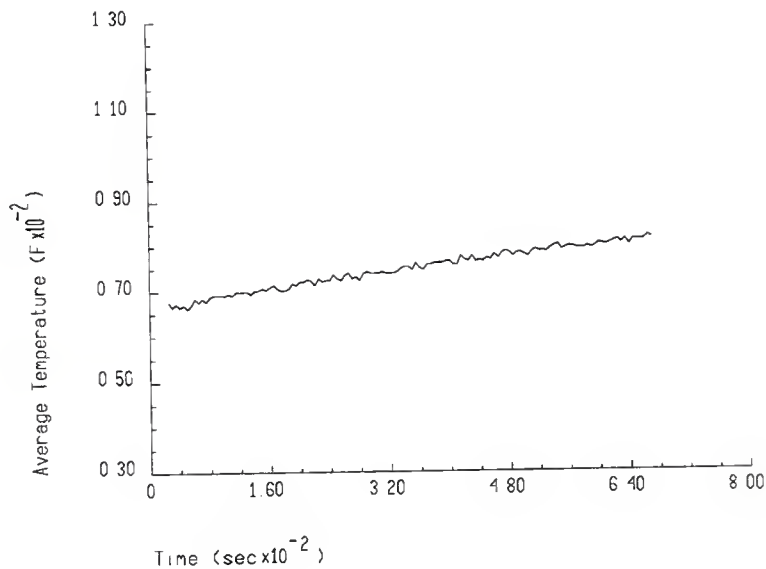


Figure 20: Variation of Average Temperature for Ammonia Liquid Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

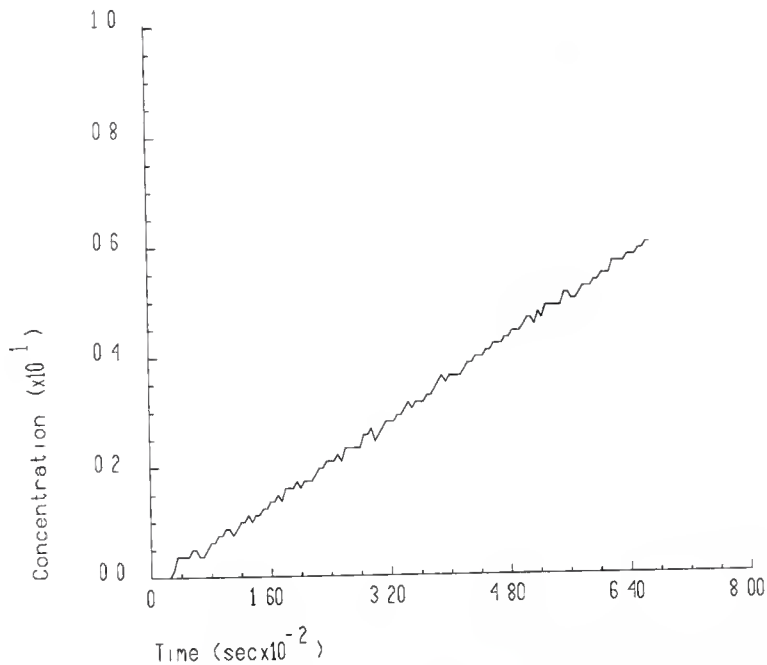


Figure 21: Variation of Concentration for Ammonia Liquid Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

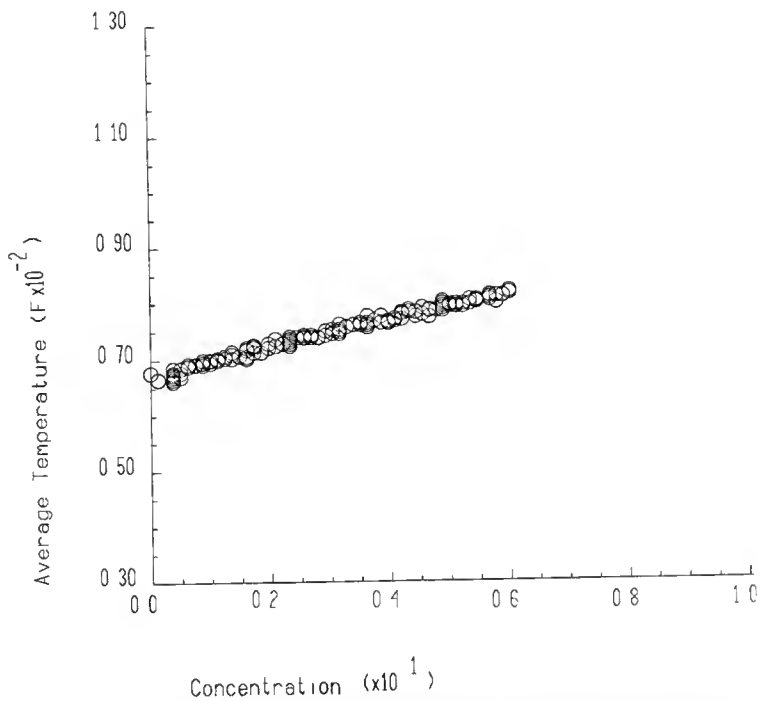


Figure 22: Concentration versus Average Temperature for Ammonia Liquid Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

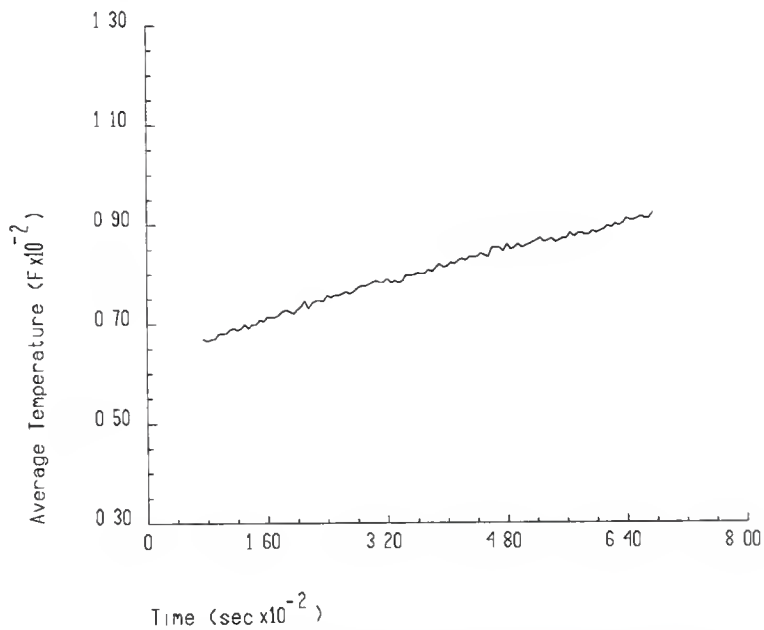


Figure 23: Variation of Average Temperature for Ammonia Liquid Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.



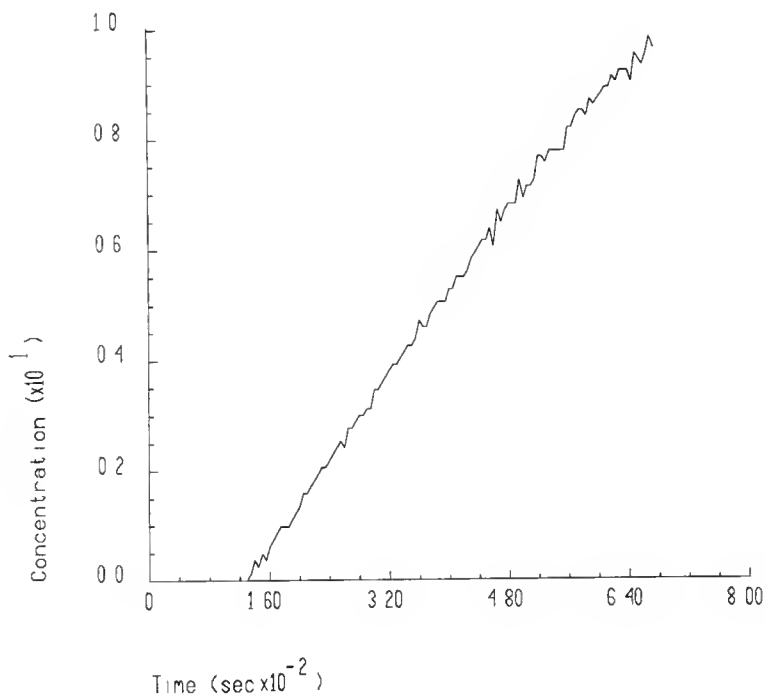


Figure 24: Variation of Concentration for Ammonia Liquid Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

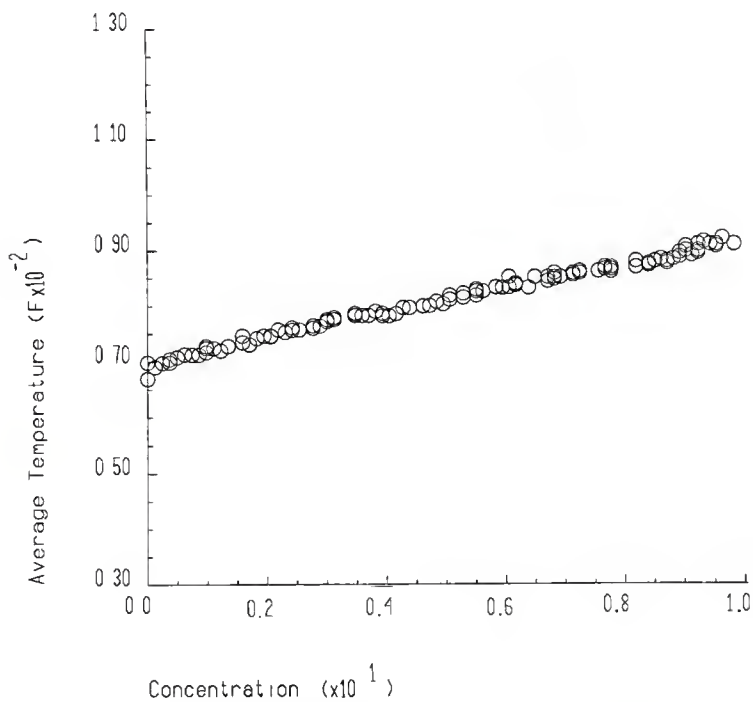


Figure 25: Concentration versus Average Temperature for Ammonia Liquid Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

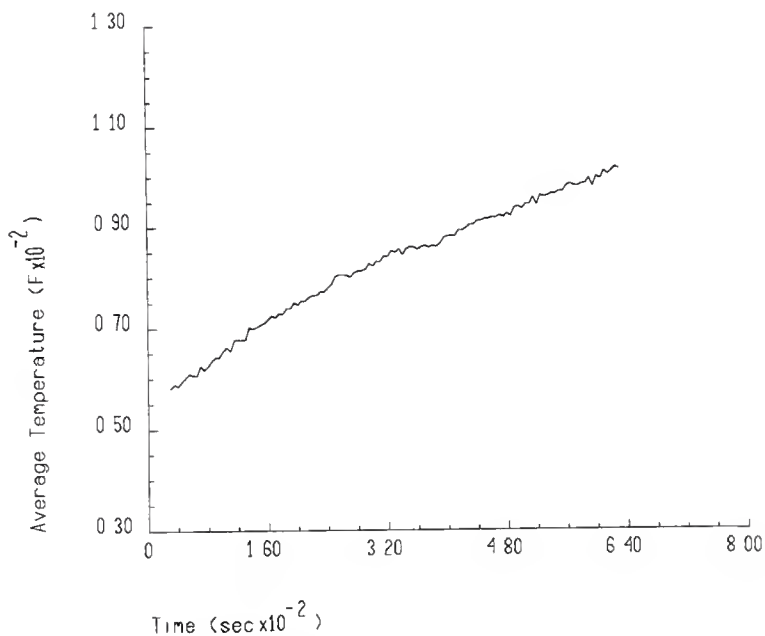


Figure 26: Variation of Average Temperature for Ammonia Liquid Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

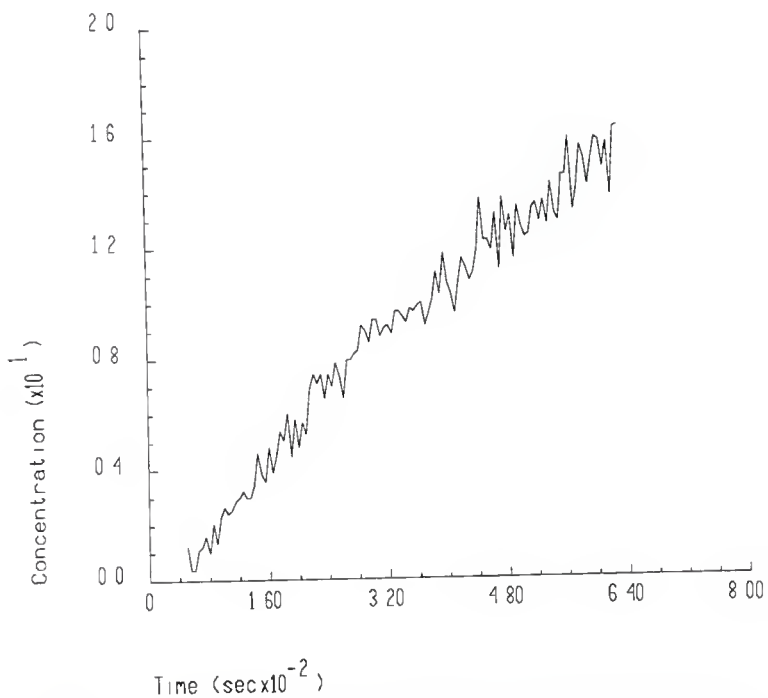


Figure 27: Variation of Concentration for Ammonia Liquid Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

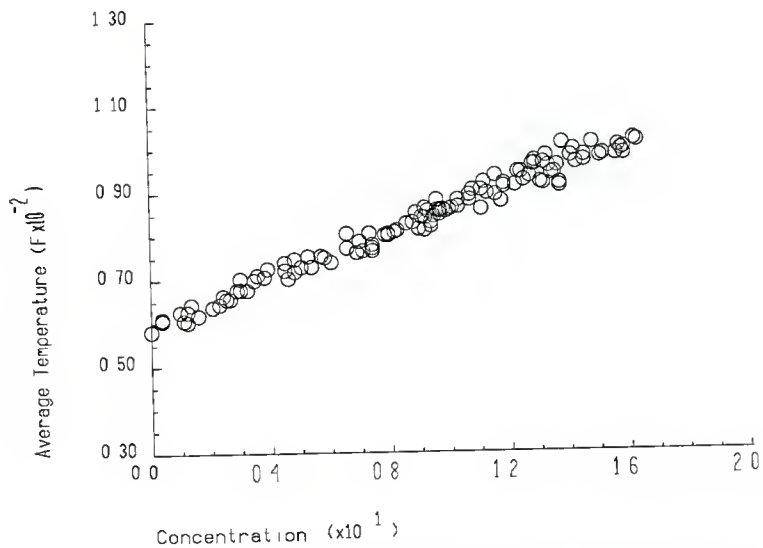


Figure 28: Concentration versus Average Temperature for Ammonia Liquid Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

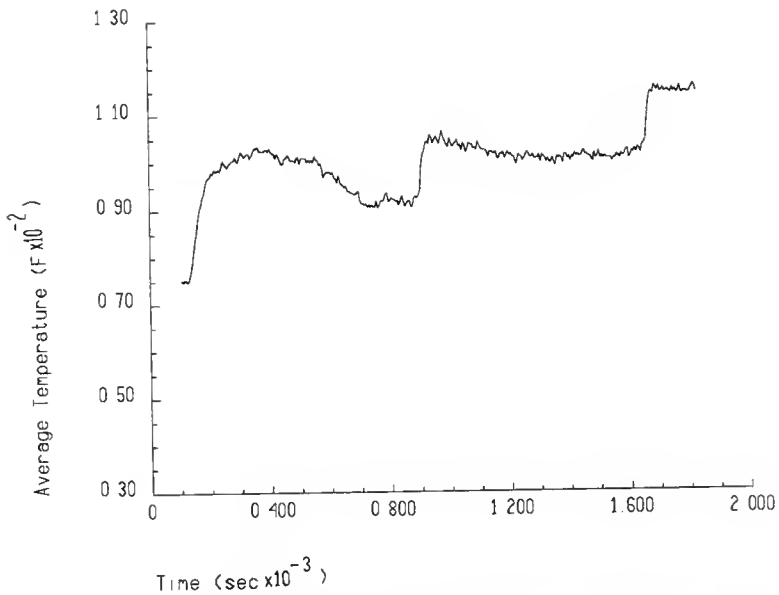


Figure 29: Variation of Average Temperature for Ammonia Vapor Absorption into Water Spray Ending at 0.5 Pound of Ammonia per Gallon of Water.

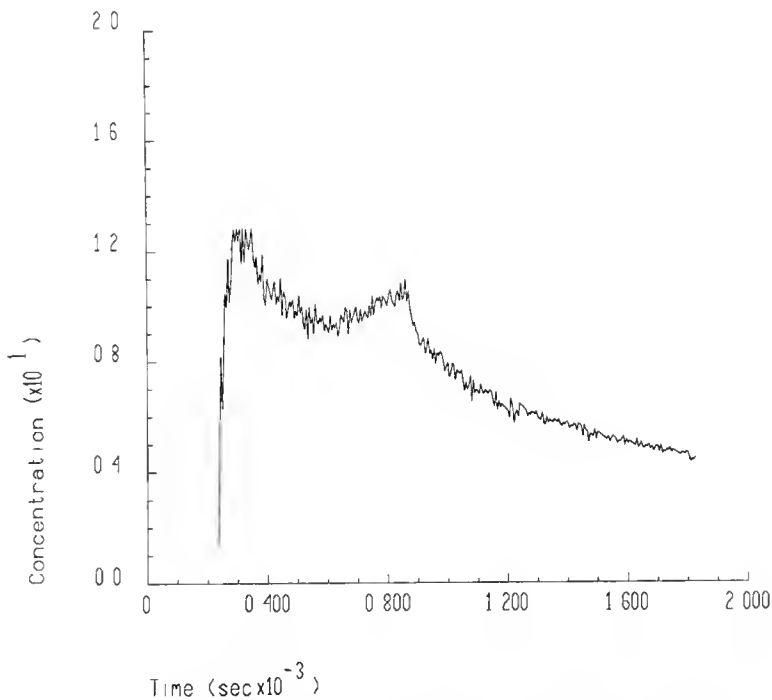


Figure 30: Variation of Concentration for Ammonia Vapor Absorption into Water Spray Ending at 0.5 Pound of Ammonia per Gallon of Water.

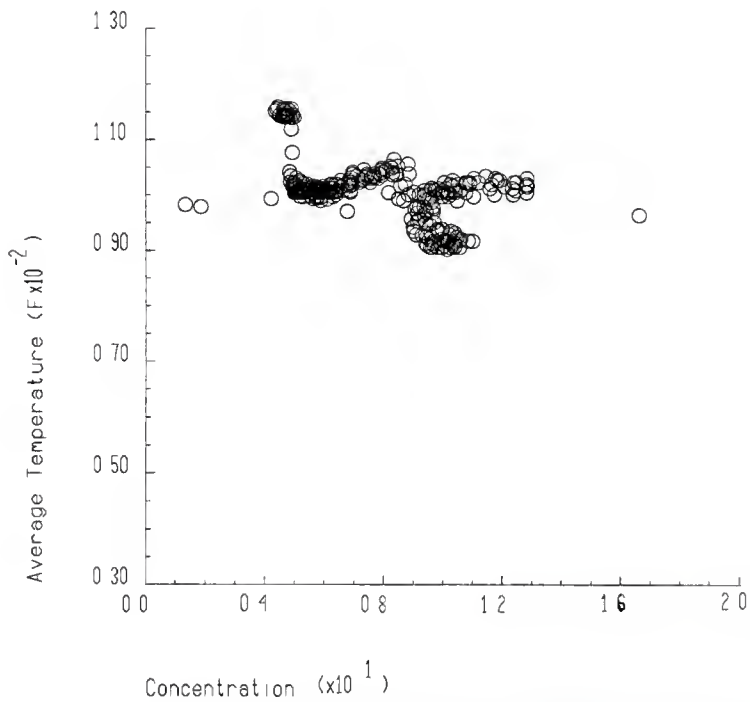


Figure 31: Concentration versus Average Temperature for Ammonia Vapor Absorption into Water Spray Ending at 0.5 Pound of Ammonia per Gallon of Water.



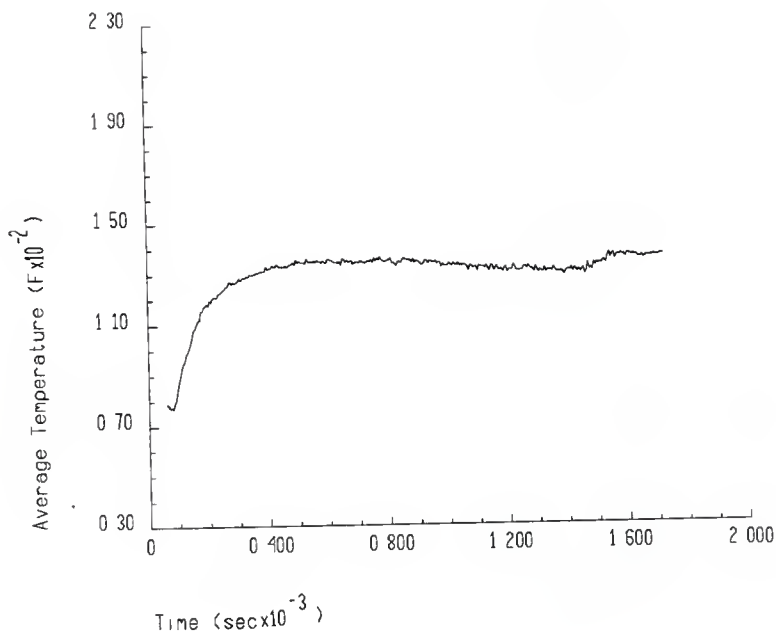


Figure 32: Variation of Average Temperature for Ammonia Vapor Absorption into Water Spray Ending at 1 Pound of Ammonia per Gallon of Water.

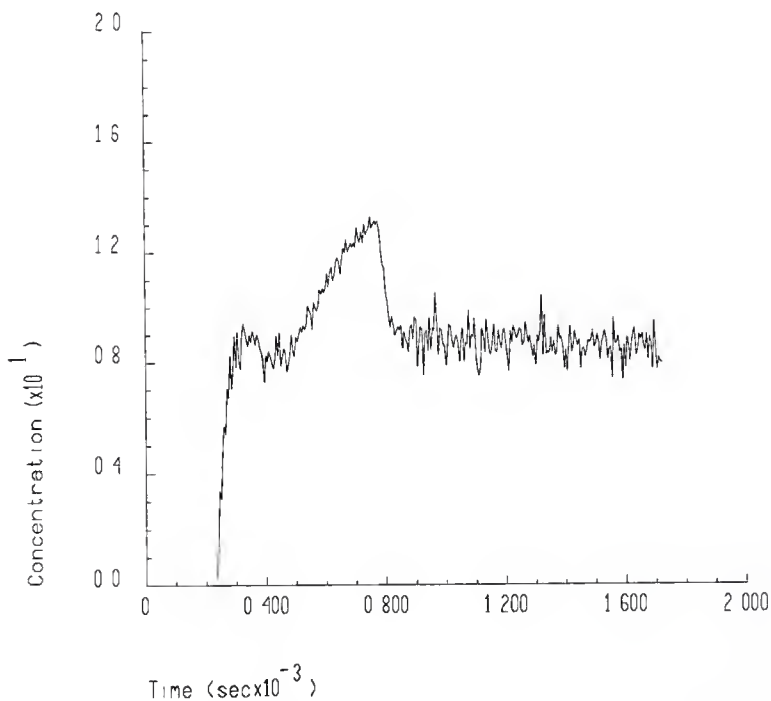


Figure 33: Variation of Concentration for Ammonia Vapor Absorption into Water Spray Ending at 1 Pound of Ammonia per Gallon of Water.

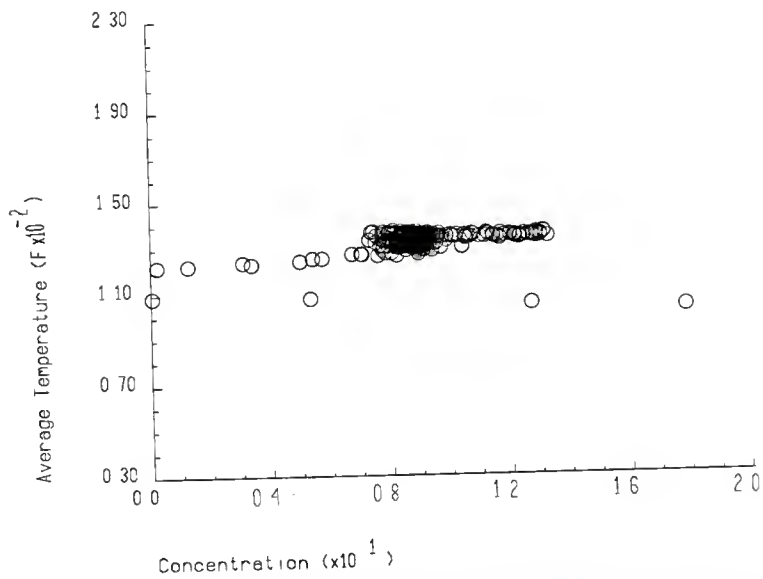


Figure 34: Concentration versus Average Temperature for Ammonia Vapor Absorption into Water Spray Ending at 1 Pound of Ammonia per Gallon of Water.

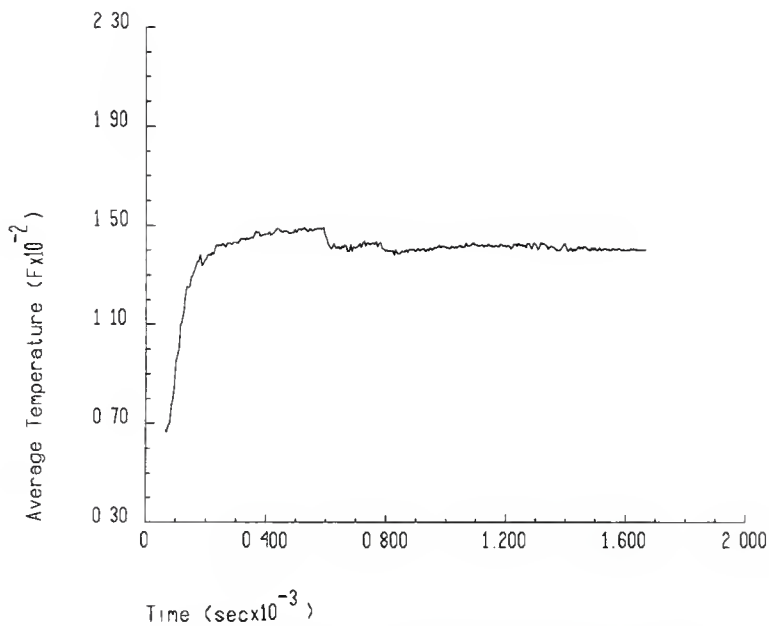


Figure 35: Variation of Average Temperature for Ammonia Vapor Absorption into Water Spray Ending at 2 Pounds of Ammonia per Gallon of Water.

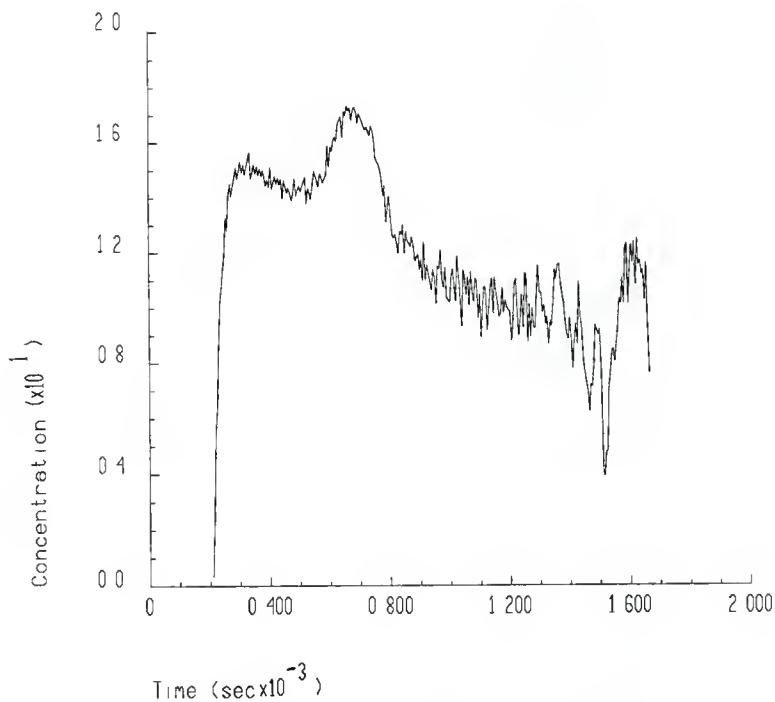


Figure 36: Variation of Concentration for Ammonia Vapor Absorption into Water Spray Ending at 2 Pounds of Ammonia per Gallon of Water.

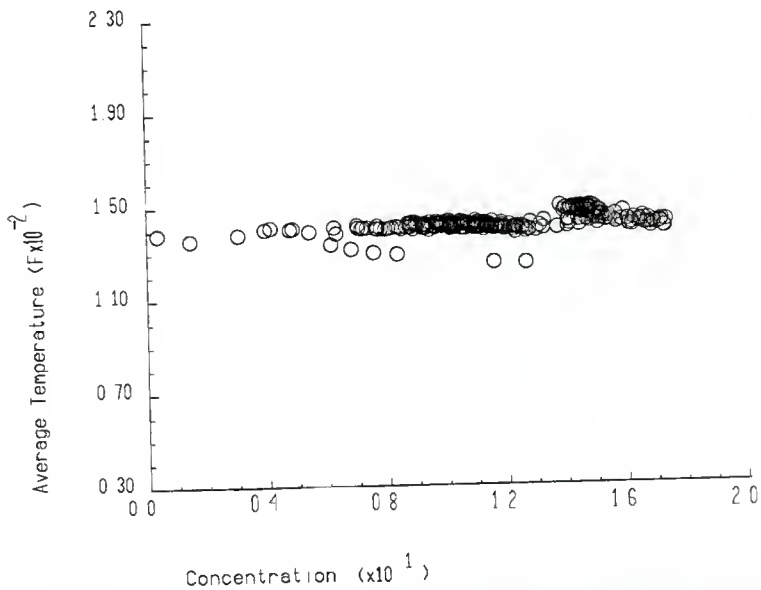


Figure 37: Concentration versus Average Temperature for Ammonia Vapor Absorption into Water Spray Ending at 2 Pounds of Ammonia per Gallon of Water.

to develop the best mixing and ammonia bubble breakup possible. It also remains that an effective configuration might be designed at a lower cost.

#### 1. Saturation Conditions

Figure 10 shows variations in the concentration of ammonia-water mixtures with temperature and pressure. The graph may be used to project saturation conditions of any ammonia-water mixture with a known initial temperature and concentration.

In this research, the initial concentrations were always 0%, and the initial temperatures ranged from 57°F (14°C) to 88°F (31°C). The projected range of saturation concentrations are about 11% at the low initial temperature to about 8.5% at the high initial temperature. Corresponding saturation temperatures are about 160°F (71°C) and 145°F (63°C).

Table 6 details the initial and saturation conditions for those experiments that reached saturation.

The Case 1 experiments at Ratios 2 and 3 can be seen to reach saturation in Figures 14, 15, 17, and 18. In Figures 14 and 17, the average temperature graph flattens at the mixture reaches its saturation temperature. The temperature ceases to rise because, at saturation, no more ammonia is being absorbed and no more energy is being liberated by the ammonia-water reaction.

In Figures 15 and 18, the concentration graphs can be seen to become very spiky as the mixture becomes saturated. The saturation (final) concentration can be read

Table 6

Initial and Saturation Conditions of Experiments

Ratio No.		T <sub>init</sub>	T <sub>final</sub>	x <sub>final</sub>
		(°F)	(°F)	(%)
Case 1	1		not saturated	
	2	71.1	154.6	9.62
	3	61.5	147.1	10.76
Case 2	1		not saturated	
	2		not saturated	
	3	58.1	101.3	16.26
Case 3	1	87.7	126.9	4.48
	2	78.7	131.3	7.93
	3	67.4	139.5	7.62

from the graph where it levels out after the ammonia release was stopped. It is not fully understood why the concentration measurements become spiky and inaccurate as the mixture reached saturation. Near the end of these experiments, the receiver vessel began to vibrate and a sound as if the mixture were churning around in the tank could be heard. It is thought that after the mixture became saturated, the high volume of ammonia bubbling through the mixture caused a churning of the liquid. This churning is thought to have created false pressure readings on the differential pressure transducer used to measure the



pressure (weight) of liquid in the tank. These false pressure readings were then used to calculate the concentration measurements rendering them inaccurate. Since the churning noise and vibration of the tank ceased when the ammonia flow was shut off, the pressure reading, and therefore the concentration measurement, at this point were thought to be a better indication of the saturation state. Note that these spiky concentration measurements are also reflected in the graphs shown in Figures 16 and 19.

The Case 2 Ratio 3 experiment cannot be seen to reach saturation in a way similar to the Case 1 experiments. This suggests that the mixture in this experiment reached saturation just before the ammonia flow was shut off.

All three Case 3 experiments can be seen to reach saturation almost immediately after the ammonia flow was started. The shoulders in the average temperature graph at Ratio 1, Figure 29, will be explained in section four of this chapter. Note that they are reflected in the graph in Figure 31. The hump in the concentration graph at Ratio 2, Figure 33, is not due to an abrupt change in the ammonia flowrate. Figure 100 in Appendix C shows that the ammonia flowrate decreased slowly and steadily during this experiment. The hump is most likely caused by an abrupt change in the water spray flowrate since the water flowrate was not controlled during the experiments. It is also not understood why the concentration decreased during both the Ratio 1 and 3 experiments except that the concentration measurements in the Case 3 experiments had a low repeatability.

The Case 1 experiments most nearly match the projected saturation conditions. The Case 2 experiments exceed the projected concentration while falling short of the temperature projection, and the Case 3 experiments fall short of both the concentration and temperature projections.

## 2. Ratio Comparison by Case

Table 7 summarizes the data in Figures 11-37 by Case:

**Table 7**  
**Comparison of Experimental Data by Case**

	Ratio No.	$m_{rel}$	$\Delta T/\Delta t$	$\Delta x/\Delta t$	$\Delta T/\Delta x$	$m_{abs}$
		(lbm)	(°F/min)	(%/min)	(°F/%)	(%)
Case 1	1	102.2	3.24	.533	606.98	100.0
	2	220.8	8.35	.962	868.34	89.0
	3	279.5	8.56	1.076	795.75	79.6
Case 2	1	102.5	1.40	.598	233.85	100.0
	2	197.7	2.32	.992	233.90	100.0
	3	403.6	4.05	1.525	265.73	91.1
Case 3	1	131.9	1.46	1.196	122.07	59.7
	2	184.3	8.88	1.942	457.26	75.7
	3	306.7	26.47	2.030	1303.94	41.9

The rate of liquid mixture average temperature rise was greater for the higher ammonia-water Ratios indicating that

more ammonia was reacting with the water, liberating more energy, and raising the liquid temperature. For Cases 1 and 2, the average temperature of the mixture increased linearly over the ammonia release whereas for Case 3, the average temperature increased to its maximum value almost immediately after the start of the ammonia release.

The rate of concentration rise was greater at the higher ammonia-water Ratios. This increased rate of concentration rise is presumed to be due to the increased ammonia flow into the receiver tank. For Cases 1 and 2, the amount of ammonia absorbed is proportional to the concentration of ammonia in the mixture. The increased rate of concentration rise indicates that the rate of ammonia absorption is greater at the higher ammonia-water ratios. This is not so for Case 3 because water is continually added to the tank. Again for Cases 1 and 2, the concentration increased linearly over the ammonia release whereas for Case 3, the concentration jumped to its maximum value almost immediately after the start of the ammonia release. It is speculated that the jump of the average temperature and concentration of the liquid in Case 3 indicates that the water droplets are absorbing the ammonia vapor midair and are individually reaching saturation conditions before falling to the bottom of the tank.

Average temperature rise versus concentration rise also tended to increase at the higher ammonia-water Ratios, indicating that the rise in average temperature was proportional to the amount of ammonia absorbed. For all Cases, the percentage of ammonia absorbed decreased at the

higher ammonia-water Ratios. Tests with less than 100% absorption of the released ammonia indicate that the mixture became saturated with ammonia. The mixture became saturated with ammonia sooner at the higher Ratios indicating that the trap was only able to absorb a limited amount of ammonia.

Summarizing the effects of ammonia-water Ratio on ammonia absorption: higher ammonia-water ratios caused 1) greater liquid average temperature rises, 2) greater rates of ammonia absorption, and 3) a higher likelihood of saturation before all of the ammonia was released to the receiver tank.

### 3. Case Comparison by Ratio

Table 8 summarizes the data in Figures 11-37 by ammonia-water Ratio. Although the average temperature rise was less for Case 3 than Case 1 at all ammonia-water Ratios, the rate of average temperature rise was greater for Case 3 than Case 1 at ammonia-water Ratios 2 and 3. This was due to the immediate rise to saturation conditions of the Case 3 experiments. For the Case 2 experiments at all ammonia-water Ratios, the average temperature rises and rates of average temperature rise were less than both the Case 1 and Case 3 experiments. It is speculated that the liquid ammonia in the Case 2 experiments must be vaporized before reacting with the water. This requires a heat transfer from the liquid mixture to the ammonia thus lowering the average temperature of the mixture. The ammonia water reaction then liberates energy increasing the average temperature of the mixture. Because the vaporous ammonia in the Case 1 and 3

experiments does not require a heat transfer from the mixture, the net average temperature rise is greater.

**Table 8**  
**Comparison of Experimental Data by Ratio**

Case No.	$m_{rel}$	$T/\Delta t$	$\Delta x/\Delta t$	$\Delta T/\Delta x$	$m_{abs}$	
	(lbm)	(°F/min)	(%/min)	(°F/%)		(%)
Ratio 1	1	102.2	3.24	.533	606.98	100.0
	2	102.6	1.40	.598	233.85	100.0
	3	131.9	1.46	1.196	122.07	59.7
Ratio 2	1	220.8	8.35	.962	868.34	89.0
	2	197.7	2.32	.992	233.90	100.0
	3	184.3	8.88	1.942	457.26	75.7
Ratio 3	1	279.5	8.56	1.076	795.75	79.6
	2	403.6	4.05	1.525	265.73	91.1
	3	306.7	26.47	2.030	1303.94	41.9

The rate of concentration rise was greatest for the Case 3 experiments. This was again due to the immediate rise to saturation conditions of the Case 3 experiments. The rate of concentration rise was greater for the Case 2 experiments than the Case 1 experiments. Since the Case 1 and Case 2 experiments had the same ammonia mass flow rate, this indicates that the mixture was able to absorb more liquid ammonia than vaporous ammonia for the flowrates

tested. Again, the ability to absorb more liquid ammonia at the flowrates tested was due to the smaller average temperature rise of the mixture during the liquid ammonia absorption resulting in a cooler liquid.

Comparing average temperature rise to concentration rise for the Case 3 experiments again showed that the mixture reached saturation conditions quickly. It is not understood why the concentration varied so much at this saturation temperature except that the concentration measurements for the Case 3 experiments had a low repeatability.

Observing average temperature rise and concentration rise for the Case 1 and 2 experiments shows the average temperature rise was less over the same concentration rise for the Case 2 experiment. This is again indicative of the liquid ammonia vaporizing before absorption resulting in a lower average temperature rise.

At ammonia-water Ratio 3, none of the situations in the Cases was able to absorb all of the ammonia released; at ammonia-water Ratio 2, only in the Case 2 situation was the mixture able to absorb all of the ammonia released; and at ammonia-water Ratio 1, the situations in both Cases 1 and 2 resulted in the mixture absorbing all of the ammonia released. For the Case 3 experiments, less than 75% of the ammonia released was absorbed at any Ratio. This indicated insufficient water spray to absorb all of the ammonia vapor. Some of the vapor passed the water droplets and escaped from the tank. The ammonia was observed escaping from the tank during each Case 3 ammonia absorption experiment.

Summarizing the Case comparison by Ratio: the situation in the Case 2 tests (liquid ammonia absorption into water) resulted in the least average temperature rise, and more ammonia absorption than in the other Cases at the ammonia-water Ratios tested. Case 3 tests were unable to trap all of the ammonia released at any Ratio tested.

#### 4. Other Phenomena Observed

For all three Cases, sounds could be heard coming from the receiver vessel during the ammonia release. These sounds were recorded and were louder at the higher ammonia-water Ratios. These sounds were thought to be associated with the ammonia-water reaction taking place in the tank during ammonia absorption, and with the ammonia bubbling through the mixture after the saturation point had been reached.

The temperature variations at different levels in the fluid as measured by the three thermocouples could also be felt on the outside of the tank and are discussed below.

1. Cases 1 and 2: Figures 38-43 show the temperature variations at each of the three thermocouples in the tank. It can be seen that the temperature at the bottom thermocouple is much lower than at the upper thermocouples for all ammonia-water Ratios. This is thought to occur because the bottom thermocouple was shielded from the ammonia-water reaction by the shroud, and the warmed liquid rose towards the top of the tank. Note that at the higher ammonia-water Ratios, the temperature of the liquid at the bottom of the tank approaches that of the rest of the

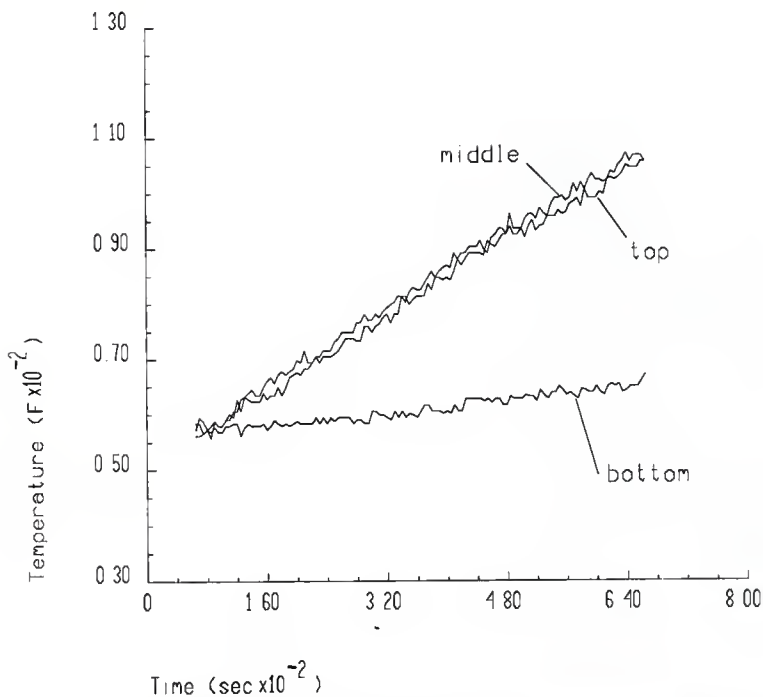


Figure 38: Variation of the Three Liquid Mixture Level Temperatures for Ammonia Vapor Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.



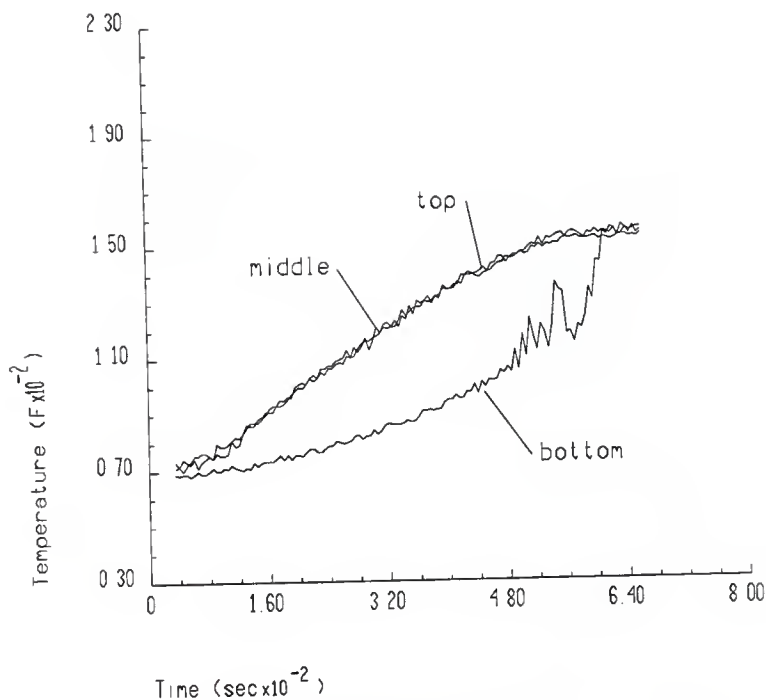


Figure 39: Variation of the Three Liquid Mixture Level Temperatures for Ammonia Vapor Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

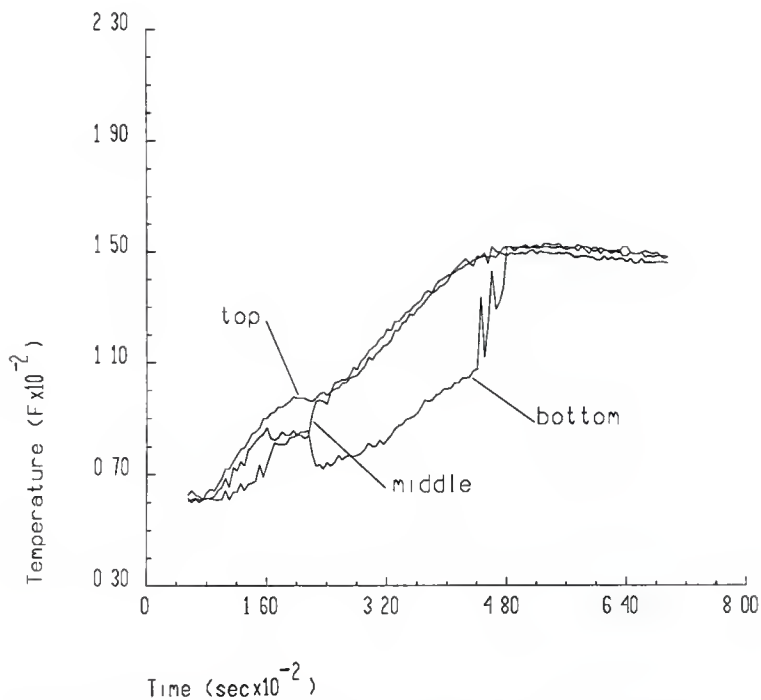


Figure 40: Variation of the Three Liquid Mixture Level Temperatures for Ammonia Vapor Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

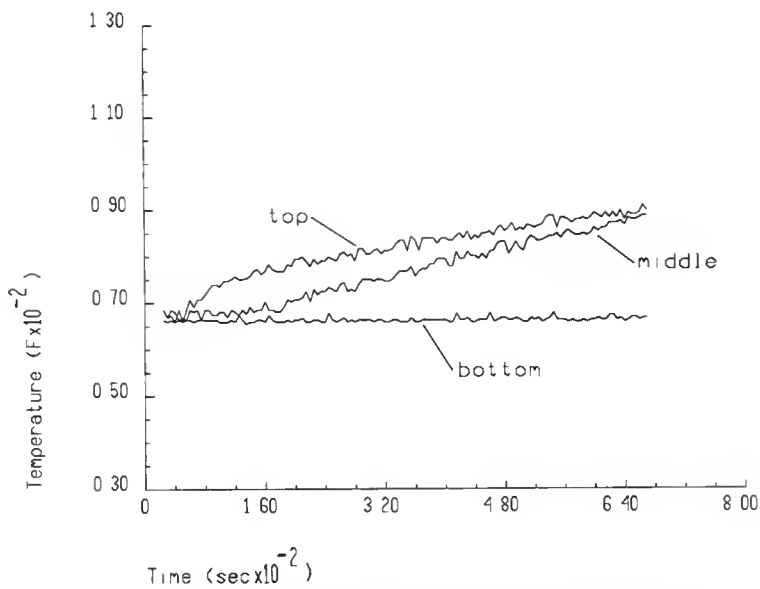


Figure 41: Variation of the Three Liquid Mixture Level Temperatures for Ammonia Liquid Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

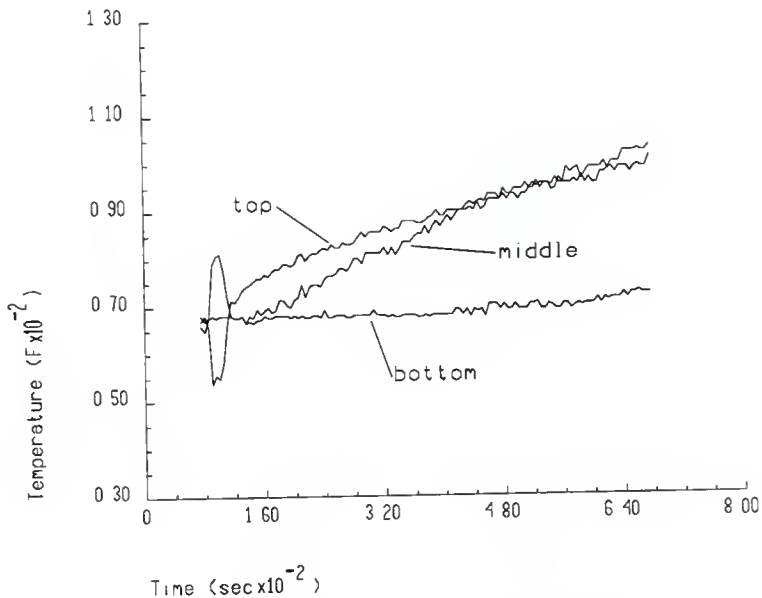


Figure 42: Variation of the Three Liquid Mixture Level Temperatures for Ammonia Liquid Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

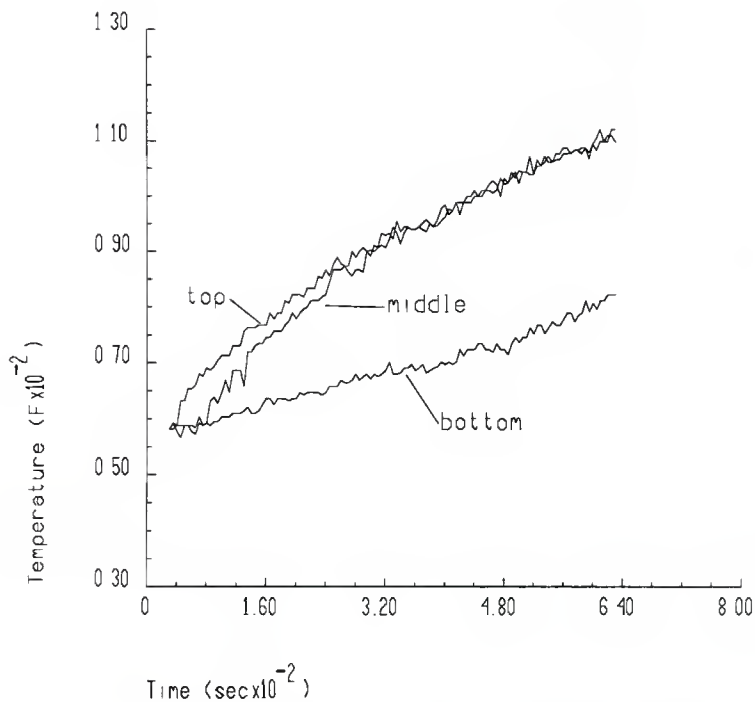


Figure 43: Variation of the Three Liquid Mixture Level Temperatures for Ammonia Liquid Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

liquid. It is thought to begin to mix with the rest of the liquid and become saturated with ammonia.

2. Case 3: Since water droplets contacted the thermocouples randomly and may have evaporated causing erratic temperature readings, the thermocouple temperature measurements were assumed to inaccurately represent the droplet cloud temperature. Thermocouple measurements were deemed accurate only after the thermocouple had become submerged in the fluid.

Ammonia vapor leaving the supply line is thought to have reacted with the water droplets until the supply line opening was submerged. Ammonia vapor bubbling through the liquid mixture was then absorbed by the liquid if unsaturated, or by the thin layer of unsaturated water droplets landing on the top of the liquid in the tank. Ammonia not absorbed by this layer was released from the liquid to react with the water droplets above the liquid.

Figure 44 shows the vertical temperature variations indicated by the three thermocouples in the tank during the Case 3 experiment at ammonia-water Ratio 1. The temperature of the liquid covering the bottom thermocouple suggests that of an unsaturated mixture. As the liquid level covered the fill pipe, this unsaturated mixture began to absorb ammonia. However, the liquid near the bottom thermocouple was again shielded from these absorption reactions. As the middle and top thermocouple were submerged, they indicated the higher temperature of the reacting mixture.

Figure 45 shows the vertical temperature variations indicated by the three thermocouples in the tank during the

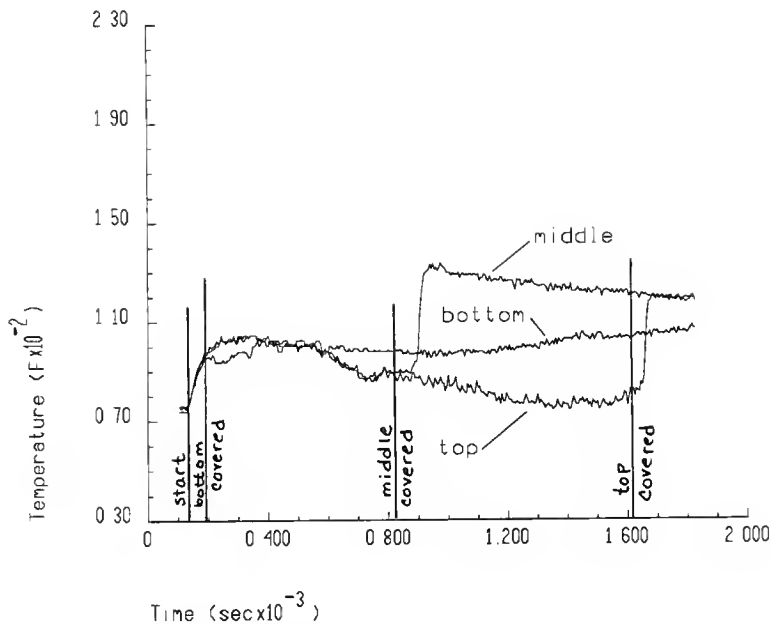


Figure 44: Variation of the Three Liquid Mixture Level Temperatures for Ammonia Vapor Absorption into Water Spray Ending at 0.5 Pound of Ammonia per Gallon of Water.

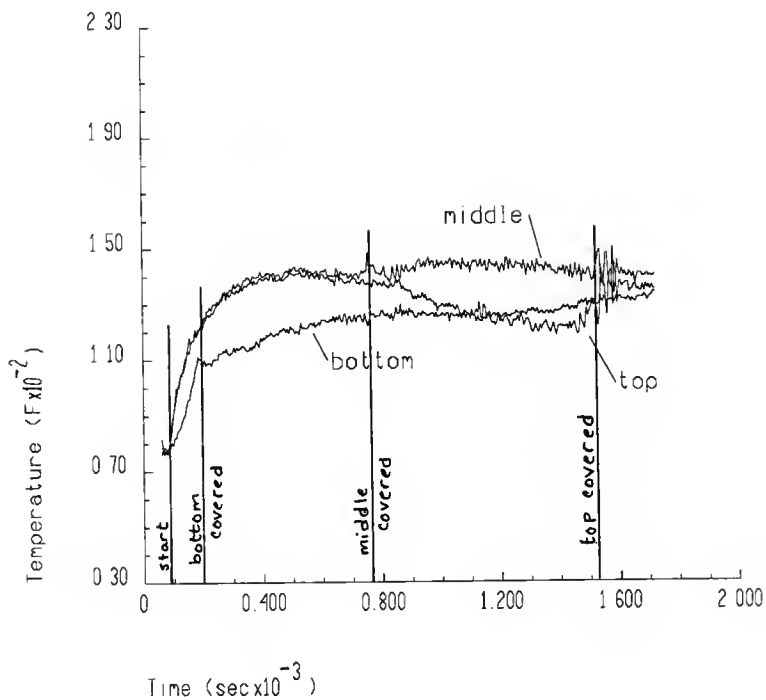


Figure 45: Variation of the Three Liquid Mixture Level Temperatures for Ammonia Vapor Absorption into Water Spray Ending at 1 Pound of Ammonia per Gallon of Water.



Case 3 experiment at ammonia-water Ratio 2. The temperature of the bottom thermocouple as it became covered was indicative of the saturated mixture temperature. The data suggests that by the time the middle thermocouple was submerged, ammonia was escaping the liquid and reacting with the droplets in the air and the temperature measurement was that of recently saturated water droplets. As the top thermocouple was covered, its temperature became nearly the same as that of the two lower thermocouples.

Figure 46 shows the vertical temperature variations indicated by the three thermocouples in the tank during the Case 3 experiment at ammonia-water Ratio 3. All of the thermocouples, as they become covered, indicated the temperature of the saturated mixture in the tank. The graph suggests that the ammonia-water Ratio was so high that the thin layer of unsaturated liquid at the top of the fluid ceased to exist and the ammonia bubbled out of the fluid to react with the water droplets above.

##### 5. Desorption Results

Table 9 shows the normalized ammonia concentration data obtained from the exposure tests. Initial ammonia concentration and actual ammonia mass are given, indicating conditions for each drum to which the later ammonia concentrations were normalized. The ammonia concentrations were determined by measurement of the mixture's specific gravity and checked against the actual weight of the liquid mixture. The control drums containing only water were simultaneously weighed with the test drums to determine the

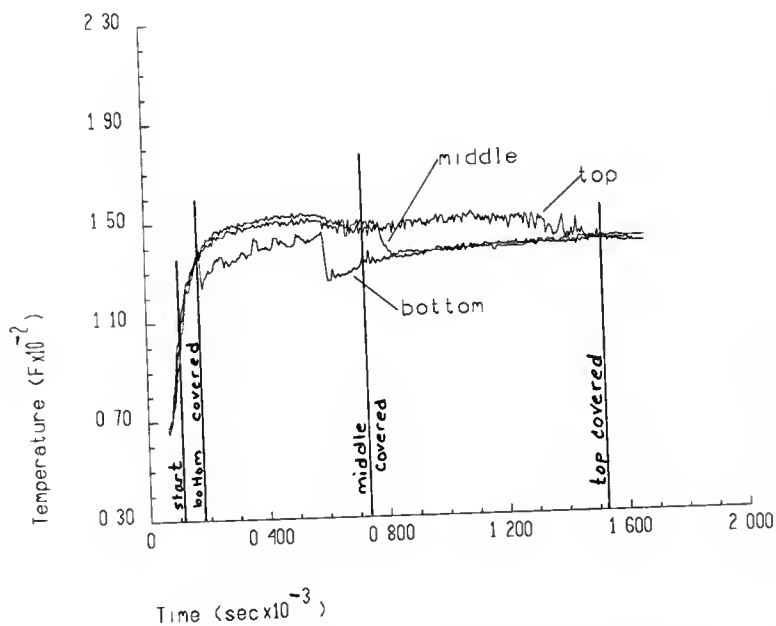


Figure 46: Variation of the Three Liquid Mixture Level Temperatures for Ammonia Vapor Absorption into Water Spray Ending at 2 Pounds of Ammonia per Gallon of Water.

**TABLE 9**  
**Normalized Ammonia Desorption Test Data for Ammonia Water Mixtures**  
**by Exposure to Ambient Conditions**

Description	Exposure (Days)	Inside Drums*						Outside Drums**					
		1	2	3	4	5	6	1	2	3	4	5	6
Initial Mass %	0	17.6	18.9	25.0	26.0	0.0	0.0	20.0	21.9	26.8	26.8	0.0	0.0
Initial NH Mass (lbm)	0	15.8	16.4	22.5	22.8	0.0	0.0	17.6	20.6	23.7	27.0	0.0	0.0
Normalized NH Conc.	0	1.00	1.00	1.00	1.00	0.0	0.0	1.00	1.00	1.00	1.00	0.0	0.0
	6	0.917	0.921	0.872	0.885	0.0	0.0	0.699	0.689	0.818	0.859	0.0	0.0
	13	0.890	0.816	0.863	0.837	0.0	0.0	0.644	0.629	0.756	0.755	0.0	0.0
	20	0.786	0.750	0.791	0.827	0.0	0.0	0.589	0.543	0.649	0.641	0.0	0.0
	27	0.724	0.654	0.754	0.716	0.0	0.0	0.536	0.564	0.658	0.645	0.0	0.0
	36	0.631	0.602	0.697	0.707	0.0	0.0	0.513	0.501	0.582	0.595	0.0	0.0
	50	0.577	0.584	0.673	0.654	0.0	0.0	0.448	0.406	0.533	0.545	0.0	0.0

\* Both control drums containing water lost 0.5 lbm of water during the 50 days.

\*\* Both control drums containing water lost 0.75 lbm of water during the 50 days.

water loss. Water loss from the controls was small -- 0.5 lbm (0.23 kg) for the inside drums, and 0.75 lbm (0.34 kg) for the drums exposed to outside conditions.

Figure 47 shows the desorption data in Table 9. Both inside and outside exposures result in a significant decrease of ammonia concentration over the 50 day period. The tanks inside released approximately 40% of the initially absorbed ammonia and the tanks exposed outside released approximately 50% over the 50 days. The outside exposure is noticed to accelerate the desorption of ammonia from the mixture by about 10% over that which occurred inside. These results only apply to summer conditions where the high ambient temperatures promote desorption rates greater than that of the winter months. The following equations were fitted to the data shown in Figure 47 yielding:

Inside Exposure:

$$\frac{X}{X_0} = 1.002 - 0.01387 N - 1.757N^2$$

(Correlation Coefficient = 0.92)

Outside Exposure :

$$\frac{X}{X_0} = 0.9523 - 0.02088 N + 0.0002392 N^2$$

(Correlation Coefficient = 0.83)

Combined Inside and Outside Exposures:

$$\frac{X}{X_0} = 0.8219 - 0.005845 N + 0.1860 \frac{1}{N}$$

(Correlation Coefficient = 0.76)

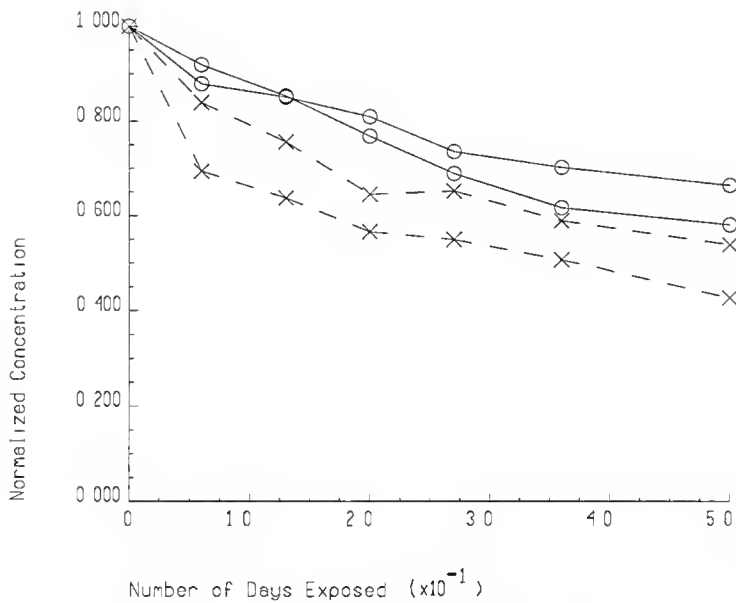


Figure 47: Ammonia Desorption from Ammonia-Water Mixture in a Drum.

where  $x$  is the ammonia concentration,  $x_0$  the initial ammonia concentration, and  $N$  the number of days exposed. Uncertainties in the exposure test data are about  $\pm 5\%$  thereby suggesting the trend observed between inside and outside exposures is tentative. Thus, the combined data correlation given above is recommended for application.

## V. Analytical Models

Each experimental situation (Case) was analytically modeled to predict the temperature and concentration of the liquid mixture in the tank as ammonia was added. These models were developed to assist in the design of industrial systems. For each experiment, the models were used with experimentally measured conditions as input parameters to predict the progression of the experiment. The model predictions were then compared to the experimental results to evaluate the model's ability to correctly predict the experimental results.

### 1. Case 1

The analytical prediction of the ammonia vapor that can be absorbed into a partially filled tank of water is developed using a physical mechanism for the absorption process. A plausible mechanism is:

1. Chemical reaction occurs upon the mixing of the ammonia vapor and water. The ammonia vapor warms to the liquid mixture temperature and the heat of reaction increases the mixture temperature.
2. Air in the receiver vessel is displaced by ammonia and water vapor above the liquid mixture.
3. Absorption of ammonia continues until the sum of the partial pressures of the ammonia and water above the liquid mixture exceeds the atmospheric pressure.

Initially, the receiving tank contains an initial mass of water and ammonia at some temperature. Ammonia entering the tank is assumed to be fully dispersed. The temperature of the liquid mixture after receiving  $\Delta M_a$ , ammonia mass, is given by rearrangement of the energy equation,

$$T_{\text{mix,new}} = T_{\text{mix,old}} + \frac{\Delta M_a [h_{\text{rxn}} - c_{\text{pa}}(T_{\text{mix,old}} - T_a)]}{M_{\text{mix}} c_{\text{pmix}}}$$

where,

$T_{\text{mix,new}}$  = liquid mixture temperature after  $\Delta M_a$  added, °K

$T_{\text{mix,old}}$  = liquid mixture temperature before  $\Delta M_a$  added, °K

$T_a$  = ammonia vapor temperature, °K

$h_{\text{rxn}}$  = heat of reaction for ammonia and water, kJ/kg  $\text{NH}_3$

$c_{\text{pa}}$  = specific heat of ammonia vapor, kJ/kg-°K

$c_{\text{pmix}}$  = specific heat of ammonia-water mixture, kJ/kg-°K

$M_{\text{mix}}$  = total mass of ammonia-water mixture, kg

$\Delta M_a$  = ammonia mass, kg

The heat of reaction is obtained from the enthalpy-concentration diagram for the ammonia-water solution [16]. The relationship, obtained by curve fitting is,

$$h_{\text{rxn}} = -5670.74 + 5589.94 \frac{T_{i,w}}{100} - 1044.19 \left( \frac{T_{i,w}}{100} \right)^2$$



The equation used for  $c_{pa}$  is,

$$c_{pa} = -0.7756 + 0.004958 T_a + \frac{437.8}{T_a}$$

The specific heat of the ammonia-water liquid mixture is based on data reported in the Chemical Engineers Handbook [17] and is,

$$\begin{aligned} c_{pmix} = & (7.706 - 0.02245 T_{mix} + 0.00003569 T_{mix}^2) + \\ & + (-298.8 + 1.923 T_{mix} - 0.003061 T_{mix}^2) x + \\ & + (1160.0 - 7.509 T_{mix} + 0.01198 T_{mix}^2) x^2 \end{aligned}$$

where  $x$  is the mass concentration of ammonia and calculated by,

$$x = \frac{M_a}{M_a + M_w}$$

where,

$x$  = mass concentration or fraction of ammonia

$M_a$  = ammonia mass in liquid mixture, kg

$M_w$  = water mass in liquid mixture, kg

The partial pressure of the water vapor above the liquid mixture obtained from the saturation steam tables is [18],

$$P_{H_2O} = 0.1509 \times 10^9 \exp \left[ \frac{-5171}{T} \right]$$

where  $P_{H_2O}$  is in kPa, and T is the mixture temperature in °K. The partial pressure of the ammonia vapor above the liquid mixture originates from data in the Chemical Engineers Handbook [17],

$$P_{NH_3} = [-9.7332 \times 10^6 + 6.3731 \left(\frac{T_i}{100}\right) - 0.987422 \left(\frac{T_i}{100}\right)^2] \\ \left\{ (3894.7699 - 23.99567 T + 0.03696 T^2) + \right. \\ \left. + (29203.743 - 259.7423 T + 0.5411 T^2) x + \right. \\ \left. + (170153.485 - 1197.155 T + 2.818166 T^2) x^2 \right\}$$

where  $P_{NH_3}$  is in kPa,  $T_i$  is the initial temperature of the liquid mixture, °K, and T is the liquid mixture temperature at the conditions of interest, °K.

A digital computer program written in FORTRAN is included in Appendix D where the above formulation is used. An input file is used to supply the information necessary to "run" the program. The total ammonia released to the receiver tank and the time duration over which the release occurs are the important variables characterizing the ammonia vapor flow. The other input variables establish the conditions for the release. An example input file is also included with the program.

To compare the analytical model to the experimental data, the computer program was run using experimentally measured conditions as the input parameters. The computer generated results were plotted with the experimental results

and are shown in Figures 48 and 49 for Ratio 1, Figures 50 and 51 for Ratio 2, and Figures 52 and 53 for Ratio 3.

At Ratio 1, the average temperature of the ammonia-water mixture predicted by the model had virtually no deviation from the average temperature during the experiment. The predicted concentration had a maximum deviation from the experimental results of 15%. The experiment verified the model's prediction that all of the ammonia released would be absorbed.

At Ratio 2, the average temperature of the ammonia water mixture predicted by the model had a maximum deviation of 8% from the experimental data. The predicted concentration had a maximum deviation from the experimental data of 18%. During the experiment 90% of the ammonia released was absorbed compared to the model's prediction that all of it would be absorbed.

At Ratio 3, the average temperature predicted by the model had a maximum deviation of 16% from the experimental data. The predicted concentration had a maximum deviation from the experimental data of 30%. During the experiment, 80% of the ammonia released was absorbed compared to the model's prediction that 90% would be absorbed.

## 2. Case 2

Analytical prediction of the ammonia liquid that can be absorbed in a tank of water required a physical mechanism for the absorption process. A plausible mechanism is:

1. Chemical reaction occurs upon the mixing of ammonia and water. The heat of reaction thereby vaporizes

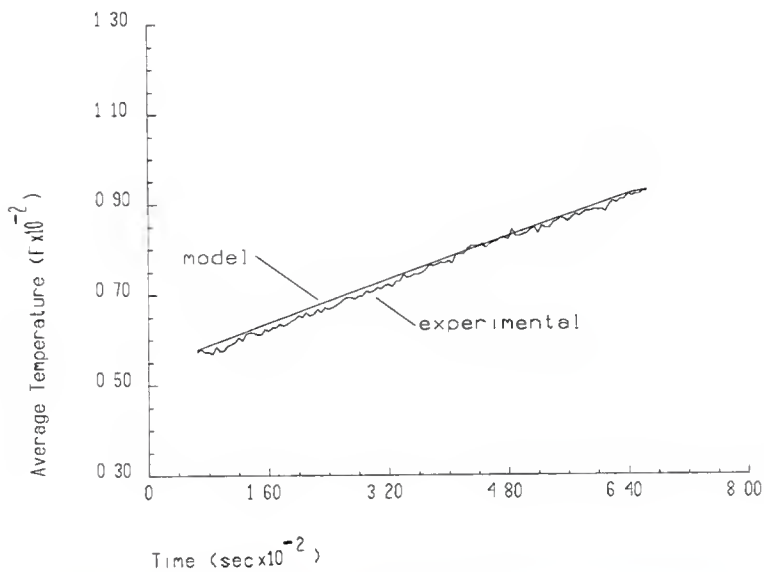


Figure 48: Experimental Results and Model Predictions of Average Temperature for Ammonia Vapor Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

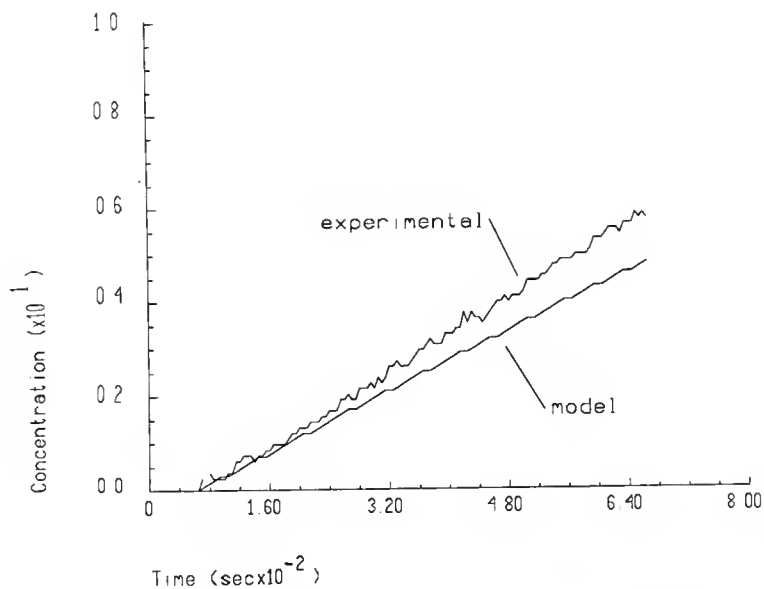


Figure 49: Experimental Results and Model Predictions of Concentration for Ammonia Vapor Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

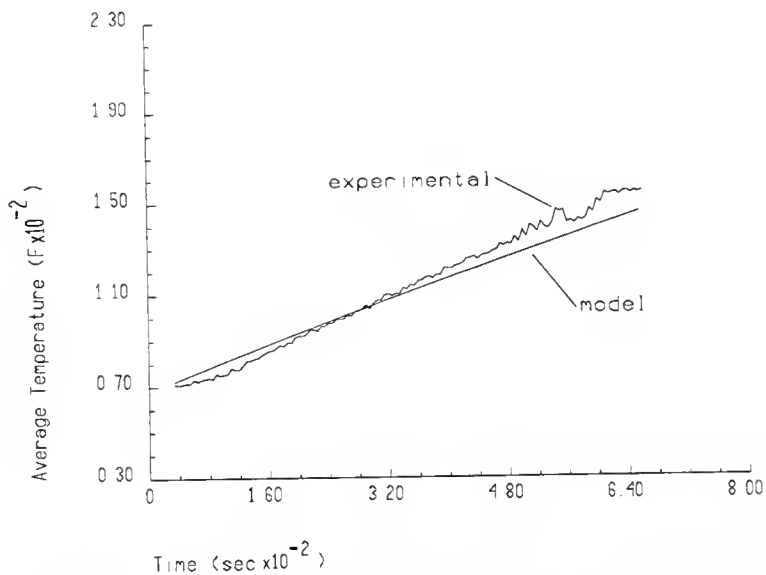


Figure 50: Experimental Results and Model Predictions of Average Temperature for Ammonia Vapor Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

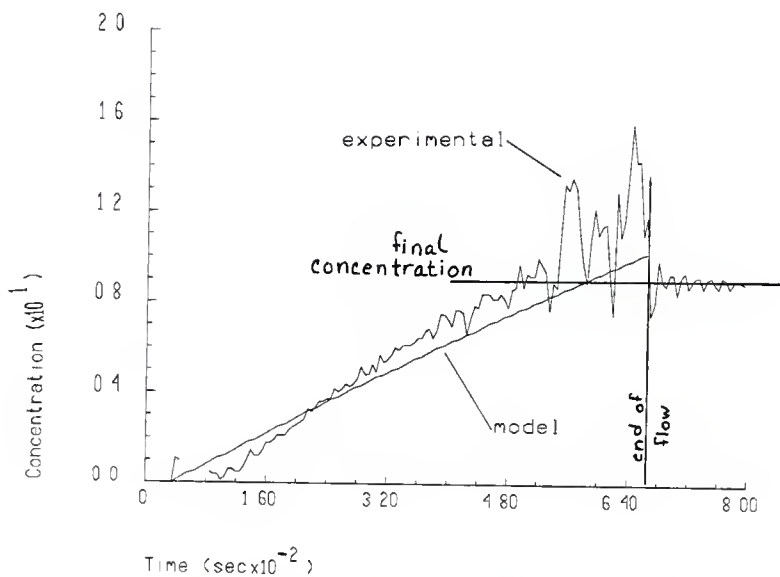


Figure 51: Experimental Results and Model Predictions of Concentration for Ammonia Vapor Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

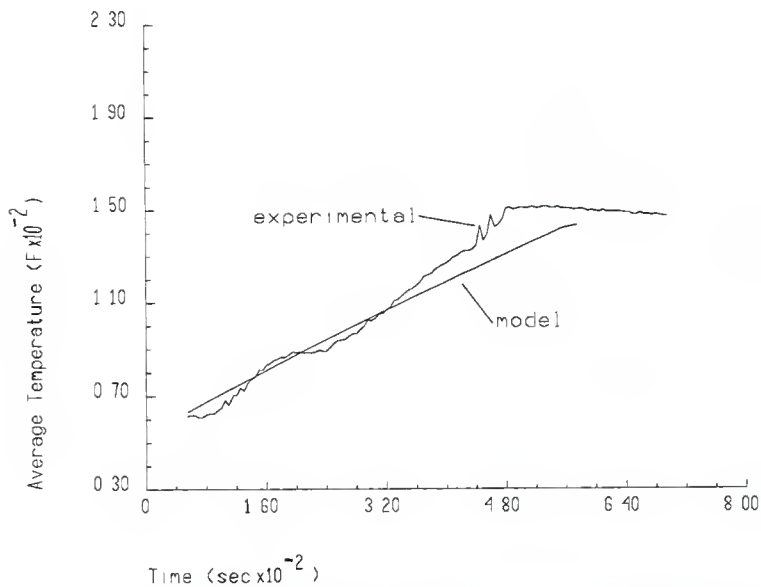


Figure 52: Experimental Results and Model Predictions of Average Temperature for Ammonia Vapor Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.



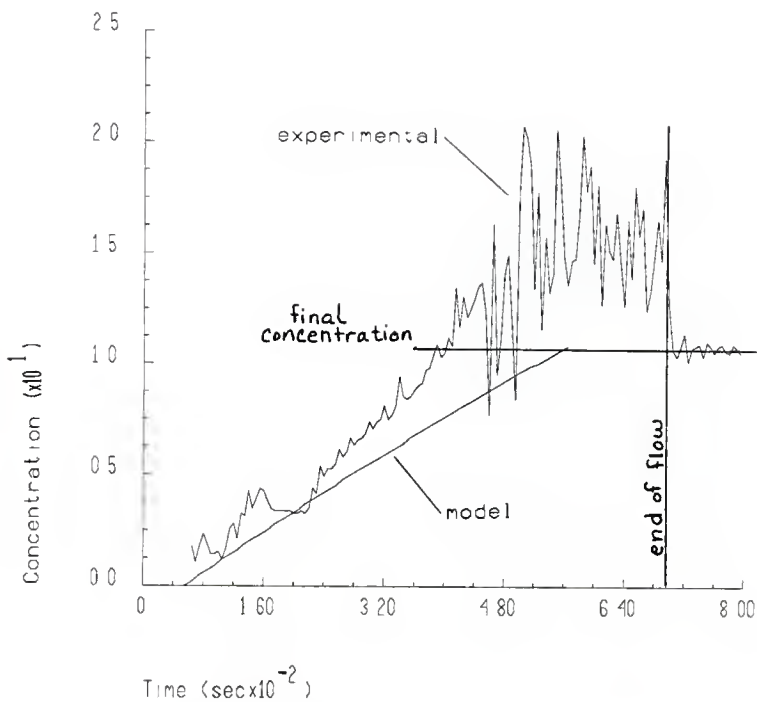


Figure 53: Experimental Results and Model Predictions of Concentration for Ammonia Vapor Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

the ammonia liquid and increases the liquid mixture temperature.

2. Air in the receiver vessel is displaced by ammonia and water vapor above the liquid mixture.
3. Absorption of ammonia continues until the sum of the partial pressures of the ammonia and water above the liquid mixture exceeds the atmospheric pressure.

Suppose that the receiving tank contains an initial mass of water and ammonia at a certain temperature. Ammonia entering the tank is assumed to be fully dispersed. Furthermore, if the heat of reaction and heat of vaporization of the ammonia are given by  $h_{rxn}$  and  $h_{fga}$  respectively, the change in liquid mixture temperature is obtained from the energy equation:

$$T_{mix,new} = T_{mix,old} + \frac{\Delta M_a (h_{rxn} - h_{fga})}{M_{mix} C_{pmix}}$$

where,

$\Delta M_a$  = mass of ammonia absorbed, kg

$h_{rxn}$  = heat of reaction for ammonia and water, kJ/kg  $NH_3$

$h_{fga}$  = ammonia heat of vaporization, kJ/kg

$M_{mix}$  = total mass of ammonia water mixture, kg

$C_{pmix}$  = constant pressure specific heat of ammonia water mixture, kJ/kg-°K

The ammonia heat of vaporization obtained from the saturated ammonia tables [18] is,

$$h_{fga} = 1416.0 + 2.507 T - 0.01123 T^2$$

The expressions developed in Case 1 for  $h_{rxn}$  and  $c_{pmix}$  are the same as for Case 2.

The partial pressure of the ammonia and water constituents in the liquid mixture are identical to those of Case 1. Additionally, the mixture is assumed to be saturated when the partial pressure of the ammonia-water mixture exceeds the atmospheric pressure.

A digital computer program written in FORTRAN is included in Appendix D where the physical mechanism outline above is modeled. This program is similar to that developed under Case 1. The ammonia release is characterized by the time duration and ammonia mass. These and other input variables are supplied to the program by means of an input file. Both the program and an example input file are included in Appendix D.

The analytical model was compared to the experimental results as in Case 1. Plots of the model predictions with the experimental data are shown in Figures 54 and 55 for Ratio 1, Figures 56 and 57 for Ratio 2, and Figures 58 and 59 for Ratio 3.

At Ratio 1, the average temperature predicted by the model had virtually no deviation from the experimental data. Concentrations predicted by the model had a maximum

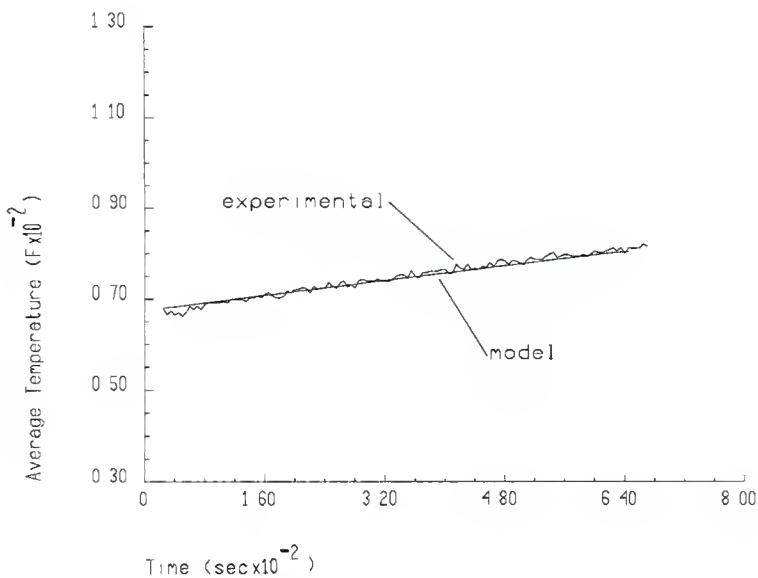


Figure 54: Experimental Results and Model Predictions of Average Temperature for Ammonia Liquid Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

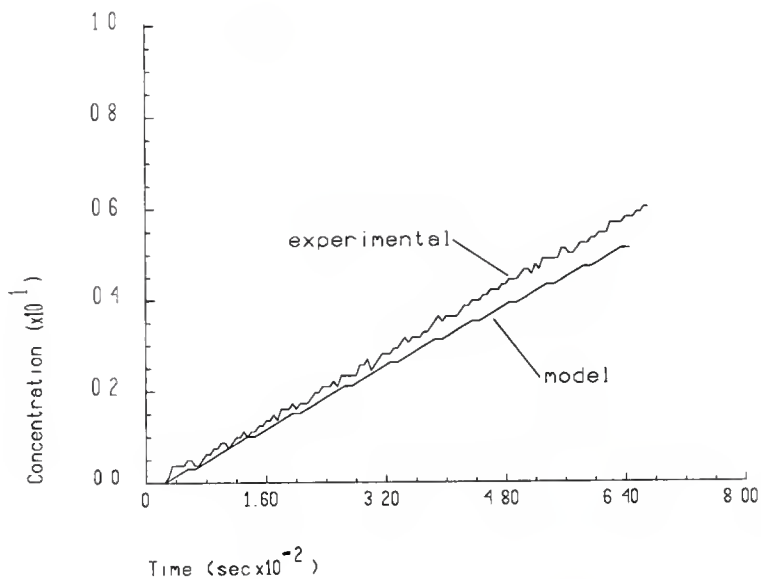


Figure 55: Experimental Results and Model Predictions of Concentration for Ammonia Liquid Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

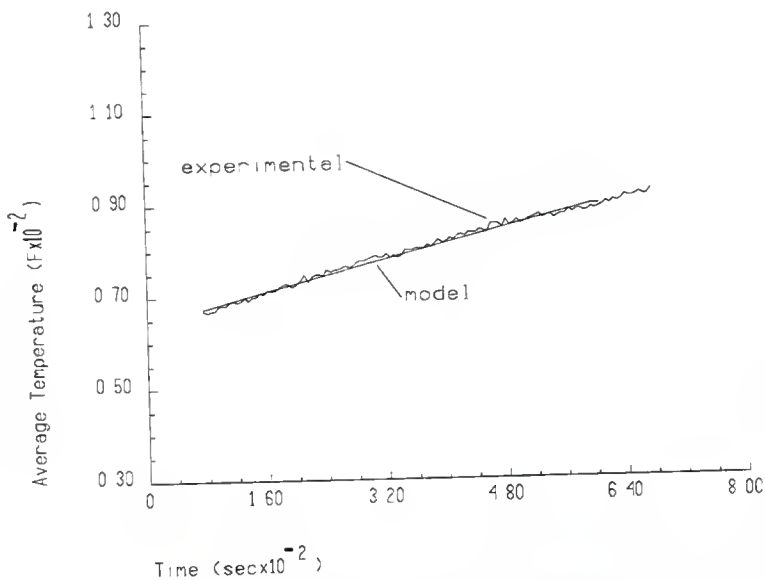


Figure 56: Experimental Results and Model Predictions of Average Temperature for Ammonia Liquid Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

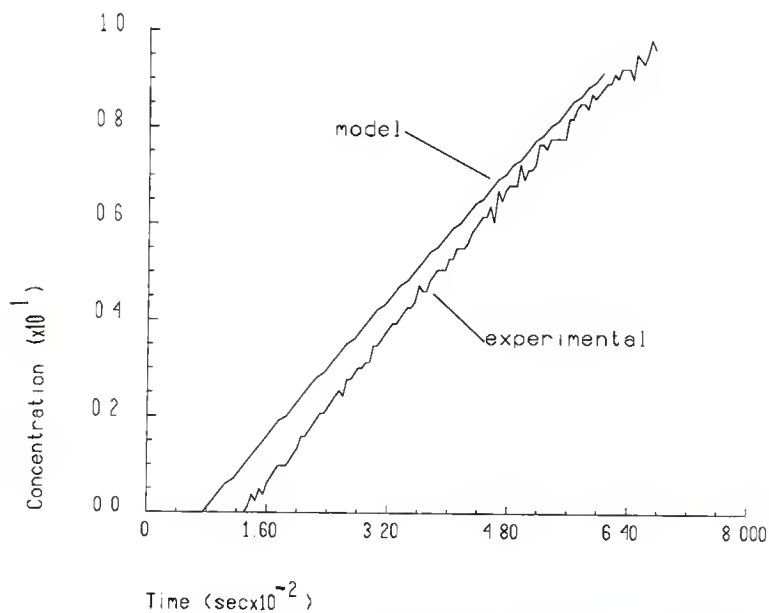


Figure 57: Experimental Results and Model Predictions of Concentration for Ammonia Liquid Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

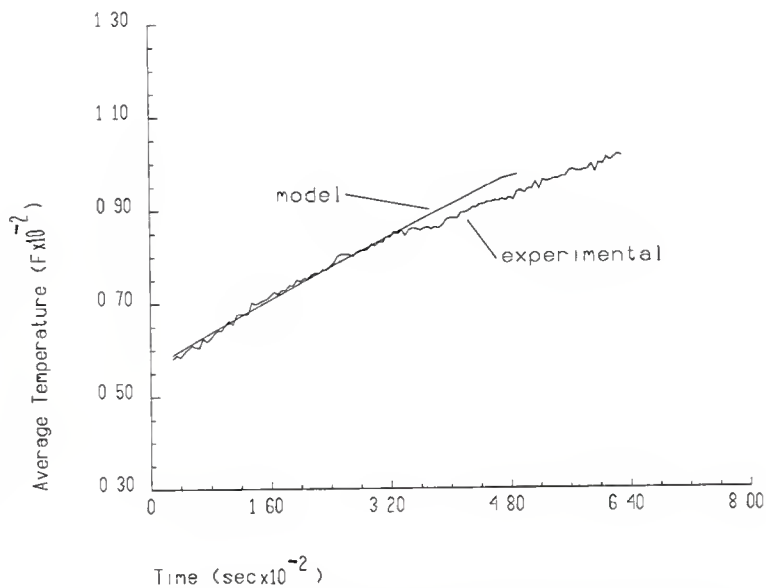


Figure 58: Experimental Results and Model Predictions of Average Temperature for Ammonia Liquid Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.



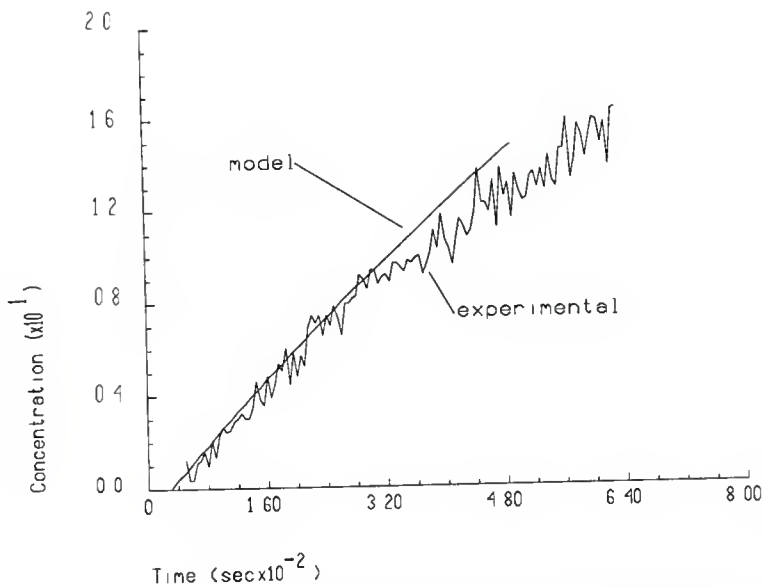


Figure 59: Experimental Results and Model Predictions of Concentration for Ammonia Liquid Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

deviation from the experimental data of 10%. The experiment verified the model's prediction that all of the ammonia released would be absorbed.

At Ratio 2, the average temperature predicted by the model had virtually no deviation from the experimental data. Concentrations predicted by the model had a maximum deviation from the experimental data of 9%. The experiment verified the model's prediction that all of the ammonia released would be absorbed.

At Ratio 3, the average temperature predicted by the model had a maximum deviation of 6% from the experimental data. Concentrations predicted by the model had a maximum deviation from the experimental data of 14%. During the experiment 91.1% of the ammonia released was absorbed compared to the model's prediction that 81% would be absorbed.

Models were also developed to include the heat transfer characteristics of the system. Results showed that accounting for heat transfer from the tank and piping changed the results less than 0.001%. Since the heat transfer characteristics of the system proved to be negligible in this Case, it was assumed to be so for the other Cases.

### 3. Case 3

The analytical model for absorption of ammonia vapor into a water spray was based on the following physical mechanism:

1. Chemical reaction occurs upon contact of the ammonia vapor with the water droplets. The ammonia vapor surrounding the water droplets warms to the droplet temperature which is increased by the heat of reaction upon absorption of the ammonia.
2. Absorption of ammonia vapor continues until the sum of the partial pressures of the ammonia and water above the liquid mixture are greater than atmospheric pressure.

The following assumptions characterize the proposed physical mechanism:

1. Air in the receiver tank is displaced by the entering ammonia vapor.
2. Ammonia absorption by water droplets occurs only during the time when the fill pipe is not submerged in the liquid mixture.
3. Ammonia absorption when the ammonia fill pipe is submerged occurs as in Case 1.
4. A single water droplet diameter characterizes the water spray and is a surface mean diameter.
5. No droplet-droplet interactions.
6. Ammonia absorption rate into droplets is proportional to the ratio,  $(x_{\text{equil}} - x)/x_{\text{equil}}$  where  $x_{\text{equil}}$  is the saturation ammonia concentration, and  $x$  is the actual ammonia concentration, in the droplet.
7. Thermodynamic equilibrium conditions prevail throughout the interior of the receiver tank.

The absorption rate of ammonia by an individual droplet [19,20] is,

$$\dot{Q}_{AW} = \pi d_p^2 k_a \rho_a$$

where,

$\dot{Q}_{AW}$  = rate of ammonia vapor absorption by droplet, kg/sec

$d_p$  = droplet diameter, m

$k_a$  = mass transfer coefficient, m/sec

$\rho_a$  = vapor density of ammonia, kg/m<sup>3</sup>

and

$$k_a = \frac{D_{AW}}{d_p} \left[ 2 + 0.60 \text{Re}^{1/2} \text{Sc}^{1/3} \right]$$

where,

$D_{AW}$  = diffusion coefficient for ammonia water, m<sup>2</sup>/sec

Re = Reynolds number,  $d_p V_p / \nu$

$V_p$  = droplet velocity, m/sec

$\nu$  = ammonia kinematic viscosity, m<sup>2</sup>/sec

Sc = Schmidt number,  $\nu / D_{AX}$

However, as the droplet absorbs ammonia, the capacity to absorb additional ammonia is reduced. Eventually, the droplet becomes saturated and further ammonia absorption is not possible. Consequently, the expression for  $\dot{Q}_{AW}$  is adjusted to accommodate this feature by a ratio of ammonia concentrations in the following manner,

$$\dot{Q}_{AW} = \pi d_p^2 k_a \rho_p \left( \frac{x_{equil} - x}{x_{equil}} \right)$$

where the concentration ratio is defined in the list of assumptions above. The water droplet velocity is approximated using the physical characteristics of the spray nozzle. The total hole area for a complete nozzle is

$$A_{total} = \sum_i^N A_i$$

where  $N$  is the number of holes and  $A_i$  is the individual hold area in  $m^2$ . With the assumption that the water stream velocity through the hole is the droplet velocity, then,

$$v_p = \frac{\dot{Q}_W}{A_{total}}$$

where  $\dot{Q}_W$  is the volumetric flowrate of water through the nozzle in  $m^3/sec$ . The diffusion coefficient,  $D_{AW}$ , is estimated using procedures in the Chemical Engineers Handbook [17],

$$D_{AW} = \frac{d_p T^{1.75} \left( \frac{1}{MWA} + \frac{1}{MWW} \right)^{0.5}}{\left( \frac{P_{atm}}{101.2} \right) \left[ (\Sigma v_a)^{0.3333} + (\Sigma v_w)^{0.3333} \right]^2}$$

where,

$T$  = droplet temperature, °K

$MWA$  = molecular weight of ammonia

$MWW$  = molecular weight of water

$P_{atm}$  = atmospheric pressure, kPa

$\Sigma v_a$  = atomic diffusion volume for ammonia, 14.9

$\Sigma v_w$  = atomic diffusion volume for water, 12.7

Considering the water droplets uniformly spaced in the receiver tank and all with diameter  $d_p$ , the mass concentration (or "cloud" density) of droplets is

$$\rho_p = \frac{\rho_{pw} \dot{Q}_w}{A V_p}$$

where,

$\rho_p$  = droplet mass or "cloud" density,  $kg/m^3$

$\rho_{pw}$  = water density,  $kg/m^3$

$A$  = cross-sectional area of the receiver tank,  $m^2$

Additionally,

$$\rho_p = \frac{M_p}{V}$$

where  $M_p$  is the mass of all the droplets in the receiver tank, kg, and  $V$  is the interior volume of the tank,  $m^3$ .

Combining the two expressions for  $\rho_p$  gives the droplet number density as,

$$N_p = 6 \left[ \frac{\rho_p}{\rho_{pw}} \right] \left[ \frac{D^2 L}{d_p^3} \right]$$

where,

$N_p$  = droplet number density, number/m<sup>3</sup>

$D$  = receiver cross-section diameter, m

$L$  = receiver tank height, m

The total absorption of ammonia in the droplet cloud inside the receiver tank is calculated by summing over all the droplets,

$$M_{a, \text{absorbed}} = N_p \dot{Q}_{AW}$$

and has units of kg/sec. In the actual calibration, the receiver tank is divided into a number of layers and the ammonia absorption that occurs during the time that the droplet occupies the layer is computed. Summation of the ammonia absorbed in each layer yields the total ammonia absorbed. Because the receiver tank is in counter flow -- ammonia vapor flowing upward and water droplet cloud flowing downward -- two calculations are required to establish the conditions in the tank. The first calculation begins at the top of the receiver tank and proceeds downward following the water droplets. From this, preliminary values for ammonia

concentration in the droplets and the droplet temperature result. The next calculation begins at the bottom of the receiver tank and proceeds upward following the ammonia vapor flow. With further calculation made in the bottom layer of the tank to accommodate the low ammonia vapor temperature, conditions in the receiver tank are known sufficiently for the determination of the ammonia absorbed by the water spray droplets.

When the volume below the bottom of the ammonia pipe is filled with liquid mixture, further absorption of ammonia occurs in the liquid mixture. Absorption takes place in the liquid mixture as water is continuously added by operation of the spray nozzles. As with Cases 1 and 2 the mixture is assumed saturated when the partial pressures of the ammonia and water exceed that of the atmosphere.

The digital computer program based on the Case 3 analytical model is given in Appendix D. The inputs are similar to those of Cases 1 and 2 except that the water spray droplets must be characterized. An example input file is also included in Appendix D.

The input variable water droplet diameter, requires discussion. Ammonia absorption into the droplet is a surface phenomena, and as such, the droplet size must reflect this feature. Therefore, the droplet surface mean diameter was computed from the cumulative volume size distribution. The mean droplet size by volume is  $d_{p,vol} = 430 \mu\text{m}$  and the associated standard deviation is  $\sigma_g = 1.54$  at a rated flowrate of 4.8 gal/min (18.2 liters/min) at 40 psig



(276 kPa) [21]. Transforming the volume mean diameter to a surface mean diameter involves the relationship [22],

$$\log_{10} d_{p,sur} = \log_{10} d_{p,vol} - 4.605 (\log_{10} \sigma_g)^2$$

where  $d_{p,sur}$  is the surface mean droplet diameter,  $\mu\text{m}$ . The surface mean diameter for the spray nozzle used in these experiments is  $296 \mu\text{m}$ . Actual nozzle operating conditions were 30 psig and thus the spray droplet size distribution varied somewhat from the rated distribution.

The analytical model was again compared to the experimental data as in Case 1. Plots of the model predictions with the experimental results are shown in Figures 60 and 61 for Ratio 1, Figures 62 and 63 for Ratio 2, and Figures 64 and 65 for Ratio 3. The analytical model was not a good predictor of the progression of the average temperature or the concentration but was a fair predictor of the final average temperature of the mixture and the average concentration of the mixture upon completion of the ammonia release.

For Case 1, the final average temperature prediction varied less than 1% from the actual final temperature. The concentration predicted varied 16.2% from the average concentration of the mixture during the experiment. During the experiment 59.7% of the ammonia released was absorbed compared to the model's prediction that all of it would be absorbed.

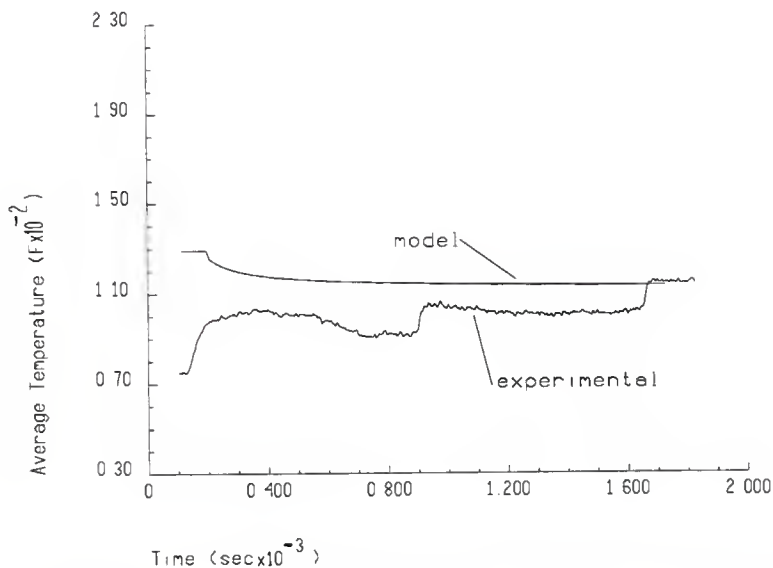


Figure 60: Experimental Results and Model Predictions of Average Temperature for Ammonia Vapor Absorption into Water Spray Ending at 0.5 Pound of Ammonia per Gallon of Water.

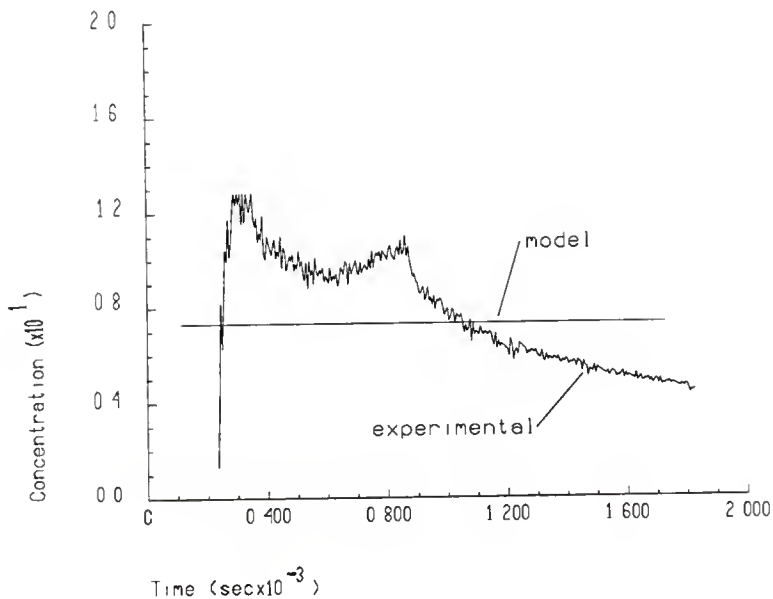


Figure 61: Experimental Results and Model Predictions of Concentration for Ammonia Vapor Absorption into Water Spray Ending at 0.5 Pound of Ammonia per Gallon of Water.

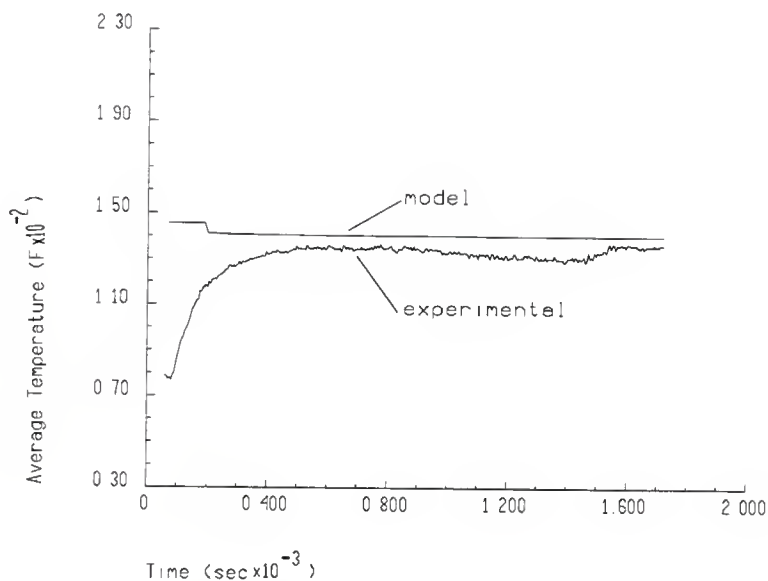


Figure 62: Experimental Results and Model Predictions of Average Temperature for Ammonia Vapor Absorption into Water Spray Ending at 1 Pound of Ammonia per Gallon of Water.

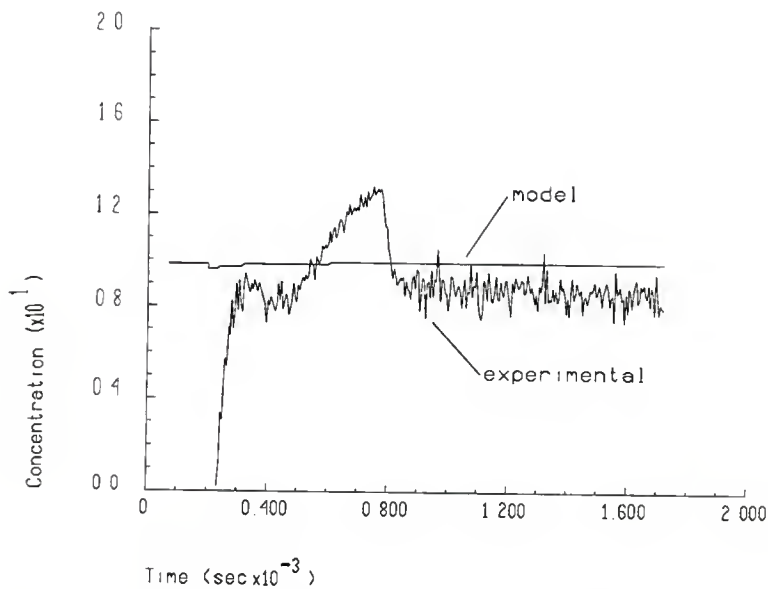


Figure 63: Experimental Results and Model Predictions of Concentration for Ammonia Vapor Absorption into Water Spray Ending at 1 Pound of Ammonia per Gallon of Water.

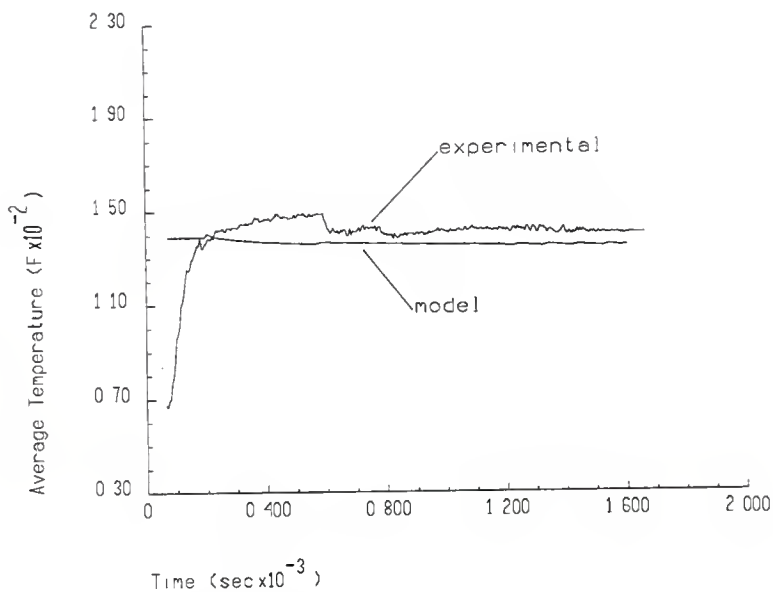


Figure 64: Experimental Results and Model Predictions of Average Temperature for Ammonia Vapor Absorption into Water Spray Ending at 2 Pounds of Ammonia per Gallon of Water.

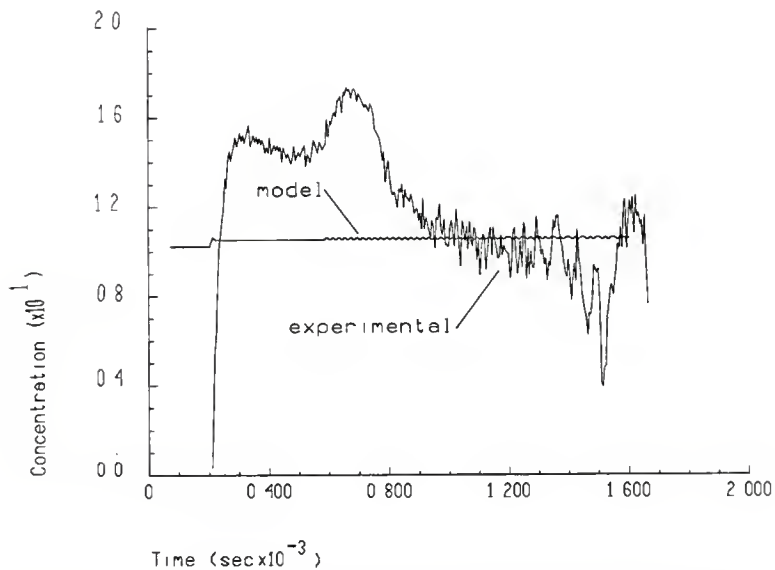


Figure 65: Experimental Results and Model Predictions of Concentration for Ammonia Vapor Absorption into Water Spray Ending at 2 Pounds of Ammonia per Gallon of Water.

For Case 2, the final average temperature prediction varied less than 7% from the actual final temperature. The concentration predicted varied only 14% from the average concentration of the mixture during the experiment. During the experiment 75.7% of the ammonia released was absorbed compared to the model's prediction that 99.7% would be absorbed.

For Case 3, the final average temperature prediction varied less than 7% from the actual final temperature. The concentration predicted varied only 2.8% from the average concentration of the mixture during the experiment. During the experiment 41.9% of the ammonia released was absorbed compared to the model's prediction that 64.2% would be absorbed.

#### 4. Use of the Models

The models developed for Cases 1 and 2 correctly predict the actual results of these experiments. The computer programs based on these models are written so that variables suitable to industrial sized equipment may be input and the programs run as performance simulations. The predictions from these simulations must be used tentatively, however, since the experiments in this research were run on a much smaller scale.



## VI. Conclusions and Recommendations

### 1. Conclusions

1. All tests were repeatable to within 25%.
2. Heat transfer characteristics of the system were negligible for the experiments in this research.
3. For the experiments in this research, higher ammonia-water Ratios caused greater average temperature rises, greater rates of ammonia absorption, and a higher likelihood of saturation before all of the ammonia was released to the receiver tank.
4. The temperature rise of the mixture was proportional to the amount of ammonia absorbed and corresponded to projections based on the equilibrium chart.
5. The situation in the Case 2 experiments (liquid ammonia absorption into water) at the ammonia-water Ratios tested resulted in the least liquid average temperature rises and more ammonia absorption than the other Cases.
6. Water was a 90% effective vaporous ammonia trap when the ammonia-water ratio was equal to or less than one pound of ammonia to one gallon of water.
7. Water was a 100% effective liquid ammonia trap when the ammonia-water ratio was equal to or less than one pound of ammonia to one gallon of water.

8. The absorption method used in the Case 3 experiments was a less than 70% effective ammonia trap at any ammonia-water ratio tested.
9. The desorption of ammonia from an ammonia-water mixture in a drum follows the equation,

$$\frac{X}{X_0} = 0.8219 - 0.005845 N + 0.1860 \frac{1}{N}$$

during the summer months.

10. The analytical models developed for Cases 1 and 2 correctly predicted the experimental data to within  $\pm 30\%$ .
11. The analytical model developed for Case 3 was only able to predict final average temperature and average concentration of the ammonia during the experiment to within  $\pm 30\%$ .
12. The rearranged energy equation,

$$T_{\text{mix,new}} = T_{\text{mix,old}} + \frac{\Delta M_a [h_{\text{rxn}} - c_{\text{pa}}(T_{\text{mix,old}} - T_a)]}{M_{\text{mix}} c_{\text{pmix}}}$$

correctly estimates the temperature change of an ammonia-water mixture as vaporous ammonia is absorbed into the mixture.

13. The rearranged energy equation,

$$T_{\text{mix,new}} = T_{\text{mix,old}} + \frac{\Delta M_a (h_{\text{rxn}} - h_{\text{fga}})}{M_{\text{mix}} c_{\text{pmix}}}$$

correctly estimates the temperature change of an ammonia-water mixture as liquid ammonia is absorbed into the mixture.

## 2. Recommendations

1. The combined correlation equation, developed for ammonia desorption from an ammonia-water mixture in a drum, is recommended for use in determining ammonia desorption during the summer months.
2. The computer models developed for Cases 1 and 2 are recommended for tentative use as performance simulators in designing systems to trap ammonia releases from industrial refrigeration systems.
3. A better model of Case 3 absorption should be developed where ammonia absorption after the fill pipe is submerged involves absorption into the liquid in the tank and the water droplets above the liquid.
4. Further investigation of Case 3 absorption may be useful since Case 3 could prove to be an effective method of absorbing ammonia at a lower ammonia-water ratio than one-half pound of ammonia to one gallon of water. Effective Case 3 absorption would eliminate problems associated with a standing tank of water.
5. Further investigation of all three Cases in a clear sided vessel may be useful in determining the actual processes taking place during ammonia absorption, especially during the absorption of vaporous ammonia into a water spray.

**APPENDIX A**  
**CALIBRATIONS**

## APPENDIX A

In this appendix, individual instrument calibrations are given for the transducers and flowmeters. All instrumentation was connected to power supplies and the DAS-8 according to manufacturers specifications [23, 24, 25, 26, 27, 28]. Electrical circuit details are provided for the thermocouples and the temperature sensitive current sources. Measurement uncertainties are determined for all measurements.

The instruments requiring calibration were:

1. Differential pressure transducer, Tobar, Inc.
2. Pressure transducer, Setra Systems, Inc.
3. Turbine flowmeter, Hoffer Flow Controls, Inc.
4. Differential pressure transducer, Dieterich Standard

1. Differential pressure transducer: Figure 66 shows the calibration obtained for the differential pressure transducer where compressed air was used to supply the pressure. Output from the transducer is a current proportional to the differential pressure (iwg). A 250  $\Omega$  precision resistor in the output circuit converted output current to a voltage that could be read by the DAS-8. The calibration curve shown incorporates the conversion of the voltage to a pressure by the equation used in the sampling program. Percent uncertainty in

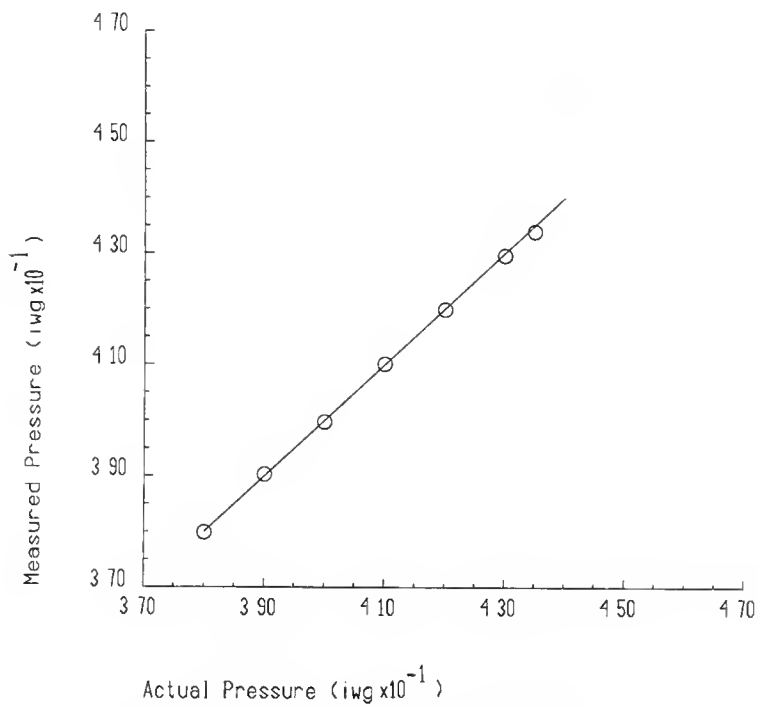


Figure 66: Calibration Curve for the Tobar Differential Pressure Transducer.

the differential pressure measurement is seen to be less than 2% at the 95% confidence interval.

2. Pressure transducer: Figure 67 shows the calibration obtained for the pressure transducer using a deadweight tester. Output from the transducer is a voltage proportional to the pressure (psi). The calibration curve shown incorporates the conversion of the voltage to a pressure by the equation used in the sampling program. Percent uncertainty in the pressure measurement is seen to be less than 2% at the 95% confidence interval.
3. Turbine flowmeter: Figure 68 shows the calibration curve for the turbine flowmeter where water was used as the fluid. Output from the turbine is a voltage proportional to the volumetric flowrate (gal/min). The calibration curve shown incorporates the conversion of the voltage to a flowrate by the equation used in the sampling program. Percent uncertainty in the flow measurement is seen to be less than 2% at the 95% confidence interval.
4. Differential pressure transducer: Figure 69 shows the calibration curve for the differential pressure transducer where compressed air was used to provide the pressure. Output from the transducer is a current proportional to the differential pressure (iwg). A 250 $\Omega$  precision resistor in the output circuit converted the output current to a voltage that could be read by the DAS-8. The calibration curve shown incorporates the conversion of the voltage to a pressure by the equation

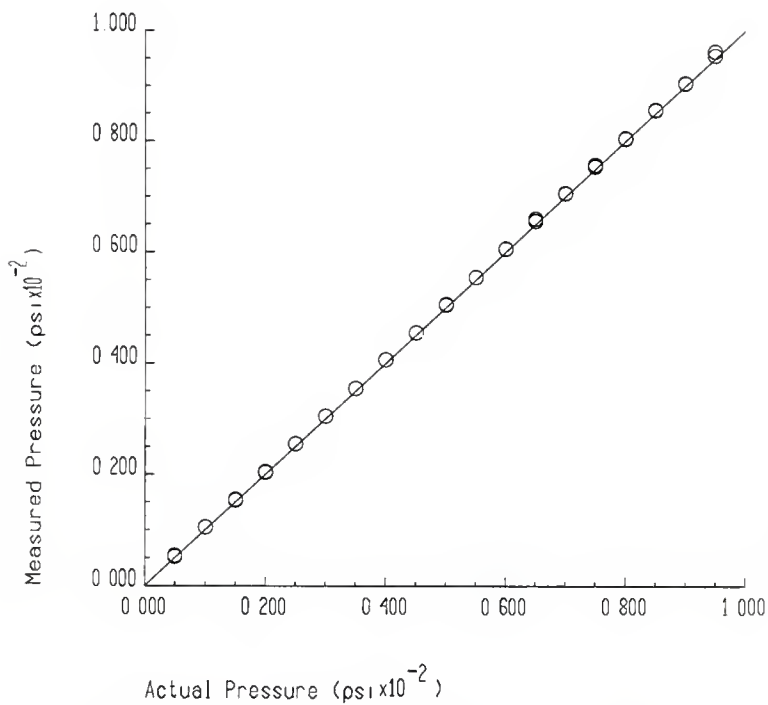


Figure 67: Calibration Curve for the Setra Pressure Transducer.



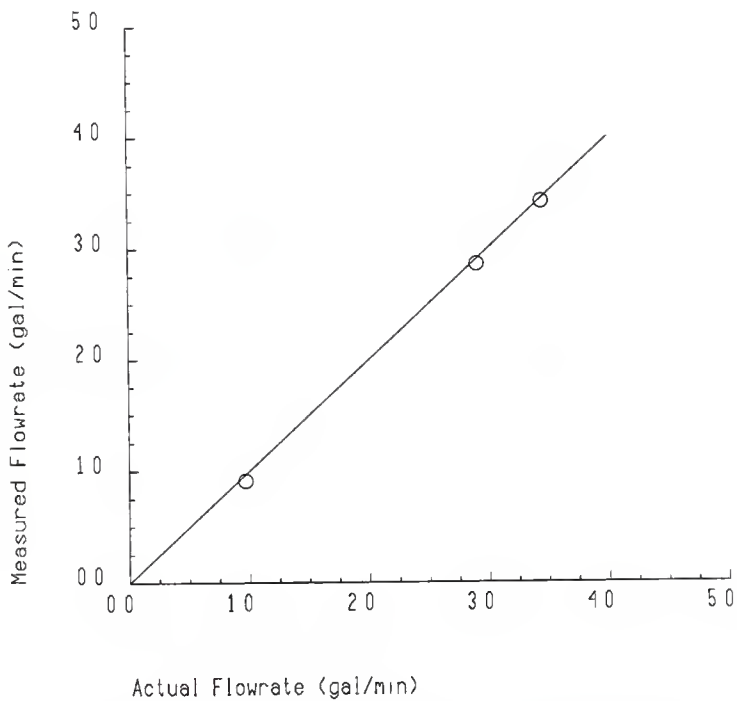


Figure 68: Calibration Curve for the Hoffer Turbine Flowmeter.

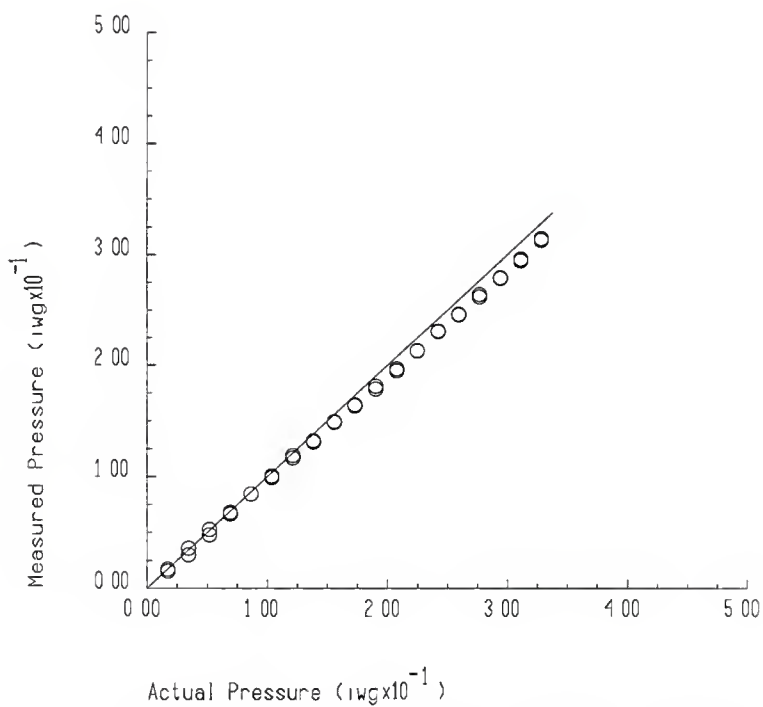


Figure 69: Calibration Curve for the Dieterich Differential Pressure Transducer.

used in the sampling program. Percent uncertainty in the differential pressure measurement is seen to be less than 5% at the 95% confidence interval.

The ammonia vapor flowrate is given by the following equation obtained from the annubar flow sensor distributor [29],

$$\dot{m} = c' dp^{1/2}$$

where,

$\dot{m}$  = mass flowrate of ammonia vapor, lbm/min

$c'$  = calculation constant provided by distributor

$dp$  = differential pressure, iwg

The calculation constant is substance specific and was provided at the transducer limits [29].  $c'$  is interpolated at the differential pressure before calculation of the flowrate and has a percent uncertainty of less than 0.01%. The percent uncertainty of the ammonia vapor mass flowrate is less than 2.5% [30].

The four thermocouples, Omega Engineering, Inc., were referenced to a large aluminum block inside a thermally insulated box as shown in Figure 70 [31]. The voltage output from each of the thermocouples was amplified 100x by an Omega Omni-Amp [32]. The temperature of the aluminum block was measured by a temperature sensitive current source in the circuit shown in Figure 71 [33]. The circuit had a voltage output of 1  $\mu\text{V}/^\circ\text{K}$  with an amplifier gain of 10. The voltage output measured by the DAS-8 was divided by 10 to get the absolute temperature in  $\mu\text{V}$ . The centigrade temperature in  $\mu\text{V}$  was obtained by subtracting 0.2372  $\mu\text{V}$

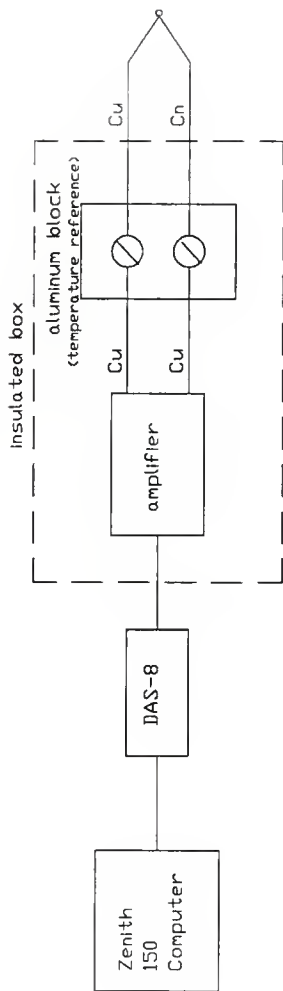


Figure 70: Diagram of the Thermocouple Reference to the Large Aluminum Block.

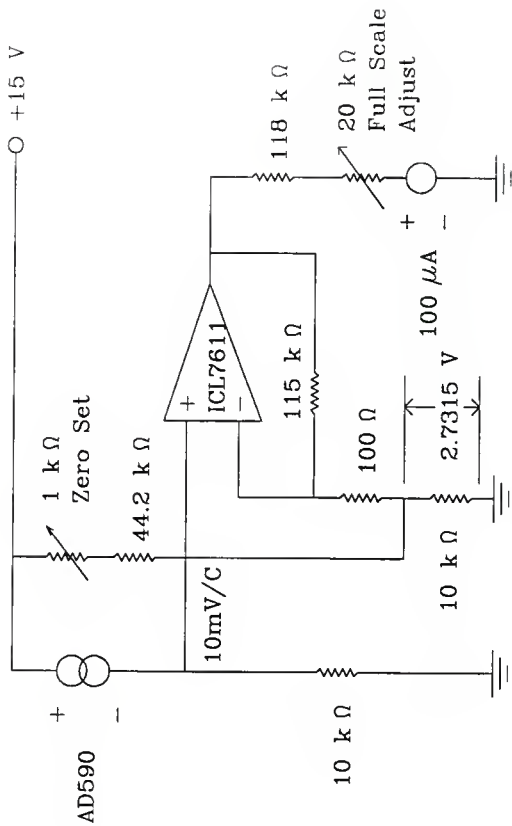


Figure 71: Diagram of the Temperature Sensitive Reference Circuit.

(273.2°K). Multiplication by 1000 yielded the measurement in °C. Uncertainty of the reference measurement was estimated to be  $\pm 2.7^{\circ}\text{F}$  ( $\pm 1.5^{\circ}\text{C}$ ).

Standard thermocouple tables [34] show that each degree centigrade change in a copper-constantan thermocouple results in a 0.04 mV change ( $\pm 0.01$  mV) in the thermocouple output for the range of these experiments ( $-10^{\circ}\text{C}$  to  $100^{\circ}\text{C}$ ). The output voltage measured by the DAS-8 was divided by 100 to get the actual thermocouple output in mV. Division by 0.04 resulted in the temperature difference between the thermocouple and the reference block. The temperature measured by the thermocouple was then obtained by adding the temperature of the reference block as measured by the temperature sensitive resistor. Because Omega thermocouples are an industry standard, the measurement of the temperature difference between the thermocouple and the reference block is taken to have a measurement uncertainty of  $\pm 0.9^{\circ}\text{F}$  ( $\pm 0.5^{\circ}\text{C}$ ), giving the actual temperature measurement an uncertainty of  $\pm 3.6^{\circ}\text{F}$  ( $\pm 2^{\circ}\text{C}$ ).

**APPENDIX B**  
**SAMPLING PROGRAMS**

## APPENDIX B

The following programs sample the eight channels on the MetraByte DAS-8 board and store the data in a disk file. Data is sampled every 5 seconds until the program is told to switch to sampling every 30 minutes. Sampling continues at this rate for 48 hours or until the program is terminated from the keyboard. Because the long term data was erratic for Cases 1 and 3 when vaporous ammonia was released, data was taken every five minutes and then averaged and recorded every 30 minutes during the long term sampling.

### 1. Case 1 and 3: SAMPL.BAS

```

:
:   This program is to sample data for Cases 1 & 3 through the DAS-8
:   and store it in a disk file. Data is sampled every 5 sec until
:   switched to long term sampling (every 30 min). Sampling
:   continues at this rate for 48 hours or until the program is
:   terminated from the keyboard. Data is stored in the following
:   format:
:
:   TIME REFTEMP TQTEMP SUPPRESS MIDTEMP PRESS BOTTEMP SUPFLOW SUPTEMP
:
:   where:
:
:   REFTEMP = temperature of thermocouple reference block, C
:   TQTEMP = temperature of thermocouple 24" above tank bottom, C
:   SUPPRESS = pressure of ammonia in supply line, PSI
:   MIDTEMP = temperature of thermocouple 12" above tank bottom, C
:   PRESS = pressure of liquid in tank, INW
:   BOTTEMP = temperature of thermocouple on tank bottom, C
:   SUPFLOW = flowrate of ammonia in supply line, gal/min
:   SUPTEMP = temperature of thermocouple in supply line, C
:
: .....
:
:   DIM LX(8), HX(8), XX(8), V(8)
:
:   Set up file data is to be written to
:
:   INPUT "ENTER FILE NAME ",IN$
:   OPEN IN$ FOR OUTPUT AS #1
:
:   Prepare to start sampling
:
:   A$ = " "
:   B$ = " "
:   PRINT
:   PRINT "Start 5 sec sampling, then start ammonia flow. After desired"
:   PRINT "amount of time, change to long term (30 min) sampling. When"
:   PRINT "ready to start 5 sec sampling hit 'S'. When ready to change"
:   PRINT "to long term sampling, hit 'L'."
```



```

      WHILE B# () "S"
        B# = INKEY#
      WEND
      PRINT
      PRINT "Short term sampling started"
    ,
    ,
      Sample every 5 seconds.
    ,
      T = TIMER
      TINIT = T
      WHILE A# () "L"
        T = T + 5
10      TIME = TIMER : IF TIME < T THEN 10
        GOSUB 100
        A# = INKEY#
      WEND
      CLOSE #1
      PRINT
      PRINT "Long term sampling started"
    ,
    ,
      Sample every 30 minutes for 48 hours.
    ,
      FOR K = 1 TO 96
        FOR I = 1 TO 8
          SUM(I) = 0
        NEXT I
        FOR L = 1 TO 6
          T = T + 300
          IF T > 86400 THEN T = T - 86400 ELSE GOTO 20
          TINIT = TINIT - 86400
20          TIME = TIMER : IF TIME < T THEN 20
          GOSUB 100
          FOR I = 1 TO 8
            SUM(I) = SUM(I) + X(I)
          NEXT I
          NEXT L
          FOR I = 1 TO 8
            X(I) = SUM(I)/6.0
          NEXT I
          GOSUB 200
        NEXT K
      END program
    ,
    ,
      CLOSE #1
      PRINT "Sampling ended"
      END
    ,
    ,
      Sampling subroutine.
100  FOR II = 1 TO 8
      IX = II - 1
      OUT &H302,IX
      OUT &H301,0
40      IF (INP(&H302) AND &H80) < 0 THEN 40
      LX(II) = INP(&H300)
      HX(II) = INP(&H301)
      X(II) = HX(II)*16 + LX(II)/16
    NEXT II
    RETURN
    ,
    ,
      Recording subroutine.
200  FOR J = 1 TO 8
      V(J) = X(J) * 10.0/4096.0 - 5.0
    NEXT J
      REFTEMP = (V(1)/10.0 - .2732) + 1000.0
      TOTTEMP = (V(2)/0.004) + REFTEMP
      MIDTEMP = (V(4)/0.004) + REFTEMP
      BOTTEMP = (V(6)/0.004) + REFTEMP
      SUPTEMP = (V(8)/0.004) + REFTEMP
      PRESS = (55.0/4.0) * (V(5) - 1.0) - 1.0
      SUPPRESS = 50.0 * (V(5) - 0.1)
      SUPFLOW = 1.9 * V(7)
      PRINT #1, REFTEMP, TOTTEMP, SUPPRESS, MIDTEMP, PRESS, BOTTEMP, SUPFLOW, SUPTEMP
      RETURN
    END

```

## 2. Case 2: SAMP2.BAS

```

*
* This program is to sample data for Case 2 through the DAS-8 and
* store it in a disk file. Data is sampled every 5 sec until
* switched to long term sampling (every 30 min). Sampling
* continues at this rate for 48 hours or until the program is
* terminated from the keyboard. Data is stored in the following
* format:
*
* TIME REFTEMP TOTTEMP SUPPRESS MIDTEMP PRESS BOTTEMP SUPFLOW SUPTEMP
*
* *****
*
* where:
*
* REFTEMP = temperature of thermocouple reference block, C
* TOTTEMP = temperature of thermocouple 24" above tank bottom, C
* SUPPRESS = pressure of ammonia in supply line, psi
* MIDTEMP = temperature of thermocouple 12" above tank bottom, C
* PRESS = pressure of liquid in tank, 1wg
* BOTTEMP = temperature of thermocouple on tank bottom, C
* SUPFLOW = flowrate of ammonia in supply line, gal/min
* SUPTEMP = temperature of thermocouple in supply line, C
*
* .....
*
* DIM LX(8), HX(8), XX(8), V(8)
*
* Set up file data is to be written to
*
* INPUT "ENTER FILE NAME ".LN$
* OPEN LN$ FOR OUTPUT AS #1
*
* Prepare to start sampling
*
* A$ = " "
* B$ = " "
* PRINT
* PRINT "Start 5 sec sampling, then start ammonia flow. After desired"
* PRINT "amount of time, change to long term (30 min) sampling. When"
* PRINT "ready to start 5 sec sampling hit 'S'. When ready to change"
* PRINT "to long term sampling, hit 'L'."
*
* WHILE B$ (0) "S"
*   B$ = INKEY$
* WEND
* PRINT
* PRINT "Short term sampling started"
*
* Sample every 5 seconds.
*
* T = TIMER
* TINIT = T
* WHILE A$ (0) "L"
*   T = T + 5
10   TIME = TIMER : IF TIME < T THEN 10
*   GOSUB 100
*   A$ = INKEY$
* WEND
* CLOSE #1
* PRINT
* PRINT "Long term sampling started"

```

```

'
' Sample every 30 minutes for 48 hours.
'
FOR K = 1 TO 96
  FOR I = 1 TO 8
    SUM(I) = 0
  NEXT I
  FOR L = 1 TO 6
    T = T + 300
    IF T > 86400 THEN T = T - 86400 ELSE GOTO 20
    TINIT = TINIT - 86400
    TIME = TIMER : IF TIME < T THEN 20
    GOSUB 100 'sample all 8 channels
    FOR I = 1 TO 8
      SUM(I) = SUM(I) + XX(I)
    NEXT I
  NEXT L
  FOR I = 1 TO 8
    YX(I) = SUM(I)/6.0 'find ave values
  NEXT I
  GOSUB 200
NEXT K
'
' End program
'
CLOSE #1
PRINT "Sampling ended"
END
'
' Sampling subroutine.
'
100 FOR II = 1 TO 8
  IX = II - 1 'convert II to channel #
  OUT &H302,IX 'set channel #
  OUT &H301,0 'start 12 bit conversion
  IF INP(&H300) AND &H80 < 0 THEN 40 'check for end of conversion
  LX(II) = INP(&H300) 'input low byte
  HX(II) = INP(&H301) 'input high byte
  YX(II) = HX(II)*16 + LX(II)/16 'combine bytes
NEXT II
RETURN
'
' Recording subroutine.
'
200 FOR J = 1 TO 8
  V(J) = XX(J) * 10.0/4096.0 - 5.0 'convert to voltage
NEXT J
REFTEMP = (V(1)/10.0 - .2752) * 1000.0
TOPTEMP = (V(2)/0.004) + REFTEMP
MIDTEMP = (V(4)/0.004) + REFTEMP
BOTTEMP = (V(6)/0.004) + REFTEMP
SUPTEMP = (V(8)/0.004) + REFTEMP
PRESS = (55.0/4.0) * (V(3) - 1.0) - 1.0
SUPRES = 50.0 * (V(5) - 0.1)
DIFPRES = (V(7) - 1.0) * 133.0/4.0
CPRIME = -9.8115E-4 * DIFPRES + 3.55248
SUPFLOW = SQR(ABS(DIFPRES)) * CPRIME
PRINT #1, REFTEMP, TOPTEMP, SUPTEMP, SUPRES, MIDTEMP, PRESS, BOTTEMP, SUPFLOW, SUPTEMP
PRINT, REFTEMP, TOPTEMP, SUPRES, MIDTEMP, PRESS, BOTTEMP, SUPFLOW, SUPTEMP
RETURN
END

```

APPENDIX C  
OTHER EXPERIMENTAL DATA

## APPENDIX C

The following Figures are plots of the measurements taken by the instrumentation during each of the absorption experiments.

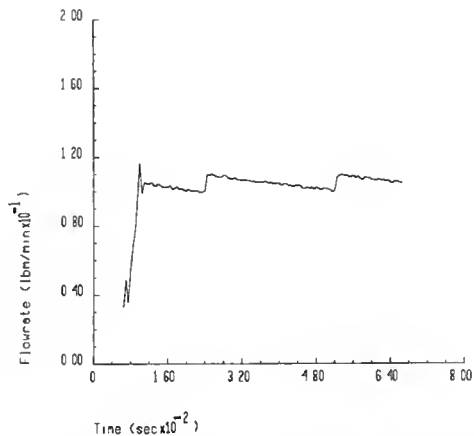


Figure 72: Variation of Ammonia Flowrate During Ammonia Vapor Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

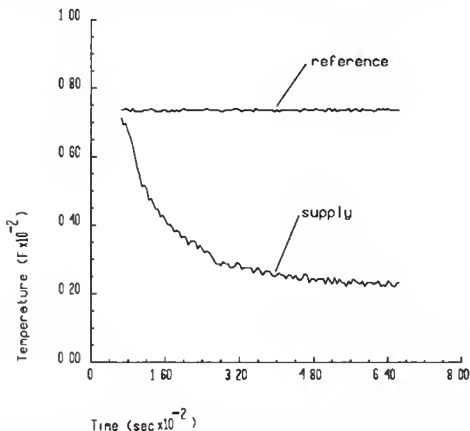


Figure 73: Variation of Ammonia Supply and Reference Block Temperature During Ammonia Vapor Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

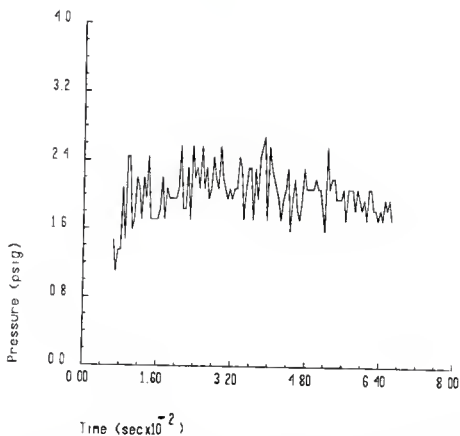


Figure 74: Variation of Ammonia Supply Pressure During Ammonia Vapor Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

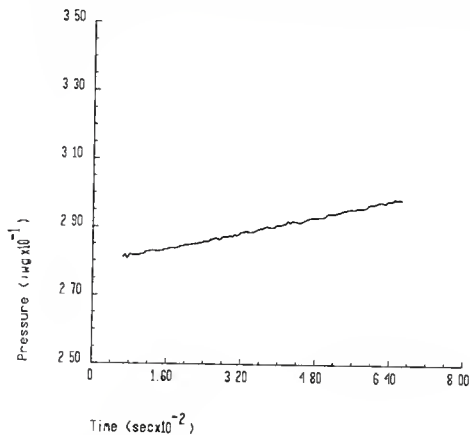


Figure 75: Variation of Tank Liquid Pressure During Ammonia Vapor Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

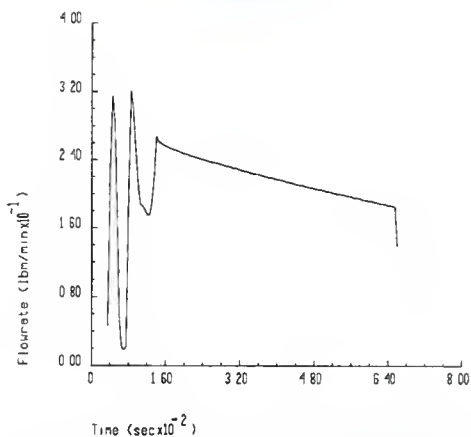


Figure 76: Variation of Ammonia Flowrate During Ammonia Vapor Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

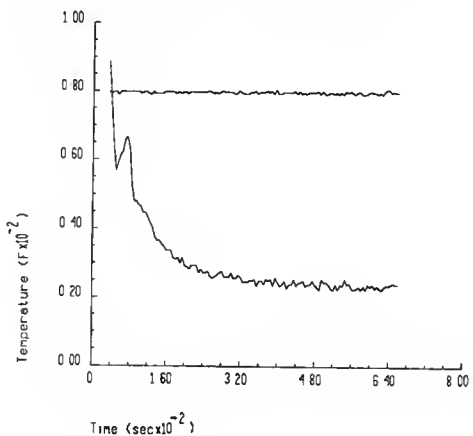


Figure 77: Variation of Ammonia Supply and Reference Block Temperature During Ammonia Vapor Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.



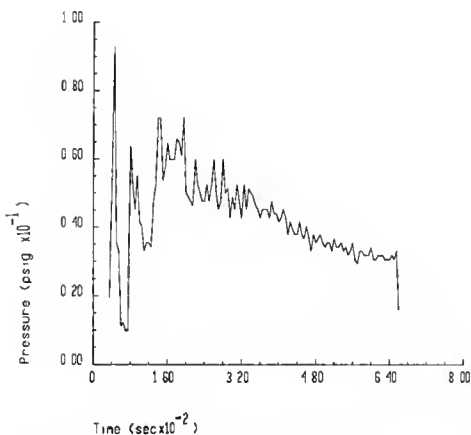


Figure 78: Variation of Ammonia Supply Pressure During Ammonia Vapor Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

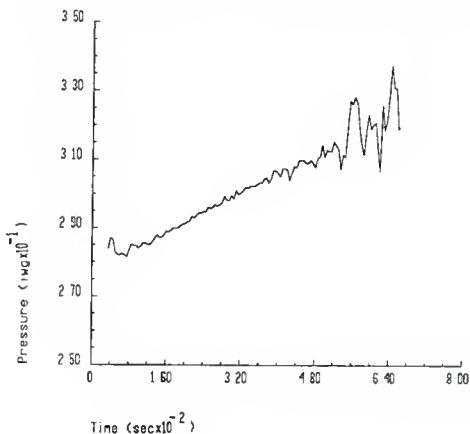


Figure 79: Variation of Tank Liquid Pressure During Ammonia Vapor Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

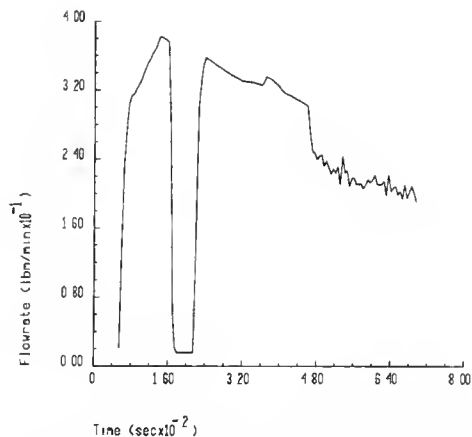


Figure 80: Variation of Ammonia Flowrate During Ammonia Vapor Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

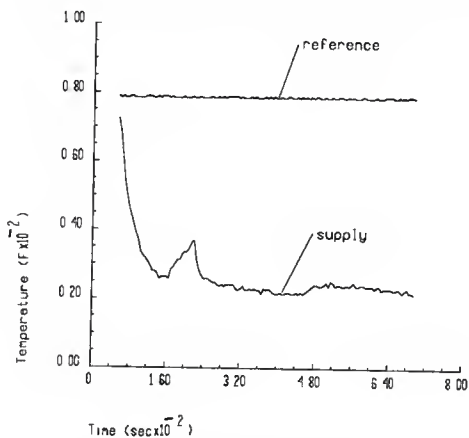


Figure 81: Variation of Ammonia Supply and Reference Block Temperature During Ammonia Vapor Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

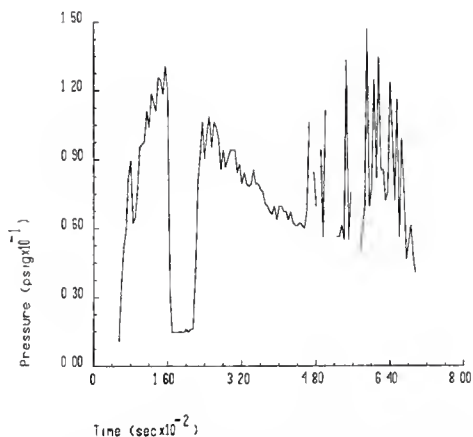


Figure 82: Variation of Ammonia Supply Pressure During Ammonia Vapor Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

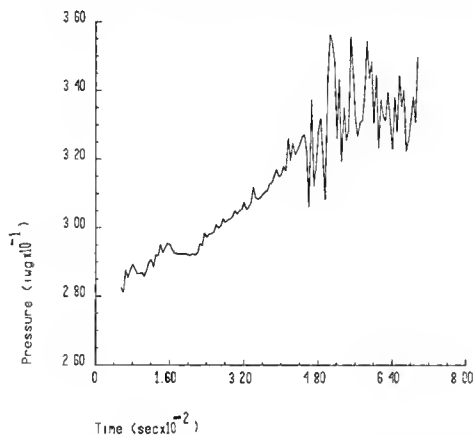


Figure 83: Variation of Tank Liquid Pressure During Ammonia Vapor Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

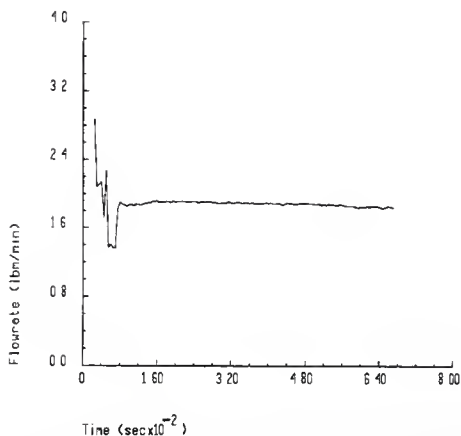


Figure 84: Variation of Ammonia Flowrate During Ammonia Liquid Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

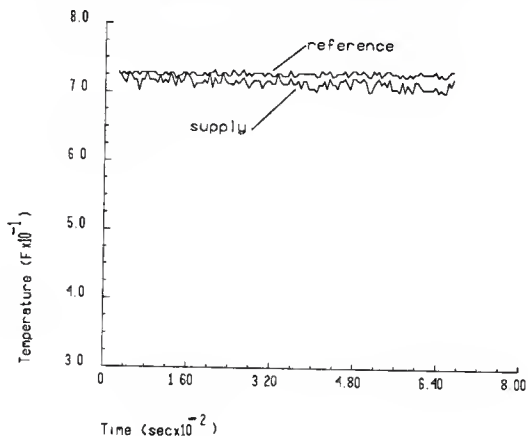


Figure 85: Variation of Ammonia Supply and Reference Block Temperature During Ammonia Liquid Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

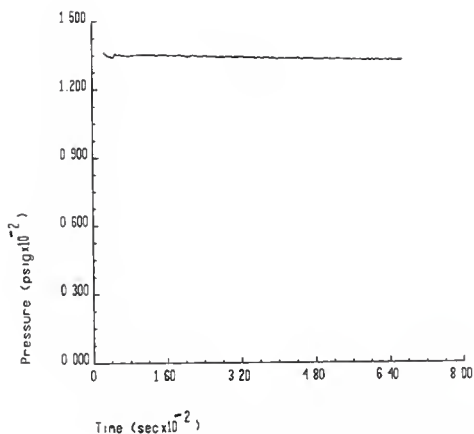


Figure 86: Variation of Ammonia Supply Pressure During Ammonia Liquid Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

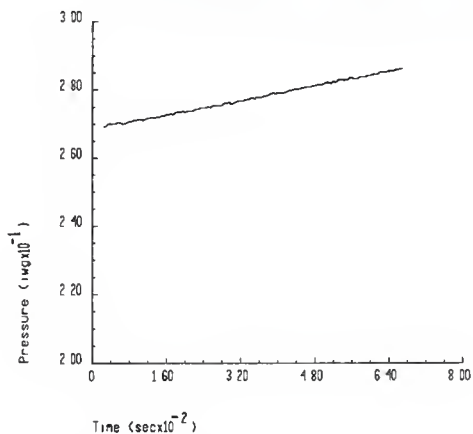


Figure 87: Variation of Tank Liquid Pressure During Ammonia Liquid Absorption into Water Ending at 0.5 Pound of Ammonia per Gallon of Water.

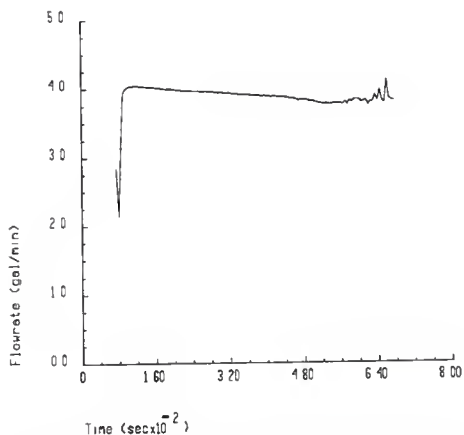


Figure 88: Variation of Ammonia Flowrate During Ammonia Liquid Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

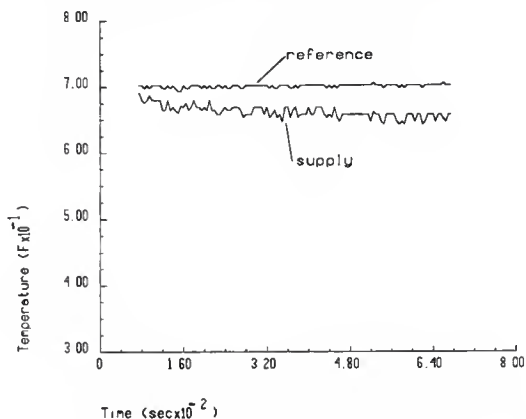


Figure 89: Variation of Ammonia Supply and Reference Block Temperature During Ammonia Liquid Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

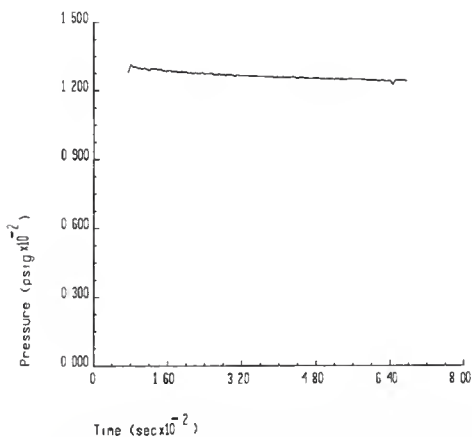


Figure 90: Variation of Ammonia Supply Pressure During Ammonia Liquid Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

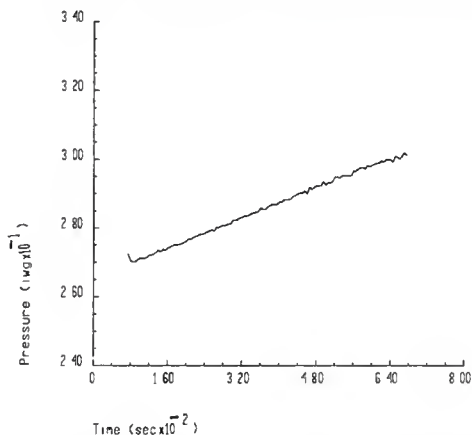


Figure 91: Variation of Tank Liquid Pressure During Ammonia Liquid Absorption into Water Ending at 1 Pound of Ammonia per Gallon of Water.

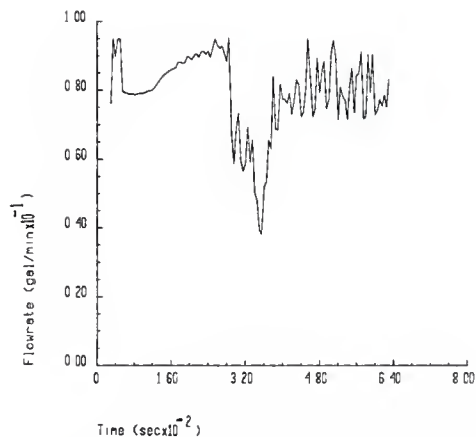


Figure 92: Variation of Ammonia Flowrate During Ammonia Liquid Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

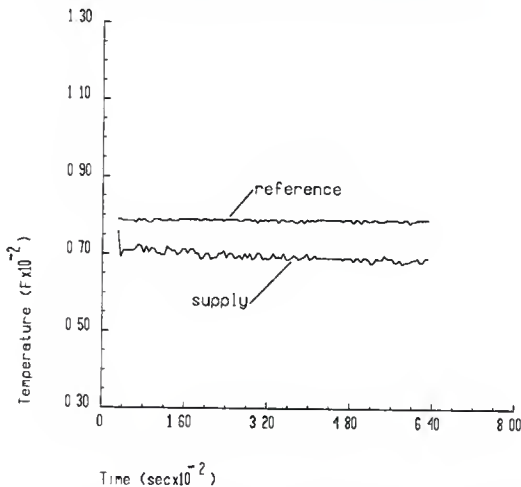


Figure 93: Variation of Ammonia Supply and Reference Block Temperature During Ammonia Liquid Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.



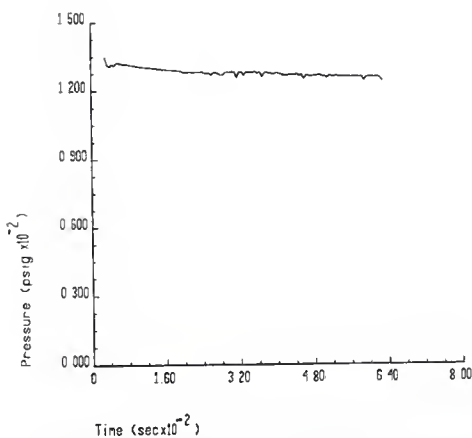


Figure 94: Variation of Ammonia Supply Pressure During Ammonia Liquid Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

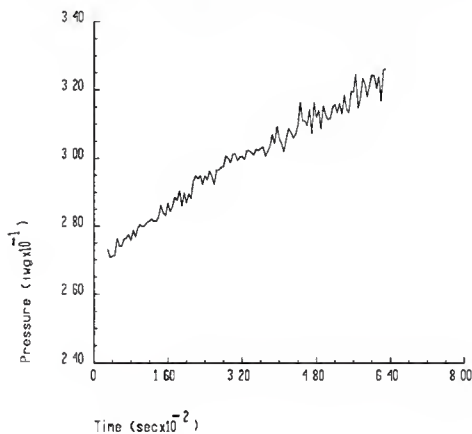


Figure 95: Variation of Tank Liquid Pressure During Ammonia Liquid Absorption into Water Ending at 2 Pounds of Ammonia per Gallon of Water.

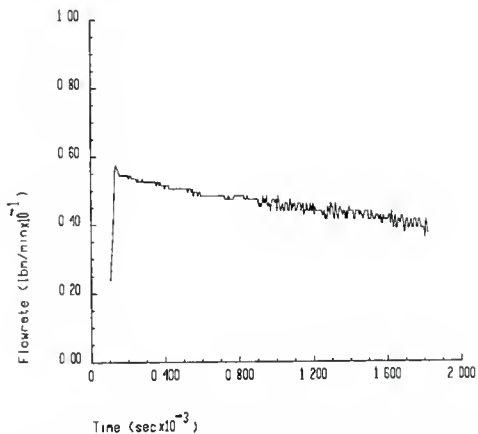


Figure 96: Variation of Ammonia Flowrate During Ammonia Vapor Absorption into Water Spray Ending at 0.5 Pound of Ammonia per Gallon of Water.

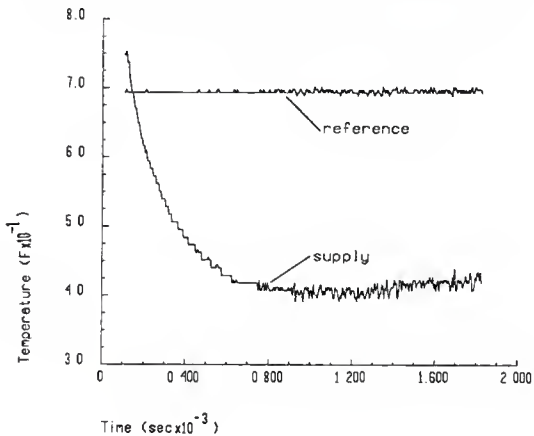


Figure 97: Variation of Ammonia Supply and Reference Block Temperature During Ammonia Vapor Absorption into

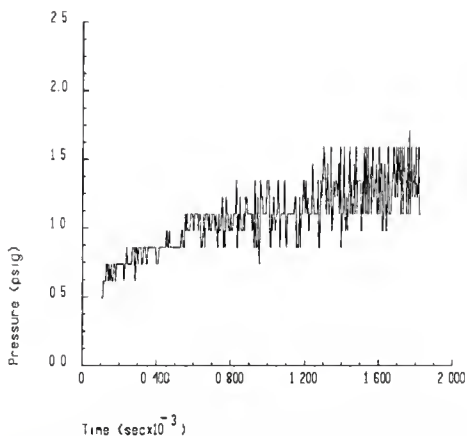


Figure 98: Variation of Ammonia Supply Pressure During Ammonia Vapor Absorption into Water Spray Ending at 0.5 Pound of Ammonia per Gallon of Water.

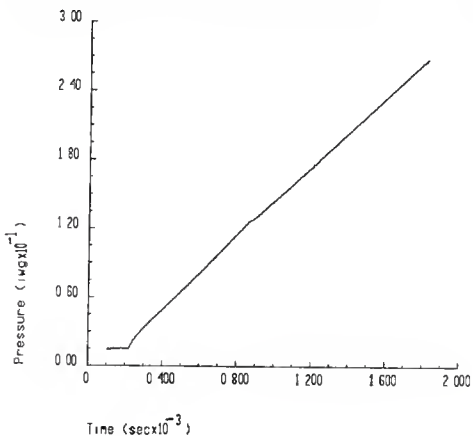


Figure 99: Variation of Tank Liquid Pressure During Ammonia Vapor Absorption into Water Spray Ending at 0.5 Pound of Ammonia per Gallon of Water.

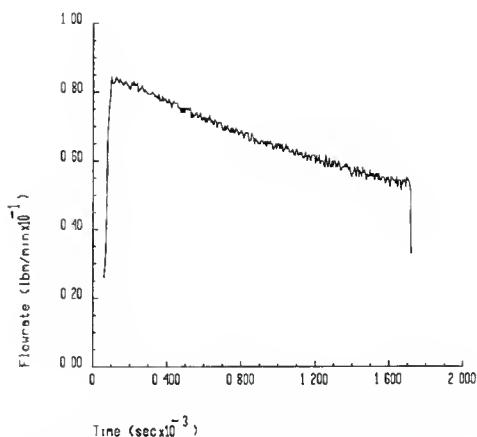


Figure 100: Variation of Ammonia Flowrate During Ammonia Vapor Absorption into Water Spray Ending at 1 Pound of Ammonia per Gallon of Water.

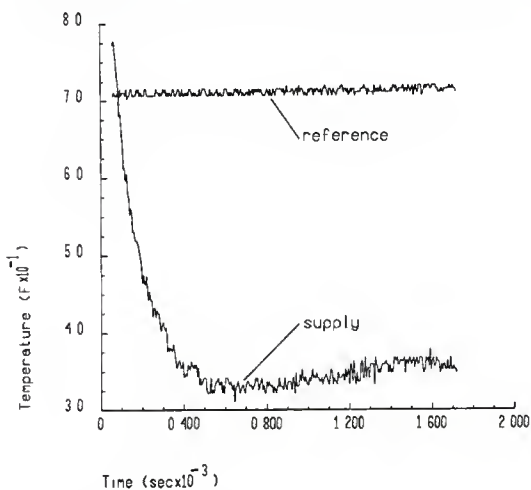


Figure 101: Variation of Ammonia Supply and Reference Block Temperature During Ammonia Vapor Absorption into Water Spray Ending at 1 Pound of Ammonia per Gallon of Water.

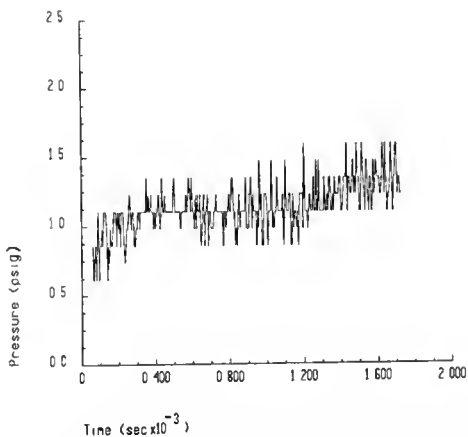


Figure 102: Variation of Ammonia Supply Pressure During Ammonia Vapor Absorption into Water Spray Ending at 1 Pound of Ammonia per Gallon of Water.

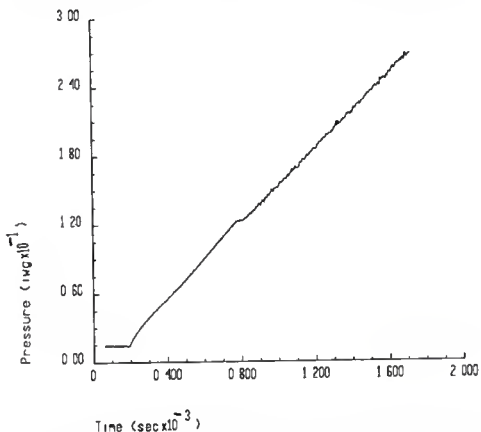


Figure 103: Variation of Tank Liquid Pressure During Ammonia Vapor Absorption into Water Spray Ending at 1 Pound of Ammonia per Gallon of Water.

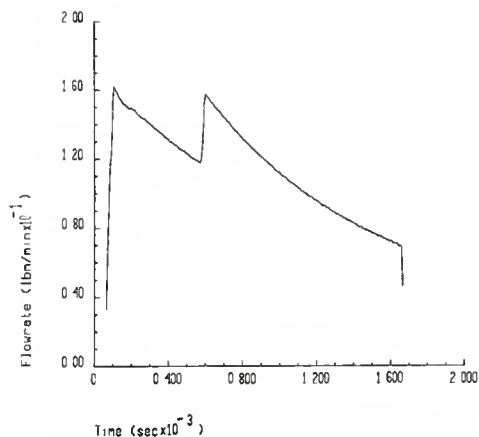


Figure 104: Variation of Ammonia Flowrate During Ammonia Vapor Absorption into Water Spray Ending at 2 Pounds of Ammonia per Gallon of Water.

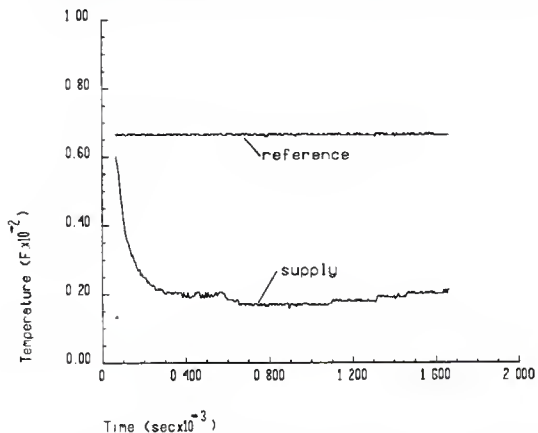


Figure 105: Variation of Ammonia Supply and Reference Block Temperature During Ammonia Vapor Absorption into Water Spray Ending at 2 Pounds of Ammonia per Gallon of Water.

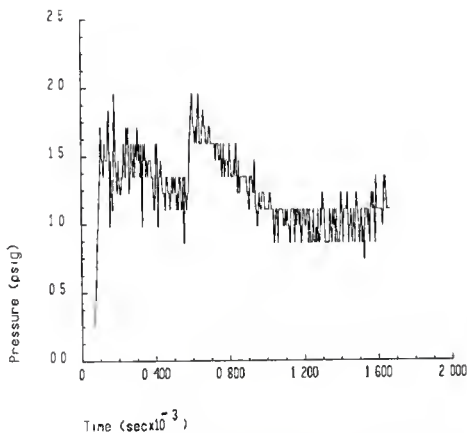


Figure 106: Variation of Ammonia Supply Pressure During Ammonia Vapor Absorption into Water Spray Ending at 2 Pounds of Ammonia per Gallon of Water.

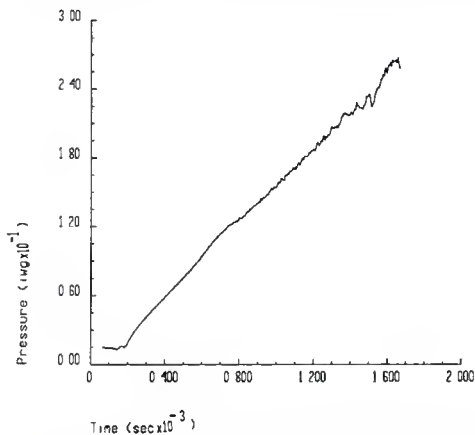


Figure 107: Variation of Tank Liquid Pressure During Ammonia Vapor Absorption into Water Spray Ending at 2 Pounds of Ammonia per Gallon of Water.

**APPENDIX D**  
**ANALYTICAL MODEL PROGRAMS**



## APPENDIX D

The following programs are used to predict the temperature history upon absorption of ammonia, and the ammonia absorption rate. Example input files are included with each program.

### 1. Case 1: AMLT1.FOR

```

C      FILE: AMLT1 FORTRAN
C
C      DYNAMIC SIMULATION OF AMMONIA LIQUID ABSORPTION
C      INTO A WATER TRAP
C
C      NOTE: "CPMIX" BASED DN AMMONIA-WATER MIXTURE DATA IN
C            CHEMICAL ENGINEERS HANDBOOK
C      "PPSATW" BASED DN SATURATED WATER DATA BY REYNOLDS
C      "PPNH3" PARTIAL PRESSURE OF AMMONIA VAPOR ABOVE
C            AMMONIA-WATER MIXTURE, BASED DN DATA IN
C            CHEMICAL ENGINEERS HANDBOOK, THE "PPAFF"
C            FACTOR IS AN ADJUSTMENT TO DUPLICATE
C            THE NH3-H2O EQUIL. CHART.
C      "HFGA" HEAT OF VAPORIZATION FOR AMMONIA AS FUNCTION
C            OF SATURATED PROPERTY DATA.
C
C      IMPLICIT DOUBLE PRECISION(A-H, O-Z)
C      DOUBLE PRECISION MA, MAREL, MIA, MI, MDOA, MMIX, MAMIX, MAOUT, MARATO,
1      MATRAP
C
C      FUNCTIONS
CPMIX(T, XX) = (7.7060D0 - 0.022450D0 * T + 0.000035690D0 * T * T)
1      + (-298.80D0 + 1.9230D0 * T - 0.0030610D0 * T * T) * XX
2      + (1160.00D0 - 7.5090D0 * T + 0.011980D0 * T * T) * XX * XX
PPSATW(T) = (0.1059D+09) * EXP((-0.5171D+04) / T)
PPNH3(T, XX) = ((3894.7699D0 - 23.99567D0 * T + 0.03696 * T * T)
1      + (29203.743D0 - 255.7423D0 * T + 0.54111D0 * T * T) * XX
2      + (170153.485D0 - 1197.155D0 * T + 2.818166 * T * T) * XX * XX)
3      * (101.325D0 / 760.0D0)
HFGA(T) = (0.1416D+04) + (0.2507D+01) * T - (0.1123D-01) * T * T
C      OPEN FILES FOR INPUT AND OUTPUT
C      OPEN(UNIT=5, FILE='AMLT1 INP', STATUS='OLD')
C      OPEN(UNIT=7, FILE='AMLT1 OUT')
C      INITIAL CONDITIONS
C      READ CONTROLING TIME PARAMETERS
C      READ(5, 910) TIME, TTIME, TSTEP
910 FORMAT (D20.4)

```

```

C   READ INITIAL CONDITIONS FOR AMMONIA LIQUID RELEASE
    READ(5,910) PATMOS,TIW,TIA,MW,MIA
C   READ TOTAL AMMONIA LIQUID MASS RELEASED TO TANK
    READ(5,910) MAREL
    MDOTA=MAREL/TTIME
C   WRITE INITIAL CONDITIONS FOR SIMULATION
    WRITE(6,920)
    WRITE(7,920)
920 FORMAT(1X,' INITIAL CONDITIONS FOR SIMULATED LIQUID RELEASE',/)
    WRITE(6,921) TIME,TTIME,TSTEP
    WRITE(7,921) TIME,TTIME,TSTEP
921 FORMAT(1X,' INITIAL TIME =',F4.1,' SEC',/,
1 IX,' TOTAL ELAPSED TIME =',F6.1,' SEC',/,
2 IX,' TIME STEP =',F4.1,' SEC',/)
    WRITE(6,922) PATMOS,TIW,TIA,MW,MIA
    WRITE(7,922) PATMOS,TIW,TIA,MW,MIA
922 FORMAT(1X,' ATMOSPHERIC PRESSURE =',F6.2,' KPA',/,
1 IX,' WATER TEMPERATURE =',F5.1,' DEG C',/,
2 IX,' AMMONIA LIQUID TEMPERATURE =',F5.1,' DEG C',/,
3 IX,' WATER VOLUME =',F6.2,' GAL',/,
4 IX,' INITIAL AMMONIA MASS IN WATER TRAP =',F6.2,' KG',/)
    TIW=TIW+273.16000
    TIA=TIA+273.16000
    PPAFF=-9.733200+6.373100*(TIW/100.000)
1 -0.98744200*(TIW/100.000)**2
    MW=MW*0.0037854000/0.001003000
    WRITE(6,923) MAREL
    WRITE(7,923) MAREL
923 FORMAT(1X,' TOTAL AMMONIA VAPOR VENTED TO TANK =',F6.2,' KG',/)
    TMIX=TIW
    TMIXC=TMIX-273.2000
    XI=MIA/(MIA+MW)
C   HEAT OF REACTION — ESTIMATED ON BASIS OF NH3-H2O EQUIL. CHT.
    DHRXN=-5670.7400+5589.9400*(TIW/100.000)
1 -1044.1900*(TIW/100.000)**2
C   CALCULATED VARIABLES
    DELMA=MDOTA*TSTEP
    DELHT=DELMA+DHRXN
    DELHFG=DELMA+HFGA(TIA)
    PPMIX=PPNH3(TMIX,XI)*PPAFF+PPSATW(TMIX)
C   WRITE INITIAL CONDITIONS
    WRITE(6,900)
    WRITE(7,900)
900 FORMAT(10X,' ESTIMATED AMMONIA-WATER MIXTURE PROPERTIES',
1 /,10X,' VARIATION UPON INPUT OF AMMONIA LIQUID',
2 //,6X,' TIME NH3 CONC. LIQ. TEMP. PRESS NH3 MASS'
3 /,6X,' (SEC) (X) (DEG. C) (KPA) (KG)')
    WRITE(6,901) TIME,XI, TMIXC, PPMIX, MIA
    WRITE(7,901) TIME,XI, TMIXC, PPMIX, MIA
901 FORMAT(1X,F10.1,5X,F6.3,4X,F10.2,3X,F10.3,3X,F8.3)
    MA=MIA

```

```

C      INCREMENT TIME FOR CALCULATION OF TEMPERATURE INCREASE
10 IF (TIME.LT.TTIME) THEN
      TIME=TIME+TSTEP
      MA=MA+DELMA
      MMIX=MW+MA
      X=MA/MMIX
      DELT=(DELHT-DELHFG)/MMIX/CPMIX(TMIX,X)
C      WRITE(6,930) DELHT,DELHFG,DELT
C 930   FORMAT(1X,3D12.4)
      TMIX=TMIX+DELT
      PPMIX=PPNH3(TMIX,X)*PPAFF+PPSATW(TMIX)
C      MAXIMUM SOLUBILITY ACHIEVED WHEN TOTAL MIXTURE VAPOR
C      PRESSURE EXCEEDS AMBIENT PRESSURE
      IF (PPMIX.GT.PATMOS) THEN
        MASAT=MA
        GOTO 20
      ENDIF
      TMIXC=TMIX-273.2000
      WRITE(6,901) TIME,X,TMIXC,PPMIX,MA
      WRITE(7,901) TIME,X,TMIXC,PPMIX,MA
      GOTO 10
ENDIF
IF (TIME.GE.TTIME) THEN
      WRITE(6,924)
      WRITE(7,924)
924   FORMAT(/,1X,'TOTAL AMMONIA MASS RELEASED IS ABSORBED')
      WRITE(6,925) MA
      WRITE(7,925) MA
925   FORMAT(1X,'TOTAL AMMONIA MASS IN WATER TRAP TANK =',
1     F6.2,' KG')
      GOTO 30
ENDIF
C      SUM REMAINING VENTED AMMONIA ENTERING TANK
20 IF (TIME.LE.TTIME) THEN
      TIME=TIME+TSTEP
      MA=MA+DELMA
      GOTO 20
ENDIF
MATRAP=MASAT-MIA
MADUT=MA-MASAT
MARATO=MADUT/MA
WRITE(6,902) MIA,MATRAP,MADUT,MARATO
WRITE(7,902) MIA,MATRAP,MADUT,MARATO

```

```

902 FORMAT(//,1X,'INITIAL AMMONIA MASS IN WATER TRAP =',F6.2,' KG',
1 /,1X,'AMMONIA MASS ABSORBED BY WATER TRAP DURING RELEASE =',
2 F6.2,' KG',
3 /,1X,'AMMONIA MASS VENTED FROM TRAP DURING RELEASE =',
4 F6.2,' KG',
5 /,1X,'VENTED AMMONIA -TO- TOTAL AMMONIA RELEASE MASS RATIO =',
6 F6.2)
30 CONTINUE
STOP
END

```

AMLT1.INP

```

00.000 TIME, "INITIAL TIME", SEC
600.0000 TTIME, "TOTAL TIME OF RELEASE", SEC
10.000 TSTEP, "TIME INCREMENT", SEC
101.000 PATMOS, "ATMOSPHERIC PRESSURE", KPA
13.800 TIW, "INITIAL WATER TEMPERATURE", DEG. C
21.400 TIA, "AMMONIA LIQUID TEMPERATURE", DEG. C
200.000 MW, "INITIAL WATER QUANTITY", GAL
00.000 MIA, "INITIAL AMMONIA MASS IN WATER", KG
90.72000 MAREL, "TOTAL AMMONIA RELEASED VENTED TO TANK", KG

```

2. Case 2: AMVT1.FOR

```
C      FILE=AMVTI.FORTRAN
C
C      DYNAMIC SIMULATION OF AMMONIA VAPOR ABSORPTION
C      INTO A WATER TRAP
C
C      SIMULATION BASED ON CURVE-FIT OF AMMONIA-WATER EQUILIBRIUM
C      CHART, NO PROPERTY EVALUATIONS, NO HEAT TRANSFER.
C
C      NOTE: "CPMIX" BASED ON AMMONIA-WATER MIXTURE DATA IN
C      CHEMICAL ENGINEERS HANDBOOK
C      "PPSATW" BASED ON SATURATED WATER DATA BY REYNOLDS
C      "PPNH3" PARTIAL PRESSURE OF AMMONIA VAPOR ABOVE
C      AMMONIA-WATER MIXTURE, BASED ON DATA IN
C      CHEMICAL ENGINEERS HANDBOOK, THE "PPAFF"
C      FACTOR IS AN ADJUSTMENT TO DUPLICATE
C      THE NH3-H2O EQUIL. CHART.
C
C      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
C      DOUBLE PRECISION MA, MAREL, MIA, MW, MDOA, MMIX, MAOUT, MARATO, MATRAP
C      FUNCTIONS
C      CPMIX(T,XX)=(7.7060D0-0.0224500D*T+0.000035690D*T*T)
C      1      +(-298.800D+1.92300D*T-0.00306100D*T*T)*XX
C      2      +(1160.0D0-7.50900D*T+0.011980D*T*T)*XX*XX
C      CPA(T)=-0.7756D0+0.0049580D*T+437.80D0/T
C      PPSATW(T)=(0.1059D+09)*DEXP((-0.5171D+04)/T)
C      PPNH3(T,XX)=((3894.7699D0-23.995670D*T+0.03696*T*T)
C      1      +(29203.743D0-259.74230D*T+0.54111D0*T*T)*XX
C      2      +(170153.485D0-1197.155D0*T+2.818166*T*T)*XX*XX)
C      3      *(101.325D0/760.000)
C      OPEN FILES FOR INPUT AND OUTPUT
C      OPEN(UNIT=5,FILE='AMVT1.INP',STATUS='OLD')
C      OPEN(UNIT=7,FILE='AMVT1.OUT')
C      INITIAL CONDITIONS
C      READ CONTROLLING TIME PARAMETERS
C      READ(5,910) TIME, TTIME, TSTEP
C      910 FORMAT(D20.4)
C      READ INITIAL CONDITIONS FOR AMMONIA VAPOR RELEASE
C      READ(5,910) PATMOS, TIW, TIA, MW, MIA
C      READ TOTAL AMMONIA VAPOR MASS RELEASED TO TANK
C      READ(5,910) MAREL
C      MDOA=MAREL/TTIME
C      WRITE INITIAL CONDITIONS FOR SIMULATION
C      WRITE(6,920)
C      WRITE(7,920)
```

```

920 FORMAT(1X,' INITIAL CONDITIONS FOR SIMULATED RELEASE',/)
WRITE(6,921) TIME, TTIME, TSTEP
WRITE(7,921) TIME, TTIME, TSTEP
921 FORMAT(1X,' INITIAL TIME = ',F4.1,' SEC',/,
1 1X,' TOTAL ELAPSED TIME = ',F6.1,' SEC',/,
2 1X,' TIME STEP = ',F4.1,' SEC',/)
WRITE(6,922) ATMOS, TIW, TIA, MW, MIA
WRITE(7,922) ATMOS, TIW, TIA, MW, MIA
922 FORMAT(1X,' ATMOSPHERIC PRESSURE = ',F6.2,' KPA',/,
1 1X,' WATER TEMPERATURE = ',F5.1,' DEG C',/,
2 1X,' AMMONIA VAPOR TEMPERATURE (FLOWMETER) = ',F5.1,' DEG C',/,
3 1X,' WATER VOLUME = ',F6.2,' GAL',/,
4 1X,' INITIAL AMMONIA MASS IN WATER TRAP = ',F6.2,' KG',/)
TIW=TIW+273.16000
TIA=TIA+273.16000
PPAFF=-9.733200+6.373100*(TIW/100.000)
1 -0.98744200*(TIW/100.000)**2
MW=MW*0.0037854000/0.001003000
WRITE(6,923) MAREL
WRITE(7,923) MAREL
923 FORMAT(1X,' TOTAL AMMONIA VAPOR VENTED TO TANK = ',F6.2,' KG',/)
TMIX=TIW
TMIX=TMIX-273.16000
XI=MIA/(MIA+MW)
CALL CALPH(XI, TMIX, PH)
C HEAT OF REACTION — ESTIMATED ON BASIS OF NH3-H2O EQUIL. CHT.
DHRXN=-5670.7400+5589.9400*(TIW/100.000)
1 -1044.1900*(TIW/100.000)**2
C CALCULATED VARIABLES
DELMA=MDDTA*TSTEP
PPMIX=PPNH3(TMIX, XI)*PPAFF+PPSATW(TMIX)
C WRITE INITIAL CONDITIONS
WRITE(6,900)
WRITE(7,900)
900 FORMAT(10X,' ESTIMATED AMMONIA-WATER MIXTURE PROPERTIES',
1 /,10X,' VARIATION UPON INPUT OF AMMONIA VAPOR',
2 //,6X,' TIME NH3 CONC. LIQ. TEMP. PRESS NH3 MASS'
3 /,6X,' (SEC) (X, PH) (DEG. C) (KPA) (KG)'')
WRITE(6,901) TIME, XI, PH, TMIXC, PPMIX, MIA
WRITE(7,901) TIME, XI, PH, TMIXC, PPMIX, MIA
901 FORMAT(1X, F10.1, 3X, F4.3, ', ', F4.1, 4X, F10.2, 3X, F10.3, 3X, F8.3)
MA=MIA
C INCREMENT TIME FOR CALCULATION OF TEMPERATURE INCREASE
10 IF (TIME.LT. TTIME) THEN
TIME=TIME+TSTEP
MA=MA+DELMA
MMIX=MA+MIA
X=MA/MMIX
CALL CALPH(X, TMIX, PH)
TMIXO=TMIX
5 TMIXN=TMIX+DELMA*(DHRXN-CPA(TIA)*(TMIXO-TIA))

```

```

1      /MMIX/CPMIX(TMIXO,X)
      IF (DABS(TMIXN-TMIXO) .GT. 0.01000) THEN
          TMIXO=TMIXN
          GOTO 5
      ENDIF
      TMIX=TMIXN
      PPMIX=PPNH3(TMIX,X)*PPAFF+PPSATW(TMIX)
C      MAXIMUM SOLUBILITY ACHIEVED WHEN TOTAL MIXTURE VAPOR
C      PRESSURE EXCEEDS AMBIENT PRESSURE
      IF (PPMIX.GT.PATMOS) THEN
          MASAT=MA
          GOTO 20
      ENDIF
      TMIXC=TMIX-273.16000
      WRITE(6,901) TIME,X,PH,TMIXC,PPMIX,MA
      WRITE(7,901) TIME,X,PH,TMIXC,PPMIX,MA
      GOTO 10
  ENDIF
  IF (TIME.GE.TTIME) THEN
      WRITE(6,924)
      WRITE(7,924)
924  FORMAT(/,1X,'TOTAL AMMONIA MASS RELEASED IS ABSORBED')
      WRITE(6,925) MA
      WRITE(7,925) MA
925  FORMAT(1X,'TOTAL AMMONIA MASS IN WATER TRAP TANK =',
1      F6.2,' KG')
      GOTO 30
  ENDIF
C      SUM REMAINING VENTED AMMONIA ENTERING TANK
20  IF (TIME .LE. TTIME) THEN
      TIME=TIME+TSTEP
      MA=MA+DELMA
      GOTO 20
  ENDIF
      MATRAP=MASAT-MIA
      MAOUT=MA-MASAT
      MARATO=MAOUT/MARAT
      WRITE(6,902) MIA,MATRAP,MAOUT,MARATO
      WRITE(7,902) MIA,MATRAP,MAOUT,MARATO
902  FORMAT(/,1X,'INITIAL AMMONIA MASS IN WATER TRAP =',F6.2,' KG',
1      /,1X,'AMMONIA MASS ABSORBED BY WATER TRAP DURING RELEASE =',
2      F6.2,' KG',
3      /,1X,'AMMONIA MASS VENTED FROM TRAP DURING RELEASE =',
4      F6.2,' KG',
5      /,1X,'VENTED AMMONIA -TO- TOTAL AMMONIA RELEASE MASS RATIO =',
6      F6.2)
30  CONTINUE
      STOP
      END

```

```

C          CALCULATE PH OF WATER-AMMONIA MIXTURE
SUBROUTINE CALPH(X,T,PH)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
DOUBLE PRECISION KB,MA,MMIX,MOLRTY,MOLWTA
SPGRAV(T,X)= (+0.1000D+01-0.8750D-04*T-0.3437D-05*T*T)
1          +(-0.3853D+00-0.2220D-02*T+0.4300D-04*T*T)*X
2          +(+0.1755D+00+0.4064D-02*T-0.1328D-03*T*T)*X*X
KB=0.1750D-04
MOLWTA=14.0080D+3.00D*1.0080D0
TC=T-273.160D0
RHMIX=SPGRAV(TC,X)*1000.0D0
MMIX=RHMIX
MA=X*MMIX
GMOLWT=MA/MOLWTA
MOLRTY=GMOLWT
CONCOH=DSQRT(MOLRTY*KB)+0.1000D-06
POH=DLOG10(1.0D0/CONCOH)
PH=14.0D0-POH
RETURN
END

```

AMVT1.INP

```

00.0D0      TIME, "INITIAL TIME", SEC
600.0D0     TTIME, "TOTAL TIME OF RELEASE", SEC
10.0D0      TSTEP, "TIME INCREMENT", SEC
101.0D0     PATMOS, "ATMOSPHERIC PRESSURE", KPA
15.4D0      TIW, "INITIAL WATER TEMPERATURE", DEG. C
0.250D0     TIA, "AMMONIA VAPOR TEMPERATURE", DEG. C
200.0D0     MW, "INITIAL WATER QUANTITY", GAL
00.0D0      MIA, "INITIAL AMMONIA MASS IN WATER", KG
90.720D0    MAREL, "TOTAL AMMONIA RELEASED VENTED TO TANK", KG

```



### 3. Case 3: AMVS1.FOR

```

C      FILE: AMVS1.FORTRAN
C
C      DYNAMIC SIMULATION OF AMMONIA VAPOR ABSORPTION
C      INTO A WATER SPRAY
C
C      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
C      DOUBLE PRECISION LTANK,MA,MA3,MALOSS,MAREL,MAOUT,
1  MAVENT,MDOTA,MDOTA3,MDOTAH,MDOTW,MMIX,MN
COMMON /CNDTNS/ PATMOS,TATMOS,PA,TIA,TIW,MDOTA,DELMW
COMMON /TANK/ DTANK,LTANK,HGAP,AXTANK
COMMON /NOZZLE/ NN,NH,DP,VOOTW,MDOTW,VP
C      FUNCTIONS
RHOW(TT)=1926.000-1.68000*TT-0.12760+06/TT
SPGRAV(T,XX)=(+0.10000+01-0.87500-04*T-0.34370-05*T*T)
1      +(-0.38530+00-0.22200-02*T+0.43000-04*T*T)*XX
2      +(+0.17550+00+0.40640-02*T-0.13280-03*T*T)*XX*XX
C      OPEN FILES FOR INPUT AND OUTPUT
C      OPEN(UNIT=5,FILE='AMVS1.INP',STATUS='OLD')
C      OPEN(UNIT=7,FILE='AMVS1.OUT')
C      CONSTANTS
C      PI=3.14159000
C      INITIAL CONDITIONS
C      READ CONTROLLING TIME PARAMETERS
910 FORMAT (D20.4)
911 FORMAT (I5)
C      READ(5,910) TIME,TTIME,TSTEP
C      READ INITIAL CONDITIONS FOR AMMONIA VAPOR RELEASE
C      READ(5,910) PATMOS,TATMOS,PAMES,TIA,TIW
C      READ TANK GEOMETRY
C      READ(5,910) DTANK,LTANK,HGAP
C      READ SPRAY NOZZLE CONFIGURATION
C      READ(5,911) NN,NH
C      READ(5,910) DP,VOOTW
C      READ TOTAL AMMONIA VAPOR MASS RELEASED TO TANK
C      READ(5,910) MAREL
C      MDOTA=MAREL/TTIME
C      WRITE INITIAL CONDITIONS FOR SIMULATION
C      WRITE(6,920)
C      WRITE(7,920)
920 FORMAT(1X,'INITIAL CONDITIONS FOR SIMULATED RELEASE',/)
C      WRITE(6,921) TIME,TTIME,TSTEP
C      WRITE(7,921) TIME,TTIME,TSTEP

```

```

921 FDMAT(1X,'INITIAL TIME = ',F4.1,' SEC',/,
  1 1X,'TOTAL ELLAPSED TIME = ',F6.1,' SEC',/,
  2 1X,'TIME STEP = ',F4.1,' SEC',/)
WRITE(6,922) PATMOS,TATMOS,PAMES,TIA,TIW
WRITE(7,922) PATMOS,TATMOS,PAMES,TIA,TIW
922 FDMAT(1X,'ATMOSPHERIC PRESSURE = ',F6.2,' KPA',/,
  1 1X,'ATMOSPHERIC TEMPERATURE = ',F5.1,' DEG C',/,
  2 1X,'AMMONIA VAPDR GAGE PRESSURE (FLOWMETER) = ',F5.1,' KPA',/,
  3 1X,'AMMONIA VAPOR TEMPERATURE (FLOWMETER) = ',F6.2,' DEG C',/,
  4 1X,'WATER SUPPLY TEMPERATURE = ',F6.2,' DEG C',/)
TATMOS=TATMOS+273.15000
PA=PAMES+PATMOS
TIW=TIW+273.15000
TIA=TIA+273.15000
WRITE(6,923) OTANK,LTANK,HGAP
WRITE(7,923) OTANK,LTANK,HGAP
923 FDMAT(1X,'TANK DIAMETER = ',F5.2,' FT',/,
  1 1X,'TANK HEIGHT = ',F6.2,' FT',/,
  2 1X,'GAP HEIGHT FROM TANK BOTTOM TO FILL PIPE = ',F5.2,' IN',/)
DTANK=OTANK*0.3048000
LTANK=LTANK*0.3048000
HGAP=HGAP*0.0254000
AXTANK=PI*DTANK*OTANK/4.000
WRITE(6,924) NN,NH,DP,VDDTW
WRITE(7,924) NN,NH,DP,VDDTW
924 FDMAT(1X,'NUMBER SPRAY NOZZLE(S) = ',I3,/,
  1 1X,'NUMBER HOLES PER SPRAY NOZZLE = ',I3,/,
  2 1X,'SURFACE MEAN SPRAY DROPLET DIA. = ',F6.1,' MICRONS',/,
  3 1X,'VOLUMETRIC WATER FLOWRATE = ',F5.2,' GAL/MIN',/)
DF=DP*1.00-06
VDDTW=VDDTW*0.0037854000/60.000
MDDTW=VDDTW*RHDW(TIW)
WRITE(6,925) MAREL
WRITE(7,925) MAREL
925 FDMAT(1X,'TDOTAL AMMONIA VAPDR RELEASED TO TANK = ',F6.2,' KG',/)
MDDTA=MAREL/TTIME
WRITE(6,900)
WRITE(7,900)
900 FDMAT(10X,'ESTIMATED AMMONIA-WATER MIXTURE PROPERTIES',
  1 /,10X,'VARIATION UPON INPUT OF AMMONIA VAPOR AND WATER SPRAY',
  2 //,6X,'TIME NH3 CONC. LIQ. TEMP. NH3 IN NH3 OUT'
  3 /,6X,'(SEC) (X,PH) (DEG. C) (KG) (KG)')
C.....SPRAY REGIME: MIXTURE COLLECTED AT BOTTOM DF TANK AND
C CONTINUES UNTIL GAP CLDSED BY LIQUID MIXTURE
C CALCULATE MIXTURE PROPERTIES FOR WATER SPRAY MIXTURE
CALL SPRAY(T3,X3,MDDTA3)

```

```

C      CALCULATE TIME TO CLOSE GAP WITH MIXTURE
      VOLGAP=HGAP*AXTANK
      RHMIX=SPBRV(T3, X3)*1000.000
      MDOTW=MDOTA-MDOTA3+MDOTW
      TIMGAP=VOLGAP+RHMIX/MDOTW
C      WRITE SPRAY REGIME CONDITIONS
      CALL CALPH(X3, T3, PH)
      MA3=0.0000
      MW=0.0000
      MALOSS=0.0000
      MAVENT=MDOTA3*TSTEP
      DELMA3=(MDOTA-MDOTA3)*TSTEP
      DELMW=MDOTW*TSTEP
      T3C=T3-273.15000
10  IF (TIME.LT.TIMGAP) THEN
      TIME=TIME+TSTEP
      MA3=MA3+DELMA3
      MW=MW+DELMW
      MALOSS=MALOSS+MAVENT
      MMIX=MA3+MW
      WRITE(6,901) TIME, X3, PH, T3C, MA3, MALOSS
      WRITE(7,901) TIME, X3, PH, T3C, MA3, MALOSS
      GOTO 10
    ENDIF
901  FORMAT(1X,F10.1,3X,F4.3,' ',F4.1,4X,F10.2,3X,F10.3,3X,FB.3)
C      RESET ACCUMULATED VALUES BACK ONE TIME STEP
      TIME=TIME-TSTEP
      MA3=MA3-DELMA3
      MW=MW-DELMW
      MALOSS=MALOSS-MAVENT
      MMIX=MA3+MW
C      GET ACCUMULATED SPRAY VALUES FOR TIMDIF
      TIMDIF=TIMGAP-TIME
      TIME=TIME+TIMDIF
      MA3=MA3+DELMA3*TIMDIF/TSTEP
      MW=MW+DELMW*TIMDIF/TSTEP
      MMIX=MA3+MW
      MALOSS=MALOSS+MAVENT*TIMDIF/TSTEP
C..... BUBBLE REGIME: ABSORPTION BY VAPOR BUBBLES IN LIQUID
C      MIXTURE
C      INITIAL CALCULATIONS
      TMIX=T3
      TMIXC=TMIX-273.16000
      XI=X3
      CALL CALPH(XI, TMIX, PH)
      MA=MA3
      X=X3

```

```

C      INCREMENT TIME FROM TIMGAP TO NEXT TSTEP
TSTEP2=TSTEP-TINDIF
TIME=TIME+TSTEP2
DELM2=MDOTA*TSTEP2
DELMW2=MDOTW*TSTEP2
TMIXO=TMIX
XO=X
CALL TEMP(TMIXO,XO,MA,MW,TMIXN1)
TMIX=TMIXN1
XCOLD=MA/(MA+MW+DELMW2)
CALL EQ(TMIX,XEQ)
IF(XEQ.GT.XCOLD) THEN
  DMAX2=(XEQ*(MA+MW+DELMW2)-MA)/(1.000-XEQ)
  IF(DELM2.GT.DMAX2) THEN
    DMA2=DMAX2
  ELSE
    DMA2=DELM2
  ENDIF
ENDIF
MW=MW+DELMW2
MA=MA+DMA2
MWX=MA+MW
X=MA/MWX
CALL AMSRP2(TMIX,X,DMA2,MA,MW,TMIXN2)
TMIX=TMIXN2
MAOUT=DELM2-DMAX2
IF(DMAX2.GT.DELM2) THEN
  MAOUT=0.0000
ENDIF
MALOSS=MALOSS+MAOUT
CALL CALPH(X,TMIX,PH)
TMIXC=TMIX-273.15000
WRITE(6,901) TIME,X,PH,TMIXC,MA,MALOSS
WRITE(7,901) TIME,X,PH,TMIXC,MA,MALOSS
C      INCREMENT TIME FOR BUBBLE REGIME
DELM2=MDOTA*TSTEP
20 IF(TIME.LT.TTIME) THEN
  TIME=TIME+TSTEP
  TMIXO=TMIX
  XO=X
  CALL TEMP(TMIXO,XO,MA,MW,TMIXN1)
  TMIX=TMIXN1
  XCOLD=MA/(MA+MW+DELMW)
  CALL EQ(TMIX,XEQ)
  IF(XEQ.GT.XCOLD) THEN

```

```

      DMAMAX=(XEQ*(MA+MW+DELMW)-MA)/(1.0D0-XEQ)
      IF (DELMW.GT.DMAMAX) THEN
        DMA=DMAMAX
      ELSE
        DMA=DELMW
      ENDIF
      ENDIF
      IF (XEQ.LE.XCOLD) THEN
        DMA=0.00D0
      ENDIF
      MW=MW+DELMW
      MA=MA+DMA
      MMIX=MA+MW
      X=MA/MMIX
      CALL AMSRP2(TMIX,X,DMA,MA,MW, TMIXN2)
      TMIX=TMIXN2
      MAOUT=DELMW-DMA
      IF (DMAMAX.GT.DELMW) THEN
        MAOUT=0.00D0
      ENDIF
      MALOSS=MALOSS+MAOUT
      CALL CALPH(X, TMIX, PH)
      TMIXC=TMIX-273.15D0D
      WRITE(6,901) TIME,X,PH, TMIXC,MA,MALOSS
      WRITE(7,901) TIME,X,PH, TMIXC,MA,MALOSS
      GOTO 20
    ENDIF
  C   WRITE RESULTS SUMMARY
      ABSRAT=MA/(MA+MALOSS)
      WRITE(6,902) TIMGAP,ABSRAT
      WRITE(7,902) TIMGAP,ABSRAT
902  FORMAT(/,1X,'GAP CLOSING TIME BY LIQUID MIXTURE = ',
1     F6.2,' SEC',/,
2     1X,'NH3 MASS ABSORBED TO MASS RELEASED RATIO = ',F7.4)
      STOP
      END
  C   CALCULATE PH OF WATER-AMMONIA MIXTURE
      SUBROUTINE CALPH(X,T,PH)
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      DOUBLE PRECISION KB,MA,MMIX,MOLRTY,MOLWTA
      SPBRAY(T,X)= (+0.1000D+01-0.8750D-04*T-0.3437D-05*T*T)
1         +(-0.3853D+00-0.2220D-02*T+0.4300D-04*T*T)*X
2         +(+0.1755D+00+0.4064D-02*T-0.1328D-03*T*T)*X*X
      KB=0.1750D-04
      MOLWTA=14.0080D+3.0D0*1.0080D0
      TC=T-273.16D0D
      RHOMIX=SPBRAY(TC,X)*1000.0D0

```

```

MMIX=RHMIX
MA=X*MMIX
GMOLWT=MA/MOLNTA
MOLRTY=GMOLWT
CONCDH=DSGRT(MOLRTY*KB)+0.1000D-06
PDH=DLG10(1.0D0/CONCDH)
PH=14.0D0-PDH
RETURN
END

C      DETERMINE MIXTURE PROPERTIES AND SPRAY REGIME CONDITIONS
SUBROUTINE SPRAY(T3,X3,MDDTA3)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
DOUBLE PRECISION KA,LI,LTANK,
1  MA1,MA2,MAAB1,MAAB2,MAI,MAPLUS,MDAB1,MDAB2,MDAD,
2  MDDTA,MDDTA1,MDDTA2,MDDTA3,MDDTW,MWI,MWTA,MWTV,
3  NUA,NP,NPI
DIMENSION MAAB1(0:40),MAAB2(0:40),MDAB1(0:40),MDAB2(0:40),
1  MDDTA1(0:40),MDDTA2(0:41),T1(0:40),T2(0:41),
2  VELA1(0:40),VELA2(0:41),VDA1(0:40),VDA2(0:41),
3  VPRA1(0:40),VPRA2(0:41),RTIM1(0:40),RTIM2(0:41),
4  XE1(0:40),XE2(0:40),X1(0:40),X2(0:41)
COMMON /CONDENS/ PATMDS,TATMDS,PA,TIA,TIW,MDDTA,DELMW
COMMON /TANK/ DTANK,LTANK,HGAP,AXTANK
COMMON /NDZLE/ NN,NH,DP,VDDTW,MDDTW,VP

C      FUNCTIONS
RHDW(TT,PP)=PP/RA/TT
RHDW(TT)=1926.0D0-1.680D0*TT-0.1276D+06/TT
NUA(TT)=0.000000120D0*TT-0.00002120D0
CPMIX(TT,XX)=(7.7060D0-0.022450D0*TT+0.000035690D0*TT*TT)
1  +(-298.80D0+1.9230D0*TT-0.0030610D0*TT*TT)*XX
2  +(1160.0D0-7.5090D0*TT+0.011980D0*TT*TT)*XX*XX
CPA(TT)=-0.7756D0+0.004956D0*TT+437.80D0/TT

C      CONSTANTS
PI=3.141590D0
MWTA=17.030D0
MWTW=18.0150D0
SUMVA=14.90D0
SUMVW=12.70D0
RA=8.314340D0/MWTA

C      SPRAY DROPLET CLOUD
CALL NDZL(DP,NN,NH,VDDTW,VP)
RHDV=RHDW(TIW)*VDDTW/AXTANK/VP
RP=DP/2.0D0
NP=0.75D0*DTANK*DTANK*LTANK*RHDV/((RP**3.0D0)*RHDW(TIW))
N=40
NPI=NP/N
LI=LTANK/N

```

```

C      INITIAL CONDITIONS
      T1(0)=TIW
      VDDTA=MDDTA/RHDA(T1(0),PATMOS)
      VELAI(0)=VDDTA/AXTANK
      VPRAI(0)=VP+VELAI(0)
      VOLWI=NP1*PI*DP*DP*DP/6.0D0
      MWI=VOLWI/RHOW(T1(0))
      RTIM1(0)=LI/VPRAI(0)
      MDDTAI(0)=MDDTA
      MAI=0.00D0
      X1(0)=0.00D0

C      DROPLET TEMPERATURE VARIATION (FROM TOP-TO-BOTTOM)
      DD 100 I=0,N-1
120  REP=DP*VPRAI(I)/NUA(T1(I))
      DD1=0.001D0*T1(I)**1.75D0
      DD2=(1.0D0/MWTA+1.0D0/MWTW)**0.50D0
      DD3=PATMOS/101.20D0
      DD4=(SUMVA**0.3333D0+SUMVW**0.3333D0)**2.0D0
      DAW=DD1*DD2/DD3/DD4/10000.0D0
      SC=NUA(T1(I))/DAW
      KA=DAW/DP*(2.0D0+0.60D0*REP**0.50D0+SC**0.3333D0)
      TI=T1(I)
      CALL EQ(TI,XEQ)
      XE1(I)=XEQ
      IF(X1(I).GE.XE1(I)) THEN
        X1(I)=XE1(I)
      ENDIF
      MDAD=PI*DP*DP*KA*RHOW(T1(I),PATMOS)*((XE1(I)-X1(I))/XE1(I))
      MDAB1(I)=NP1*MDAD
      MARB1(I)=MDAB1(I)*RTIM1(I)
      MAI=MAI+MARB1(I)
      X1(I+1)=MAI/(MAI+MWI)
      TT=T1(I)
      XX=X1(I+1)
      MAPLUS=MARB1(I)
      CALL AMSRP1(TT,XX,MAPLUS,MAI,MWI,TNEW)
      T1(I+1)=TNEW
      CALL EQ(TT,XEQ)
      XE1(I+1)=XEQ
      MDDTAI(I+1)=MDDTAI(I)-(X1(I+1)-X1(I))*MDDTW
      IF(MDDTAI(I+1).LT.0.00D0) THEN
        MDDTAI(I+1)=0.00D0
      X1(I+1)=MDDTA/(MDDTA+MDDTW)
      MAPLUS=(X1(I+1)-X1(I))*MDDTW*RTIM1(I)
      TT=T1(I)
      XX=X1(I+1)
      MAI=MAI+MAPLUS-MARB1(I)
      CALL AMSRP1(TT,XX,MAPLUS,MAI,MWI,TNEW)

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```

      T1(I+1)=TNEW
      TT=T1(I+1)
      CALL EQ(TT,XEQ)
      XE1(I+1)=XEQ
C      ASSUME FURTHER DOWNWARD CONDITIDNS ARE SAME
      DD 130 II=I+1,N
          X1(II)=X1(I+1)
          T1(II)=T1(I+1)
          XE1(II)=XE1(I+1)
          MDDTA1(II)=MDDTA1(I+1)
130      CONTINUE
          GDTD 140
      ENDIF
          VDA1(I+1)=MDDTA1(I+1)/RHDA(T1(I+1),PATMDS)
          VELA1(I+1)=VDA1(I+1)/AXTANK
          VPRAI(I+1)=VP+VELA1(I+1)
          RTIM1(I+1)=LI/VPRAI(I+1)
100 CONTINUE
C      RE-ORDER DROPLET CONDITIONS
140 DD 150 J=0,N
          X2(J)=X1(N-J)
          XE2(J)=XE1(N-J)
          T2(J)=T1(N-J)
150 CONTINUE
C      CONDITIONS FOR UPWARD CALCULATION.
      MA2=0.00D0
      MDDTA2(0)=MDDTA
      VELA2(0)=VDDTA/AXTANK
      VPRAI(0)=VP+VELA2(0)
      RTIM2(0)=LI/VPRAI(0)
      X2(N+1)=0.00D0
      T2(N+1)=TIW
C      UPWARD CALCULATION
      DD 200 J=0,N
          REP=DF*VPRAI(J)/NUR(T2(J))
          DD1=0.001D0*T2(J)**1.75D0
          DD2=(1.0D0/MNTA+1.0D0/MNTW)**0.50D0
          DD3=PATMDS/101.20D0
          DD4=(SUMVW**0.3333D0+SUMVW**0.3333D0)**2.0D0
          DAW=DD1*DD2/DD3/DD4/10000.0D0
          SC=NUR(T2(J))/DAW
          KR=DAW/DP*(2.0D0+0.60D0*REP**0.50D0*SC**0.3333D0)
          MDAD=PI*DP*DF*(KA+RHDA(T2(J),PATMDS))*((XE2(J)-X2(J))/XE2(J))
          MDAB2(J)=NPI*MDAD
          MARAB2(J)=MDAB2(J)*RTIM2(J)
          MA2=MA2+MARAB2(J)
          MDDTA2(J+1)=MDDTA2(J)-(X2(J)-X2(J+1))*MDDTW
          VDA2(J+1)=MDDTA2(J+1)/RHDA(T2(J+1),PATMDS)
          VELA2(J+1)=VDA2(J+1)/AXTANK
          VPRAI(J+1)=VP+VELA2(J+1)
          RTIM2(J+1)=LI/VPRAI(J+1)
200 CONTINUE

```



```

C      EQUILIBRIUM TEMPERATURE AND CONCENTRATION AT TANK BOTTOM
      MA1=LI*AXTANK*RHDA(TIA,PATMDS)
      T2OLD=TIA
210  T2NEW=(MA1*CPA(TIA)*TIA+MWI*CPMIX(T2(0),X2(0))*T2(0))/
      I  (MA1*CPA(T2OLD)+MWI*CPMIX(T2OLD,X2(0)))
      IF(DABS(T2NEW-T2OLD).LE.0.10D0) THEN
        GOTO 220
      ELSE
        T2OLD=T2NEW
      GOTO 210
      ENDIF
220  T2(0)=T2NEW
      CALL EQ(T2NEW,XEQ)
      XE2(0)=XEQ
C      RECALCULATE AMMONIA ABSORPTION AT BOTTOM LAYER
      REP=DP*VPA2(0)/NJA(T2(0))
      DD1=0.001D0*T2(0)**1.75D0
      DD2=(1.0D0/MWTA+1.0D0/MWTW)**0.50D0
      DD3=PATMDS/101.20D0
      DD4=(SUMWA**0.3333D0+SUMVW**0.3333D0)**2.0D0
      DAW=DD1*DD2/DD3/DD4/10000.0D0
      SC=NJA(T2(0))/DAW
      KA=DAW/DP*(2.0D0+0.60D0*REP**0.50D0*SC**0.3333D0)
      MDAD=PI*DP*DP*KA*RHDA(T2(0),PATMDS)*((XE2(0)-X2(0))/XE2(0))
      MDAB2(0)=MPI*MDAD
      MARB2(0)=MDAB2(0)*RTIME(0)
      MA2=MA2+MARB2(0)
      X2NEW=MA2/(MA2+MWI)
      MDDTA2(N)=MDDTA2(N)-(X2NEW-X2(0))*MDDTW
      IF(MDDTA2(N).LT.0.00D0) THEN
        X2NEW=X2(1)
        MDDTA2(N)=0.00D0
      ENDIF
      X2(0)=X2NEW
      TT=T2(0)
      MAPLUS=MARB2(0)
      CALL AMSRP1(TT,X2NEW,MAPLUS,MA2,MWI,T2NEW)
      T2(0)=T2NEW
      T3=T2(1)
      X3=X2(1)
      MDDTA3=MDDTA2(N)
      RETURN
      END
C      DETERMINE SPRAY DROPLET VELOCITY
      SUBROUTINE NDZL(DP,NN,NH,VDDTW,VP)
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)

```

```

PI=3.141590D0
RHDL=PI*DP*DP/4.0D0
ATDT=NN*NH*RHDL
VSPRAY=VDDTW/ATDT
VF=VSPRAY
RETURN
END

C   DETERMINE EQUILIBRIUM CONCENTRATION GIVEN TEMPERATURE
SUBROUTINE EQ(T1,XEQ)
IMPLICIT DOUBLE PRECISION(A-H,I-Z)
DOUBLE PRECISION MDDTA
COMMON /CNDTNS/ PATMOS,TATMOS,PA,TIA,TIW,MDDTA,DELMW
PPSATW(TT)=(0.1059D+09)*DEXP((-0.5171D+04)/TT)
PPNH3(TT,XX)=(13894.7699D0-23.99567D0*TT+0.03696*TT*TT)
1      +(29203.743D0-259.7423D0*TT+0.54111D0*TT*TT)*XX
2      +(170153.485D0-1197.155D0*TT+2.818166*TT*TT)*XX*XX)
3      *(101.325D0/760.0D0)
PPAFF(TT)=-9.7332D0+6.3731D0*(TT/100.0D0)
1      -0.987442D0*(TT/100.0D0)**2
XX=0.0D0
TT=T1
DELX=0.0010D0
10 PPMIX=PPNH3(TT,XX)*PPAFF(TT)+PPSATW(TT)
IF (PPMIX.LT.PATMOS) THEN
    XX=XX+DELX
    GOTD 10
ELSE
    XEQ=XX
ENDIF
RETURN
END

C   DETERMINE MIXTURE TEMPERATURE WITH WATER ADDITION
SUBROUTINE TEMP(TMIXO,XO,MATDT,MWDT,TMIXN)
IMPLICIT DOUBLE PRECISION(A-H,I-Z)
DOUBLE PRECISION MATDT,MDDTA,MWDT
COMMON /CNDTNS/ PATMOS,TATMOS,PA,TIA,TIW,MDDTA,DELMW
CPMIX(TT,XX)=(7.7060D0-0.022450D0*TT+0.000035690D0*TT*TT)
1      +(-298.80D0+1.9230D0*TT-0.0030610D0*TT*TT)*XX
2      +(1160.0D0-7.5090D0*TT+0.011980D0*TT*TT)*XX*XX
CPW(TT)=6.073D0-1181.0D0/TT+0.1841D+06/TT/TT
A=(MATDT+MWDT)*CPMIX(TMIXO,XO)*TMIXO
B=DELMW*CPW(TIW)*TIW
C=(MATDT+MWDT+DELMW)*CPMIX(TMIXO,XO)
TMIXN=(A+B)/C
RETURN
END

```

```

C      DETERMINE DROPLET TEMPERATURE WITH NH3 ABSORPTION
SUBROUTINE AMSRP1(T2,X2,MABS,MA,MW,TNEW)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
DOUBLE PRECISION MA,MABS,MAINP,MATOT,MDOA,MW
COMMON /CNDTNS/ PATMDS,TATMDS,PA,TIA,TIW,MDDTA,DELMW
CPMIX(TT,XX)=(7.7060D0-0.022450D0*TT+0.000035690D0*TT*TT)
1      +(-298.80D0+1.9230D0*TT-0.0030610D0*TT*TT)*XX
2      +(1160.0D0-7.5090D0*TT+0.011980D0*TT*TT)*XX*XX
DHRXN(TT)=-5670.74D0+5589.94D0*(TT/100.0D0)
1      -1044.19D0*(TT/100.0D0)**2
TT=T2
XX=X2
MATOT=MA
MAINP=MABS
      DELA=DHRXN(TT)
      DELB=MAINP/(MATOT*MW)
      DELT=DELA*DELB/CPMIX(TT,XX)
TNEW=TT+DELT
RETURN
END

C      DETERMINE MIXTURE TEMPERATURE WITH NH3 VAPOR ABSORPTION
SUBROUTINE AMSRP2(TMIXO,X,DMA,MA,MW,TMIXN)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
DOUBLE PRECISION MA,MDDTA,MW
COMMON /CNDTNS/ PATMDS,TATMDS,PA,TIA,TIW,MDDTA,DELMW
CPMIX(TT,XX)=(7.7060D0-0.022450D0*TT+0.000035690D0*TT*TT)
1      +(-298.80D0+1.9230D0*TT-0.0030610D0*TT*TT)*XX
2      +(1160.0D0-7.5090D0*TT+0.011980D0*TT*TT)*XX*XX
CPA(TT)=-0.7756D0+0.004958D0*TT+437.80D0/TT
DHRXN(TT)=-5670.74D0+5589.94D0*(TT/100.0D0)
1      -1044.19D0*(TT/100.0D0)**2
TMIX=TMIXO
10  TMIXN=TMIX+DMA*(DHRXN(TIW)-CPA(TIA))*(TMIXO-TIA)
1      / (MA+MW) / CPMIX(TMIXO,X)
      IF (DABS(TMIXN-TMIXO).GT.0.010D0) THEN
          TMIXO=TMIXN
          GOTO 10
      ENDIF
RETURN
END

```

AMVS1.INP

00.0000	TIME, "INITIAL TIME", SEC
600.000	TTIME, "TOTAL TIME OF RELEASE", SEC
10.000	TSTEP, "TIME INCREMENT", SEC
101.000	PATMOS, "ATMOSPHERIC PRESSURE", KPA
23.000	TATMOS, "ATMOSPHERIC TEMPERATURE", DEG. C
10.6400	PAWES, "AMMONIA VAPOR GAGE PRESSURE", KPA
-1.600	TIA, "AMMONIA VAPOR TEMPERATURE", DEG. C
32.000	TIW, "INITIAL WATER TEMPERATURE", DEG. C
4.000	OTANK, "TANK DIAMETER", FT
12.000	LTANK, "TANK HEIGHT", FT
4.000	HGAP, "GAP FROM TANK BOTTOM TO NH3 PIPE", IN
2	NN, "NOZZLE NUMBER", --
12	NH, "HOLE NUMBER PER NOZZLE", --
295.6000	DP, "WATER SPRAY DROPLET DIAMETER", MICRONS
9.6000	VDOTW, "VOLUMETRIC WATER FLOWRATE", GAL/MIN
90.72000	MAREL, "TOTAL AMMONIA RELEASED VENTED TO TANK", KG

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ABSORPTION OF AMMONIA INTO WATER

by

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AN ABSTRACT OF A THESIS

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Ammonia is a flammable and toxic material. The ANSI/ASHRAE Standard 15-1978 suggests a procedure for trapping the ammonia when released, and provides a means for safe release to the atmosphere. A private code agency recently added Standard 15-1978 10.4.8.2 as a requirement for large ammonia refrigeration systems. Actual performance of the suggested procedure is unknown. This paper addresses the effectiveness of trapping the vaporous or liquid ammonia release with water as suggested: one gallon of water for every pound of ammonia released.

Three ammonia absorption cases were tested and analytically modeled: (1) vaporous ammonia absorbed into a partially filled vessel of water; (2) liquid ammonia absorbed into a partially filled vessel of water; and (3) vaporous ammonia absorbed into a water spray. For each case, three ammonia-water ratios were tested: (1) nominal ratio - one pound of ammonia per gallon of water; (2) twice the nominal ratio - two pounds of ammonia per gallon of water; and (3) half the nominal ratio - one-half pound of ammonia per gallon of water.

The receiver tank was 4 feet in diameter and 11 feet tall erected vertically. Ammonia was supplied from a 1000 gallon tank filled with saturated liquid ammonia. The water trap for Cases 1 and 2 consisted of 200 gallons of water. For Case 3, an equivalent quantity of water was sprayed at the top of the receiver tank and ammonia was introduced at the bottom as with Cases 1 and 2. The experiments measured how much ammonia was absorbed by the water under those conditions and the temperature rise of the ammonia-water

mixture as ammonia was absorbed. This data determined the limiting factors on each Case and the effectiveness of each Case as an ammonia trap. Each Case was also analytically modeled predicting the effectiveness of the trapping technique.

For Case 1, experiments determined that for the half nominal ratio all of the ammonia was absorbed, for the nominal ratio 90% of the ammonia was absorbed, and for the twice nominal ratio, 80% of the ammonia was absorbed. The temperature rise was greater for the higher ammonia-water ratios. For Case 2, experiments determined that for the half nominal and the nominal ratios all of the ammonia was absorbed, and for the twice nominal ratio, 90% of the ammonia was absorbed. As found in Case 1, the temperature rise was greater for the higher ammonia-water ratios. Whereas the vaporous and liquid ammonia released into a vessel of water absorbed approximately the same amount of ammonia for each ammonia-water ratio, the vaporous release resulted in a higher temperature. For Case 3, experiments determined that for all ammonia-water ratios, less than 75% of the ammonia was absorbed. Also, the temperature rise was greater for the higher ammonia-water ratios and occurred simultaneously with introduction of the ammonia. During Case 3, water coming into the receiving tank apparently reached the saturation condition and the greatest possible temperatures very quickly.

For all Cases, a maximum amount of ammonia that the water could absorb was observed, and this maximum value was

a function of two variables -- temperature of the ammonia-water mixture and the amount of ammonia initially in the mixture. The method used in Case 1 was determined to be an effective ammonia trap at the half nominal ammonia-water ratios. The method used in Case 2 was determined to be an effective ammonia trap at the nominal and half nominal ammonia-water ratios. The method used in Case 3 was determined to be less than 75% effective as an ammonia trap at all Ratios.

The analytical models developed for Cases 1 and 2 correctly predicted the experimental results to within  $\pm 10\%$ . The model for Case 3 only accounts for the essential features of the absorption process and therefore only predicted the end results to within  $\pm 20\%$ .