

AMMONIA VOLATILIZATION DURING LAND
APPLICATION OF SWINE LAGOON
EFFLUENT

By

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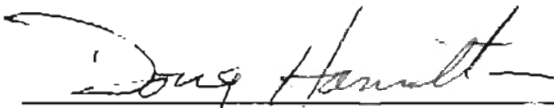
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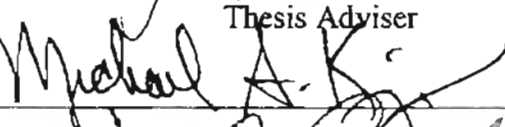
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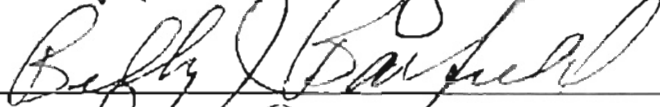
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LIST OF SYMBOLS

C	Flow coefficient, dimensionless
C_A	Droplet surface area, m^2
C_G	Concentration of the odorant in the free air surrounding the droplet, mg/L
C_L	Concentration of odorant in the liquid droplet, mg/L
C_{Sg}	Concentration of the odorant at the surface of the droplet in the gas phase, mg/L
C_D	Drag coefficient, m/s
D	Droplet diameter, m
E	Elevation of the test site, m
g	Acceleration due to gravity, m/s^2
h	Head difference across the orifice, m
h_m	Gas-phase film mass transfer exchange coefficient, m/s
K	Mass diffusivity of water vapor in gas, m^2/s
K_{od}	Mass diffusivity of odorant in gas, m^2/s
m	Mass of the droplet, kg
M_{IN}	Quantity of odorant mass generated within the droplet, kg
M_m	Mean molecular weight of the gas mixture, 29 g/mole for air
M_O	Mass of odorant inside the droplet, kg
M_{OUT}	Quantity of odorant mass being released from the droplet, kg

M_v	Molecular weight of the diffusing water vapor, g/mole
P_o	Atmospheric pressure, atm
P_f	Atmospheric pressure, atm
P_s	Saturation pressure at wet bulb temperature, atm
P_v	Saturation pressure at the dry bulb temperature, atm
ΔP	Vapor pressure difference, atm
r	Droplet radius, m
R	Air resistance, kgm/s^2
Re	Reynolds Number, dimensionless
Sc	Schmidt Number, dimensionless
Sh_w	Sherwood Number for water vapor, dimensionless
t	Time, s
T_k	Water temperature, K
V	Droplet volume, L
V_o	Velocity of the droplet, m/s
V_h	Horizontal projection of resultant velocity vector, m/s
V_r	Resultant velocity vector, m/s
V_w	Wind velocity, m/s
V_x	Wind speed in the x-direction, m/s
V_y	Wind speed in the y-direction, m/s
V_z	Wind speed in the z-direction, m/s

- x Horizontal distance, m
- α Angle about the z-axis, degrees
- ρ_o Density of dry air, kg/m³
- ρ_d Density of water vapor, kg/m³
- θ Angle the droplet makes with the horizontal, degrees
- θ_v Angle that the resultant velocity vector makes within the x-y plane, degrees
- ν Kinematic viscosity, m²/s

CHAPTER 1

INTRODUCTION

Background

The pig dates back 40 million years to fossils that indicate that wild pig-like animals roamed forests and swamps in Europe and Asia. By 4900 B.C. pigs were domesticated in China, and were being raised in Europe by 1500 B.C. Hernando de Soto could be dubbed “the father of the American pork industry.” He landed with America’s first 13 pigs at Tampa Bay, Florida in 1539 (NPPC, 2000). Today the United States is the second largest exporter of pork and is gaining rapidly on world leader Denmark. U.S. production accounts for about 10 percent of the total world pork supply (USDA, 1996).

Pork production in the United States is a vital part of the agricultural economy, with over 19 billion pounds of pork meat processed from about 99 million hogs in 1998. The economic impact of the industry on rural America is immense. Annual farm sales usually exceed \$11 billion, while the retail value of pork sold to consumers exceeds \$30 billion (NPPC, 2000). The “value-added” nature of pork provides employment well beyond the farm. The United States pork industry is responsible for over \$64 billion in total domestic economic activity. The pork industry supports over 600,000 jobs and adds over \$27 billion of value to basic production inputs such as corn and soybeans. There are approximately 139,000 pork operations today compared to nearly three million in the 1950’s. Farms have grown in size with over 80 percent of the hogs grown on farms that

produce 1000 or more hogs per year (NPPC, 1999). Between 1969 and 1992 there has been a decrease of 73% of those farms that produce less than 1000 hogs. In contrast, there has been a 320% increase in the number of farms which produce 1000 hogs or more (USDA, 1996).

This increase in farm size leads to many environmental concerns. Environmental management is an integral part of the pork production system today. Key factors in the success of today's pork producers are management of manure, water, soil and air. Manure management at pork operations has become recognized as a significant factor in protecting the natural environment and maintaining the overall acceptance of the pork industry (Jongbloed and Lenis, 1998).

Manure is a by-product of the livestock industry. It can be considered a waste, or it can be treated as a resource for crop production. The direct land application of animal manure is an efficient utilization alternative. The cost of application is consistently lower than that of treatment and the nutrient benefits derived from the manure help build and maintain soil fertility. Manure can also improve soil tilth, increase water-holding capacity, lessen wind and water erosion, improve aeration, and promote beneficial organisms (Johnson and Eckert, 1997).

Although manure can provide valuable plant nutrients, land application of swine lagoon effluent, however, faces growing scrutiny because of potential surface and groundwater contamination, and odor nuisances. Odor has long been associated with swine production. In general, the feed and body odors are not regarded as offensive, but those odors generated from manure and its decomposition during collection, handling, storage, and land application are often found to be offensive (Mackie et.al., 1998). The

most significant complaint about odor from swine manure by the public is during and after surface spreading to the land (Sharpe and Harper, 1997).

Scientists have identified hundreds of odor causing compounds, called odorants, forming these smells known as farmstead odors. The odor that our noses detect can be combinations of 60 to 150 different compounds (Williams et al., 1998; Jongbloed and Lenis, 1998; Fulhage, 1993; Mackie et al., 1998). The types of odors and gases produced are dependent upon the amount and type of microbial activity associated with the decomposition of manure and other organic matter.

Land application can lead to gaseous emissions of ammonia, one of the most documented swine lagoon effluent odorants. Ammonia is easily recognized by its sharp, pungent odor. As a highly volatile compound, ammonia is also one of the first compounds to be detected and recognized as an odor produced by a swine production facility.

Ammonia is also the primary neutralizing agent for atmospheric acids and is a common component of atmospheric aerosols. There is a growing realization of the importance of ammonia emissions and their role in acidification and eutrophication of terrestrial ecosystems. Natural ecosystems are thought to be sinks for ammonia (Sharpe and Harper, 1997; Van Hove et al., 1987; Hutchinson et al., 1972). Ammonia emitted from agricultural sources has also been implicated in forest decline (McLeod et al., 1990; Nihlgard, 1985) and species changes in the heathlands of Europe (Van Hove et al., 1987). Volatilization of ammonia is also being investigated as a possible cause of diminished atmospheric visibility and eutrophication of surface water (Sutton et al., 1998).

The volatilization of ammonia during irrigation of swine lagoon effluent and release into the atmosphere is dependent upon several variables. The method of land application will affect the mass concentrations of ammonia released into the atmosphere. The real-time weather conditions also help determine the release of ammonia. The difficulties in estimating volatilization rates suggest that modeling may help make understanding and estimating the influence of these different factors on volatilization more accessible, and make comparing the experimental results obtained under different conditions a practical possibility (Genermont and Cellier, 1997).

As rural populations of both people and pigs have increased, people and pigs have come into proximity, and odor emissions have increasingly become an issue, especially in locations where animal operations are near areas of public sensitivity, such as housing developments, shopping and non-agricultural business centers, schools and recreational facilities. A model that predicts the mass concentration of ammonia volatilization during land application of swine lagoon effluent would prove beneficial to both swine production facilities and their neighboring communities.

Objectives

There were two primary objectives in this work. The first objective was to develop a simple model to determine the release of ammonia during land application of swine lagoon effluent. Simple in this context means using simplified algorithms to model the mass transfer process while minimizing the number of inputs. The second objective was to determine whether the model yielded valid results as compared to available field data in the literature.

CHAPTER 2

LITERATURE REVIEW

Introduction

The literature was reviewed to determine the contribution of land application of swine lagoon effluent to increased odorant concentrations, particularly ammonia. The human physiological and psychological responses to odors are examined, as well as odor generation, emission, and measurement. The literature review documented a relationship between land application and higher mass concentrations of ammonia in the surrounding atmosphere, and mathematical models of dispersion were reviewed to predict how management and application practices impacted ammonia volatilization. A discussion of irrigation application practices and their effects on ammonia volatilization concludes this chapter.

The Olfactory Process

Physiological Response

The brain and the nose work together to create what an individual identifies as an odor. Odor perception begins well up in the nasal cavity where humans are outfitted with a collection of highly specialized receptor cells. As individual odorous molecules are drawn into the nasal cavity, a portion is dissolved in the mucous film that covers these specialized detectors (Minor, 1995). Once an odorous molecule is captured in the

system, it will become attached to one or more of the individual receptor cells based on a shape match. Depending upon the molecule, it may be captured by one or several of the specifically shaped receptors. Once a receptor has been stimulated, an electrical signal is transmitted to the brain and the amazing process of identifying odors begins (Campbell, 1990).

Once a signal is generated, the brain takes over and a person responds. When smelling an odor, the reaction may be to flee because of an association with danger or it may be to linger because of the perceived desirable situation. It has been asserted that human beings can detect over ten thousand different odors even though humans can identify only a small percentage of these (Mackie et al., 1998; Minor, 1995). This sense of smell is much more precise than is our ability to describe the odor we have perceived.

Psychological Response

The psychological response to odor is more complex and far less understood than the physiological process discussed above. Evidence suggests that each individual learns to like or dislike certain odors. Children like almost all smells (Campbell, 1990). It is only as we mature and begin to talk about the odors that we develop a sense of likes and dislikes. Obviously, individuals react differently to the smell of any one odor source. A person's perceptions about an odor are based on experiences that they have had throughout their life. For some individuals, this experience includes agricultural production, and therefore some level of farm odor may be acceptable to them. For others who may not have been exposed to such situations, any livestock odor may be perceived as very offensive and unacceptable. To these people livestock odor is a nuisance. Nuisance has been defined as the presence of offensive odorous air at such intensity,

concentration, frequency, and duration as to “materially interfere” with the normal use and enjoyment of property (Sweeten and Minor, 1993).

McFarland and Easterling (1995) found that the offensiveness or inoffensiveness of an odor is often influenced by a person’s background. In the study of 30 people, including those with both agricultural and non-agricultural backgrounds, the general results found that people with agricultural backgrounds were more likely to be familiar with the agricultural odors tested and found these odors offensive at a lower dilution level (higher concentrations) than the panelists with non-agricultural backgrounds.

Studies by Engen and Mower (1977) clearly showed that if an odor is unfamiliar, a person is unlikely to rate it as pleasant, while more pleasant odors are also generally familiar. People tend to be more tolerant of familiar odors than of unfamiliar odors, thus, reactions to odors are greatly influenced by experience. Differences in experience can cause large variations in offensiveness measurements, and the average judgment of a panel of observers must be tempered by knowledge about the background of each panelist.

Odors and gases are emitted from all swine livestock enterprises. The odors vary greatly, and the offensiveness of each odor is dependent upon the person smelling the odor. The animals and the dander from their bodies generate some odors; some odors are from the animals’ feed. And some odors, usually the strongest and most offensive, are from the livestock manure and the decomposition of that manure (Schmidt and Jacobsen, 1995; Fulhage, 1993; Jongbloed and Lenis, 1998; Minor, 1995; Muehling, 1969).

Odor and Gas Generation

Scientists have identified hundreds of odor causing compounds, called odorants, forming the smells known as farmstead manure odors. The odor that our noses detect can be combinations of 60 to 150 different compounds (Williams et al., 1995; Jongbloed and Lenis, 1998; Fulhage, 1993; Mackie et al., 1998). The types of odors and gases produced are dependent upon the amount and type of microbial activity associated with the decomposition of manure and other organic matter.

The types of compounds produced during degradation of manure depend on the types of biological processes that take place within the manure. There are three primary factors that control these processes: bacteria, temperature and moisture (Jacobs, 1994). The bacteria that are found in manure are responsible for creating odorous gases as they break down organic material. Anaerobic bacteria, which thrive in the absence of oxygen, tend to produce odorous compounds such as ammonia and hydrogen sulfide. Aerobic bacteria, which require oxygen to survive, produce mainly carbon dioxide, but may also produce ammonia. The type of bacteria present may vary at different locations throughout the manure.

Temperature is the second factor that controls the type of odorous compounds produced during degradation. Temperature controls the rate of bacterial action: the higher the temperature, the faster the biological action and therefore the greater the gas production. For example, as temperature decreases, microbial activity slows down; consequently, during the winter months, microbial activity is lower and therefore fewer odors are generated. On the other hand, warm, moist conditions favor bacterial action, and therefore increase decomposition and odor generation. In the spring, for example,

the sudden release of odor-causing compounds is caused by the combination of warmer temperatures and the buildup of organic matter in the winter.

The third factor affecting odor production is the moisture content of the manure. Moisture is required for biological activity to take place. The bacterial activity slows and can be stopped as manure is dried. Moisture also makes anaerobic conditions more likely in manure and thereby encourages the activity of odor-causing anaerobic bacteria. In summary, biological processes are sensitive to moisture content, temperature, oxygen concentration, and other environmental factors. Any changes in these parameters will alter odor and gas generation.

Some principal odorous compounds found in swine manure are ammonia, amines, sulfur-containing compounds, volatile fatty acids, indoles, skatole, phenols, alcohols, and carbonyls (Schmidt and Jacobsen, 1995; Mackie et. al., 1998; Fuhlage, 1993; Zahn et al., 1997). Odorants are grouped into families based on their chemical structure. Many of the odorants and their respective odorant families associated with swine production are listed in Table 2.1. These compounds are not only responsible for unpleasant odors but also affect the comfort, health, and production efficiency of animals as well as the comfort and health of human workers (Sweeten and Minor, 1993).

Unfortunately, most manure degradation takes place under anaerobic conditions. There is rarely enough oxygen available to convert manure organic matter aerobically. More than 75% of the swine production systems in the United States store and process swine wastes anaerobically (Safley et al., 1992) due to greater economic feasibility (Sievers and Iannotti, 1982) and the extremely high biological oxygen demand (Sievers and Iannotti, 1982; Kobayashi and Kobayashi, 1995). Currently, the most common

anaerobic storage and anaerobic processing systems for swine manure are anaerobic lagoons (Zahn et al., 1997). The types of manure treatment and storage systems used by grower/finisher operations are illustrated in Figure 2.1.

Table 2.1 Common Manure Odorants and Odorant Families.

Family Name					
	Organic Acids	Phenolic Compounds	Alcohols, Aldehydes, Ketones	Sulfur Compounds	Nitrogen Compounds
Odorant	Acetic Acid	Phenol	Methanol	Hydrogen Sulfide	Ammonia
	Propionic Acid	p-Cresol	Formaldehyde	Methyl Mercaptan	Methyl Amine
	Butanoic Acid		Acetaldehyde	Dimethyl Sulfide	Dimethyl Amine
	Iso-valeric Acid		Acetone	Diethyl Sulfide	Diethyl Amine
	Pentanoic Acid		Methyl ethyl ketone		Indole
					Skatole

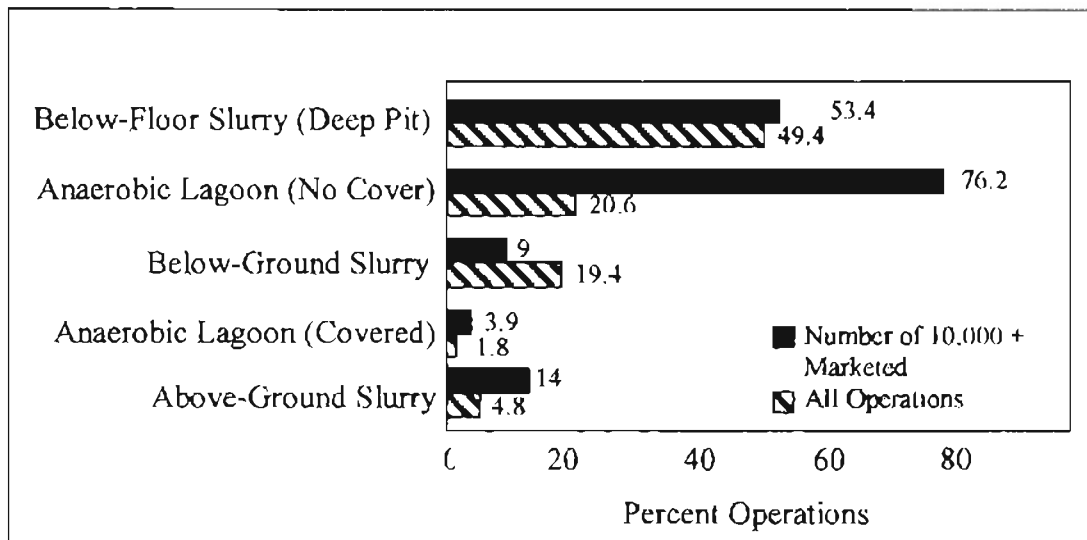


Figure 2.1. Grower/Finisher Operation by Use of Manure Storage Systems (Adapted from United States Department of Agriculture, 1996).

Most of the odorous gases associated with swine manure are created in this anaerobic environment. Anaerobic digestion follows three steps: hydrolysis, acid formation, and methane formation. The production and utilization of odorous compounds under anaerobic conditions are shown in Figure 2.2. Ammonia is one of the end products of anaerobic degradation, as seen in Figure 2.2.

Atmospheric ammonia is produced from decomposing feces and hydrolysis of urea in the urine (Sharpe and Harper, 1997). Nitrogen in the feces comprises undigested dietary nitrogen, endogenous nitrogen and microbial nitrogen, partly present in nucleic acids. Ammonia is the most highly reduced form of nitrogen occurring in nature (Minor and Hazen, 1969). The properties and physiological effects of ammonia gas exposure are listed in Table 2.2. Humans recognize ammonia as a sharp, pungent odor. With a detection level of only 17 ppb, ammonia can cause frequent odor complaints from neighbors surrounding swine production facilities.

The concern with ammonia is not limited to those odor conditions adversely affecting humans and pigs. Ammonia is also the primary neutralizing agent for atmospheric acids and is a common component of atmospheric aerosols. There is a growing realization of the importance of ammonia emissions and their role in acidification and eutrophication of terrestrial ecosystems. Natural ecosystems are thought to be sinks for ammonia (Sharpe and Harper, 1996; Van Hove et al., 1987; Hutchinson et al., 1972; McLeod et al., 1990; Nihlgard, 1985).

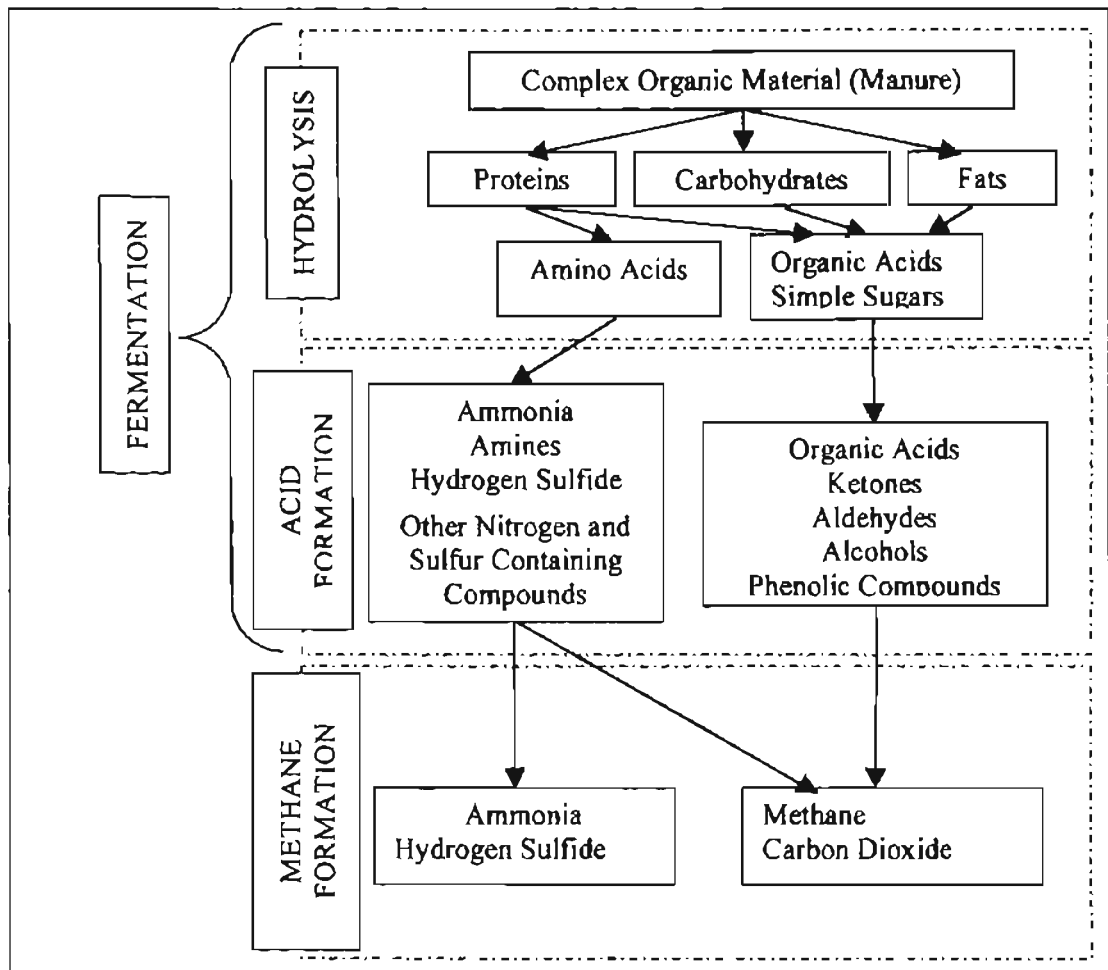


Figure 2.2. Compounds Formed During Anaerobic Degradation of Manure.

Odor Quantification

Measuring odor is an imprecise science. Odor quantification is difficult because no instrument has been found to successfully measure manure odor and all of its components. Because of the lack of instrumentation for odor measurement, standard odor quantification currently depends solely on the human nose (Schmidt and Jacobsen, 1995; Williams et al., 1998). A variety of odor measurement methods are available, while others are being developed. Four methods are briefly discussed here: olfactometry, scentometer, electronic nose, and chemical methods. The importance of accurate odor

measurement affects the validity of an odor model. For this research, the correct measurement of ammonia will directly impact the calculation of percent volatilization during irrigation of swine lagoon effluent.

Olfactometry

Although much progress has been made in the area of developing instrumentation for measuring odor, olfactometry, which makes use of the human nose, is currently accepted as the most valid procedure for odor measurement (Williams et al., 1998; Schmidt and Jacobsen, 1995). Olfactometry involves collecting odor samples: odorants are contained in a volume of air or adsorbed onto a media such as cotton fabric. These samples are then presented to an odor panel (a group of people trained to detect odor). The panelists' responses are recorded and the data is analyzed.

The lowest concentration at which panel members can still detect an odor is called the detection threshold. The detection and recognition levels of ammonia are listed in Table 2.3, along with other nitrogen compounds found in swine manure. The detection level is the concentration (in parts per billion) at which the average, healthy person first notices an odor. People cannot recognize the odor at the detection level, but they know they smell something. At the recognition level concentration, the brain begins to recognize the odorant as a distinct scent. The average human recognizes the scent of ammonia cleanser when the concentration of ammonia gas reaches 37,000 parts per billion (ASAE, 1996).

The olfactometer system works well for comparing odorous samples of air; however, it is both time consuming and expensive. Another drawback of the

olfactometer is that there has been no standard design for the dilution equipment and therefore different labs give different results for the same sample (Schmidt and Jacobsen, 1995.)

Table 2.2. Properties and Physiological effects of Ammonia (Adapted from Fublage, 1993)

AMMONIA	
Property	Value
Density ¹	0.77 Grams/Liter
Specific Gravity ²	0.58
Odor	Sharp, Pungent
Color	None
Maximum Allowable Concentration	50 ppm
400 ppm concentration ³	Physiological effects ⁴ : Throat Irritation
700 ppm concentration ³	Physiological effects ⁴ : Eye Irritant
1,700 ppm concentration ³	Physiological effects ⁴ : Coughing and Frothing
3,000 ppm concentration ³	Exposure period ⁵ : 30 minutes Physiological effects ⁴ : Asphyxiating
5,000 ppm concentration ³	Exposure period ⁵ : 40 minutes Physiological effects ⁴ : Could be fatal
Odor Threshold ⁶	17 ppb
<p>¹ Density: Density of gas in grams per liter at 32 degrees F. Density of air is 1.29 grams/liter</p> <p>² Specific Gravity: The ratio of the weight of pure gas to that of atmospheric air. If the number is less than 1, the gas is lighter than air; if greater than 1, it is heavier than air.</p> <p>³ Concentrations: In parts of pure gas per million parts of atmospheric air. To change to percent by volume, divide by 10,000.</p> <p>⁴ Physiological effects: Those found to occur in adult humans. A 150-pound pig would feel similar effects. Lighter pigs would be affected sooner at lower rates</p> <p>⁵ Exposure Period: The time during which the effects of the noxious gas are felt by an adult human or a 150-pound pig.</p> <p>⁶ Odor Threshold: The lowest concentration at which the odor is detected. This figure can only be approximate.</p>	

Table 2.3. Detection Level and Recognition Level for Nitrogen Compounds (Adapted from ASAE, 1996).

	Detection Level (ppb)	Recognition Level (ppb)
Ammonia	17	37,000
Methylamine	-	2.1
Dimethylamine	37	37
Diethylamine	-	500
Indole	1.0	-
Skatole	1.2	470

Scentometer

The scentometer is a hand-held device that allows on-site sampling of odorous air. The person taking the measurement holds the device up to his or her nose and breathes through the scentometer. The air that a person smells reaches the sniffer's nose through two holes, one for odorous air and a second, equipped with an activated carbon filter, for nonodorous air. The analyst chooses dilution factors by selecting the size of the hole passing unfiltered air. Advantages of the scentometer are it is portable, simple to use, and it gives immediate values for odor concentration (Sweeten and Rodriguez-Akabani, 1994). The main disadvantage is that the analyst's ability to distinguish odors diminishes the longer he or she is exposed to odors. Currently, there is no standard for describing the various dilution to threshold levels.

Electronic Nose

An electronic nose may eventually prove to be the convenient, objective, inexpensive, and portable tool needed to measure odor in the field. Electronic noses mimic the human olfactory system using polymer sensors to simulate receptors in the nose and a computer to simulate the brain. The sensors respond by producing changes in electrical resistance in direct proportion to the concentration of the odorant (Williams et

al., 1998). The main use of an electronic nose is to compare differences between mixtures of odors. The main drawback of the electronic nose is that it must be “taught” a pattern of sensor responses before it can make future comparisons. If properly trained, however, electronic noses may prove valuable in measuring odor character and offensiveness.

Chemical Methods

Chemical methods are used to determine the actual concentration of individual odorants in a sample taken from the field. The most common instrument used in odorant analysis is a gas chromatograph with a mass spectrometer detector (Williams et al., 1998). Similar to the electronic nose, a gas chromatograph distinguishes compounds by comparing to a reference standard. The main drawback to chemical methods is the large number of potential odorants that require analysis in a single sample of farmstead odors. The search for potential odorants may become less exhaustive using a universal set of reference odorants for farm odors.

Measurement Significance

Not only does the measuring device complicate odor measurement, but the variability in meteorological conditions during the sampling period will also affect odor quantification. Odor emissions and concentrations change with time, as does the movement of odorous air. The intensity and location of the odorous air changes with wind speed and direction. At any particular location, the current odor measurement says little about the odor concentration of an hour ago, or an hour from now. An

understanding of these factors is important when attempting to validate the model of ammonia emissions and volatilization during irrigation of swine lagoon effluent.

Models for Estimating Ammonia Volatilization

Many models have been developed that will predict the extent to which pollutants and odors can be dispersed downwind of the source. Mathematical dispersion models are valuable tools for regulatory agencies. The models allow for the simulation of the emission of pollutants for a new or proposed expansion of a manufacturing facility or power plant. These mathematical models generally perform many calculations using information such as the strength or emission rate of the pollutant or odor source, the location of the release point, the topography of the land, and meteorological information, including wind speed, wind direction and the mixing height of the atmosphere (Williams, et al., 1998, Wark et al, 1998). The problem with these models is not the dispersion component, but the emission rate. Odor emission is defined as the amount of odor released by a source over time. Mathematically, the emission rate is the volume of odorant produced divided by the time it takes to release the odorant to the atmosphere. There is no standard method, however, for determining odor emissions from a livestock facility. A dispersion model may estimate how much odor is being generated, give an estimate of where the odor will go, and predict how much dilution will take place, but it cannot define how much odor is a nuisance.

There have been many experimental studies on ammonia volatilization and nitrogen balance using wind tunnels or micrometeorological measurements in the field (Denmead et al., 1977; Lockyer, 1984; Hargrove, 1988; Jarvis and Pain, 1990; Pain, et al., 1990a,b; Sommer et al., 1991; Moal et al., 1995; Katz, 1996; Montes and Chastain,

2000). But integrating these findings is difficult, because volatilization factors and experimental conditions vary greatly. Ammonia losses depend on the nature of the slurry, soil conditions, agricultural practices and climate (Hargrove and Massey, 1960; Faurie and Bardin, 1979a,b; Terman, 1979; Pain et al., 1990; Montes and Chastain, 2000). It is also difficult to estimate ammonia losses because they may depend on how the measurements are made (Hargrove and Kinnison, 1990a, b; Pain et al., 1991; Denmead and Raupach, 1993; Montes and Chastain, 2000). Consequently, accurate, reliable data obtained under field conditions are scarce (Hargrove, 1988).

Numerous researchers have also reported on the volatilization of ammonia from liquid and slurry wastes. There is a wide range of reported ammonia losses during and immediately following application of liquid wastes. A summary of data from several studies is presented in Table 2.4. In these studies, ammonia losses were estimated using several approaches: micrometeorological mass balance (Beauchamp et al., 1982; Gordon et al., 1988; Pain et al., 1989), wind tunnel (Wright et al., 1987; Lockyer et al., 1989) and concentration difference (Wright et al., 1987). Most of this reported research on ammonia loss has been done using wind tunnel data on relatively dilute anaerobic lagoon liquid.

The difficulties in estimating emissions suggest that model development requires a better understanding and estimating the influence of the different factors on ammonia volatilization, accessible, and make comparing the experimental results obtained under different conditions a practical possibility (Genermont and Cellier, 1997).

Table 2.4. Reported Ammonia Losses from Applied Liquid Wastes (Adapted from Safley et al, 1992).

Waste Type	Application Technique	Conditions	Ammonia Loss (% of Applied)	Source
Liquid Swine Manure	Surface Applied to Soil	Spring; 90 t/ha of manure; 3.5 day measurement	14.0	Hoff et al. (1981)
Liquid Swine Manure	Surface Applied to Plastic	Spring; 90 t/ha of manure; 3.5 day measurement	65.8	Hoff et al. (1981)
Liquid Swine Manure	Surface Applied to Soil	Greenhouse conditions; 8 day measurement	82.5	Hoff et al. (1981)
Sewage Sludge	Surface Applied	Spring; 5 day test; 150 kg ammonia/ha	60	Beauchamp et al. (1978)
		Fall; 7 day test; 89 kg ammonia/ha	56	
Swine Slurry	Surface Applied to Grassland	22.9 kg ammonia/ha; 4 day test	53.0	Lockyer et al. (1989)
		73.4 kg ammonia/ha; 4 day test	56.9	
		139.6 kg ammonia/ha; 4 day test	36.1	
		48.4 kg ammonia/ha; 5 day test	77.6	
		44.1 kg ammonia/ha; 3 day test	60.4	
Swine Slurry	Surface Applied to Grassland	106 kg ammonia/ha; 3 day test	24.1	Pain et al. (1989)
		57 kg ammonia/ha; 3 day test	61.9	
Dairy Cattle Slurry	Surface Applied	197 kg ammonia/ha; 6 days; spring	30	Beauchamp et al. (1982)
		176 kg ammonia/ha; 7 days; spring	33	
		145 kg ammonia/ha; 6 days; spring	24	
Swine Lagoon Liquid	Sprinkler Irrigation	Overnight; spring and summer	9-23	Westerman et al. (1982)

Irrigation of Swine Lagoon Effluent

Land application is the final step in most swine manure handling schemes. This step is a frequent cause of odor complaints because it creates a large surface area from which volatile compounds can escape. Irrigation equipment has been adapted for disposal of liquid manure and wastewaters on cropland. The primary concern is to dispose of the wastes in an environmentally acceptable manner. Dilute wastes with relatively low solids content, similar to lagoon effluent, can be readily applied through conventional small-head, multi-sprinkler systems.

High trajectory guns with small droplet size are the worst combination for odor release and transport. The small droplet size increases wind effects on the drift of these droplets, spreading potential odors. Using less pressure results in larger droplet size and less intense odors. Droplets are less susceptible to wind drift, the application is more efficient, and the effluent is applied where intended. While several types of sprinkler systems can be used, center pivot systems are usually preferred for the dilute wastewater contained in an anaerobic lagoon primarily because of the technology advancements and economics.

The center pivot type of sprinkler system rotates around the pivot point and has the lowest labor requirements of most systems. It is constructed using a span of pipe connected to moveable towers. It will irrigate approximately 132 acres out of a square quarter section. Center pivot system can be either electric, water or oil-driven and can handle slopes up to 12 percent (Jensen, 1983). At any properly managed swine production facility the slope of the land will be limited to control the surface runoff and contamination of either the groundwater or surface water by the applied effluent. The

effluent application amount is controlled by the speed of rotation. The annual volume of effluent applied is primarily dependent upon the nitrogen and phosphorus requirements for the specific crop as well as the groundwater limits. Center pivots are also adaptable for any height crop and are particularly suited for coarser textured soils (Jensen, 1983).

The sprinkler device on the pivot system is also a factor to be considered when modeling ammonia volatilization during irrigation. The results from Yonts et al. (1997a) evaluating water loss from both impact sprinklers and spray nozzles is summarized in Table 2.5

The air evaporation of the water droplets will affect the quantity of ammonia that volatilizes into the atmosphere. This amount of nitrogen lost to volatilization depends on other factors of the irrigation system. Operative factors that determine water droplet size, such as nozzle diameter and operating pressure, affect droplet evaporation. The trajectory of the sprinklers and height above the crop canopy also affect the amount of evaporation during effluent application. Conditions that increase droplet evaporation and drift losses will increase ammonia release and transport off the field site.

Table 2.5 Sprinkler Water Losses and Application Efficiency for 1-inch Water Application (Adapted from Yonts et al., 1997a)

Water Loss Component	Impact Sprinkler Water Loss	Spray Head Water Loss
Air Evaporation and Drift	0.03 in.	0.01 in.
Net Canopy Evaporation	0.08 in.	0.03 in.
Plant Interception	0.04 in.	0.04 in.
Evaporation From Soil	Negligible	Negligible
Total Water Loss	0.15 in.	0.08 in.
Application Efficiency	85%	92%

CHAPTER 3

AMMONIA VOLATILIZATION MODEL DESCRIPTION

Introduction

Effluent that is applied to crops and land is most effective as a fertilizer if that effluent enters the transpiration stream and contributes directly to dry matter accumulation. Unfortunately, some of the effluent may be lost by water evaporation and chemical volatilization. A wide range of losses has been reported in the literature due to the many physical parameters and environmental factors involved. The most promising method of separating these components and evaluating the true water evaporation and chemical volatilization is by using mathematical models. Measurement of both water drop evaporation and chemical volatilization is important for evaluation and validation of this model.

The purpose of this model is to predict ammonia volatilization during land application of swine lagoon effluent. The model is composed of two primary components: water droplet evaporation and ammonia volatilization. Each component was developed independently. The two components were then combined and tested as a unit. A flowchart describing the model structure is presented in Figure 3.1. The FORTRAN code for this model is contained in Appendix A.

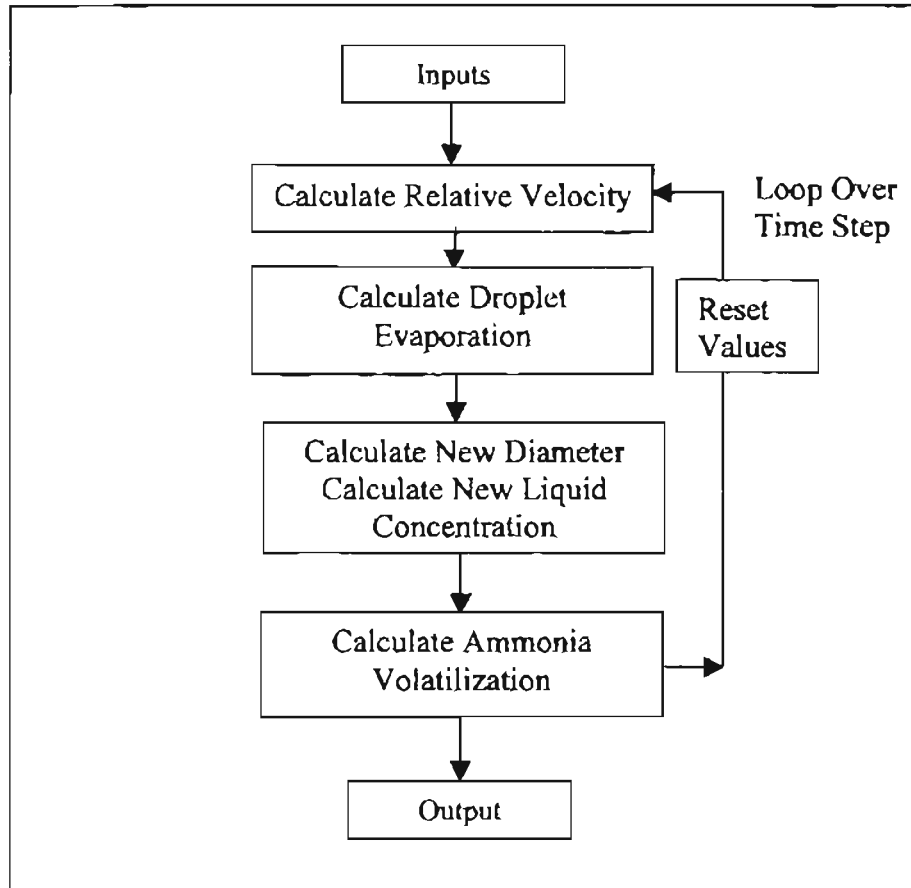


Figure 3.1. Ammonia Volatilization Model Flowchart.

Model Assumptions

This is a first generation model. It evaluates the ammonia volatilization during land application of swine lagoon effluent. To simplify the approach, this model considers the application of swine lagoon effluent removed from an uncovered, anaerobic lagoon. A center pivot type of irrigation system is considered using two types of sprinkler devices: impact sprinklers and low-pressure spray nozzles. The wind speed is assumed to be less than 5 m/s in this simplified model. These low wind speeds insure that wind drift during irrigation does not occur. Although this may be inaccurate at some times, this assumption allows for the completion of this first generation model. For the case of odor

generation from land application using a center pivot system, land slopes of less than 4% will be considered. At any properly managed swine production facility the slope of the land will be less than this 4% to prevent runoff and contamination of either groundwater or surface water.

Water Droplet Component

Droplet Evaporation

The heat and mass transfer analogy approach to water droplet evaporation offers a sound theoretical basis for the explanation of evaporation from falling sprinkler droplets. Numerous investigators have used the heat transfer analogy theory to describe the evaporation from droplets, and most all of these have referenced the work of Ranz and Marshall (1952). Their model was based on boundary layer equations and the equations for heat and mass transfer.

Water droplet evaporation is dependent on the diffusion of water molecules away from the drop and the transfer of heat by conduction and convection into the droplet to sustain the evaporative process (Ranz and Marshall, 1952a,b; Orr, 1966; Kincaid and Longley, 1989). The following equation is used to determine the rate of diameter change of an evaporating droplet:

$$\frac{dD}{dt} = -2 \left(\frac{M_v}{M_m} \right) \left(\frac{K}{D} \right) \left(\frac{\rho_a}{\rho_v} \right) \left(\frac{\Delta P}{P_f} \right) \text{Sh}_w \quad (3.1)$$

where D is the droplet diameter (m), t is the time (s), K is the mass diffusivity of water vapor in the air (m^2s^{-1}), ρ_a and ρ_v are densities of dry air and water vapor, respectively (kgm^{-3}), Sh_w is the Sherwood Number for water vapor (dimensionless), P_f is the

atmospheric pressure (atm), and ΔP is the vapor pressure difference (atm), M_m is the mean molecular weight of the gas mixture in the transfer path (29 g/mole for air), and M_v is the molecular weight of the diffusing water vapor (g/mole). Equation (3.1) is similar to that used by Goering et al (1972) and agrees with numerous other references given by Marshall (1954) with respect to the form of the equation, as recently reviewed by Kincaid and Longley (1989) and Thompson et al. (1993a).

All of the quantities in parentheses are dimensionless, with the exception of K/D , which has dimensions of m/s. The diffusivity K , is a function of both air temperature and pressure and is taken from List (1963) as:

$$K = \left(\frac{101.3}{P_a} \right) 8.8 * 10^{-10} T_k^{1.81} \quad (3.2)$$

where T_k is the water temperature (K) and P_a is the atmospheric pressure (atm). Previous authors (Goering et al., 1972; Williamson and Threadgill, 1974; Edling, 1985) have assumed the diffusivity is a function of temperature alone. Equation (3.2) provides a better agreement between data collected in Kincaid and Longley (1989) than did the above functions previously used by Goering et al. (1972), Williamson and Threadgill (1974), and Edling (1985).

In the case of a sprinkler droplet falling through a moving airstream, forced convection is the process under which evaporation takes place. For this situation, Froessling (1938) developed the following empirical relation for the mass transfer number, Sh_w (Sherwood number). The exponents and coefficient preceding the Reynolds and Schmidt numbers in Equation (3.3) vary slightly from reference to reference. The equation presented here is the Froessling expression for the Sherwood number to account

for the mass transfer from a droplet under forced convection (Thompson et al., 1993a; Kincaid and Longley, 1989).

The Sherwood number for a water sphere is calculated by:

$$Sh_w = 2.0 + 0.6 \cdot Re^{\frac{1}{2}} \cdot Sc^{\frac{1}{3}} \quad (3.3)$$

where Re is the Reynold's number (dimensionless) and Sc is the Schmidt number (dimensionless) defined by the following equations:

$$Re = \frac{DV_r}{\nu} \quad (3.4)$$

$$Sc = \frac{\nu}{K} \quad (3.5)$$

where V_r is the resultant velocity vector of the droplet with respect to the air (m/s), K is the diffusivity of water vapor in air (m^2/s), D is the diameter of the droplet (m) and ν is the kinematic viscosity of the air at the temperature of the air and droplet (m^2/s).

The air pressure is determined by:

$$P_a = 101.3 \left(1 - 2.257 \cdot 10^{-5} E\right)^{5.255} \quad (3.6)$$

where E is the elevation of the test site (m).

In the Goering (1972) models, the droplet temperature was assumed to be the same throughout and equal to the wet bulb temperature. Consequently, the vapor pressure difference is:

$$\Delta P = P_s - P_w \quad (3.7)$$

where P_w is the vapor pressure at the dry bulb temperature (or saturation pressure at the dewpoint) and P_s is the saturation pressure at the wet bulb temperature of the air.

Because the airstream contains only air and water vapor, the total pressure P_a (atmospheric) is the sum of the partial pressures of the air and water vapor, and

$$\frac{\Delta P}{P_f} = \frac{(P_s - P_v)}{(P_a - P_v)} \quad (3.8)$$

All quantities on the right side of (3.1) are now known and the evaporation rate dD/dt can be calculated for any time step dt , knowing the initial droplet size.

Droplet Flight and Size Distribution

Droplet size and trajectory are related, and both can have considerable influence on droplet mass lost by evaporation; thereby influencing the mass of odorant also lost between the sprinkler nozzle and the canopy or ground surface (Thompson et al., 1993a). The equations for describing droplet trajectory provide a means for estimating the effect of flight time and relative velocity with the air on droplet evaporation. Assuming that droplets remain as spheres during flight (Seginer, 1965), it is possible to model the trajectory of various droplets using ballistics equations.

Bilanski and Kidder (1958) presented the following differential equation for computing droplet trajectory:

$$m \frac{d^2 x}{dt^2} = -R \cos(\theta) \quad (3.9)$$

where m is the mass of the droplet (kg), R is the air resistance ($\text{kg} \cdot \text{m/s}^2$), θ is the angle the droplet makes with the horizontal (degrees), and x is the horizontal distance (m). Based on a graphical solution using Laws (1941) data, Seginer (1965) concluded that a reasonable expression for R would be:

$$R = C_2 V_r^2 \quad (3.10)$$

where C_2 is the drag coefficient of the drop (m/s). A solution of the trajectory equations in three dimensions is required to include the effect of wind on droplet flight. The

velocity vectors describing the trajectory of a given irrigation sprinkler droplet are illustrated in Figure 3.2.

Note that V_w , the wind velocity, is fixed in a position parallel to the x-axis and in the positive x-direction. Therefore, relative velocity of the droplet with the air (V_r) in the x-direction becomes $V_x - V_w$. Assuming that the application pattern of a sprinkler is symmetric about its axis, rotating the angle α through 360° about the z-axis will simulate a wind from any horizontal direction. V_h represents the horizontal projection of V_r in the x-y plane, and θ is the angle the V_r lies about this plane. (Thompson, et al., 1993a). By substituting Equation (3.10) into Equation (3.9) and eliminating the mass term, the differential equations for acceleration can be written as:

$$\frac{d^2x}{dt^2} = -C_2 V_r (V_x - V_w) \quad (3.11)$$

$$\frac{d^2y}{dt^2} = -C_2 V_r V_y \quad (3.12)$$

$$\frac{d^2z}{dt^2} = -C_2 V_r V_z - g \quad (3.13)$$

where $V_x, V_y,$ and V_z are the resultant velocity vector in the x, y and z directions, respectively, and g is the acceleration due to gravity (m/s^2). The resultant velocity vector of the droplet with respect to air can be represented by the following equation:

$$V_r = \left[(V_x - V_w)^2 + V_y^2 + V_z^2 \right]^{0.5} \quad (3.14)$$

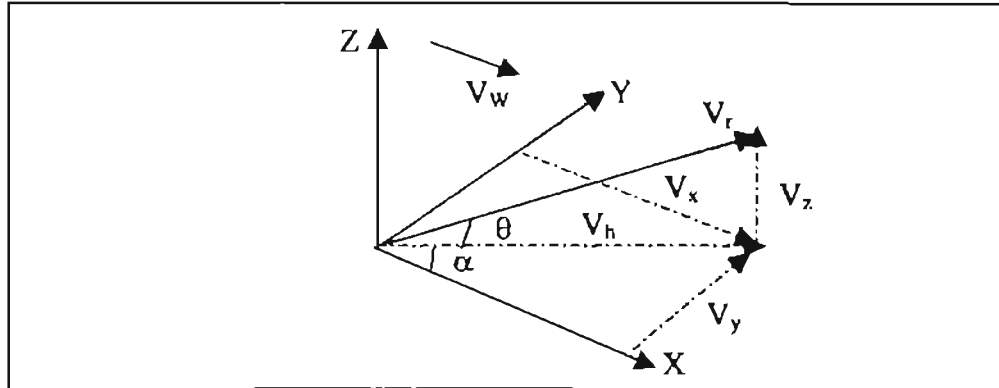


Figure 3.2. Diagram of Velocity Vectors Describing the Trajectory of a Given Irrigation Sprinkler Droplet (Adapted from Thompson et al., 1993).

To solve these three equations, C_2 must be known. Values of C_2 as a function of droplet size were reported by von Bernouth and Gilley (1984), based on results from Laws (1941), Green (1952), and List (1966) for droplet up to 6 mm in initial diameter. These values assume those droplets are at or near terminal velocity (Seginer, 1965). Therefore, by specifying the initial velocity vector of a droplet, equations (3.11), (3.12), and (3.13) can be used to calculate the position, velocity, and distance traveled of any given droplet (Thompson et al., 1993a).

The implementation of equations (3.11), (3.12), and (3.13) requires knowledge of a droplet size distribution. Mogle and Evans (1951) proposed a log-normal probability distribution to describe droplet size from spray nozzles, with the maximum droplet size limited by aerodynamics. They referred to this three-parameter function as an Upper Limit Log Normal (ULLN). Bezdek and Solomon (1983) state that the ULLN distribution can account for bimodality and a finite maximum, as well as left or right skewedness. This makes it a desirable model for sprinkler droplet distributions.

Ammonia Volatilization

Mass Flux of an Odorant

The mass flux of odorant is defined by the following equation:

$$\frac{dM_o}{dt} = M_{IN} - M_{OUT} \quad (3.15)$$

where M_{IN} is the quantity of odorant mass being generated within the droplet (mg/s),

M_{OUT} is the quantity of odorant mass being released from the droplet (mg/s), and $\frac{dM_o}{dt}$ is

the change in odorant mass concentration within the droplet with time (mg/s).

An expression for M_{OUT} can be formed based on a finite difference approximation to Fick's Law of Diffusion, which can be written as

$$M_{OUT} = h_{m,od} C_A (C_{SG} - C_G) \quad (3.16)$$

where h_m is a gas-phase film mass transfer exchange coefficient (m/s), C_A is the droplet surface area (m^2), C_{SG} is the concentration of odorant at the surface of the droplet in the gas phase (mg/m^3), and C_G is the concentration of odorant in the free air surrounding the droplet (mg/m^3). Knowing the surface area of a sphere droplet, $C_A = 4\pi r^2 = \pi D^2$, where r is the droplet radius (m) and D is the droplet diameter (m), Equation (3.16) can be simplified:

$$M_{OUT} = h_{m,od} \pi D^2 (C_{SG} - C_G) \quad (3.17)$$

For the time scales typical of a drop falling through the air, generated odorant in the droplet will be small. Combining equations (3.15) and (3.17), assuming that the ammonia generation within the drop is zero ($M_{IN} = 0$) and no odorant mass is accumulating within the droplet:

$$\frac{dM_o}{dt} = -M_{OUT} = -h_{m,od} \pi D^2 (C_{\infty} - C_G) \quad (3.18)$$

Odorant Concentration

The initial concentration within each droplet can also be calculated using the following equation:

$$M_o = C_L V \quad (3.19)$$

where M_o is the mass of odorant inside the droplet (mg), C_L is the initial concentration in the liquid droplet (mg/m³) and V is the droplet volume (m³). Equation (3.19) can be simplified with the assumption that the droplets formed at the nozzle are spherical (Seginer, 1965), knowing the volume of a sphere is:

$$V_{sphere} = \frac{4}{3} \pi r^3 \quad (3.20)$$

Expanding Equation (3.19):

$$M_o = C_L \cdot \frac{4}{3} \cdot \pi r^3 = \frac{\pi}{6} C_L D^3 \quad (3.21)$$

where r is the droplet radius (m) and D is the droplet diameter (m).

Taking the derivative of Equation (3.21) with respect to time yields the following equation:

$$\frac{dM_o}{dt} = 3 \cdot \frac{\pi}{6} D^2 C_L \frac{dD}{dt} + \frac{\pi}{6} D^3 \cdot \frac{dC_L}{dt} \quad (3.22)$$

Simplifying Equation (3.22):

$$\frac{dM_o}{dt} = \frac{\pi}{6} D^2 \left(3C_L \cdot \frac{dD}{dt} + D \frac{dC_L}{dt} \right) \quad (3.23)$$

Combining Equations (3.23) and (3.18):

$$\frac{dM_o}{dt} = \frac{\pi}{6} D^2 \left(3C_L \cdot \frac{dD}{dt} + D \cdot \frac{dC_L}{dt} \right) = -\pi h_{m,od} D^2 (C_{\infty} - C_G) \quad (3.24)$$

Simplifying Equation (3.24):

$$\frac{\pi}{6} D^2 \left(3C_L \cdot \frac{dD}{dt} + D \cdot \frac{dC_L}{dt} \right) = -\pi h_{m,od} D^2 (C_{Si} - C_G) \quad (3.25)$$

The gas phase exchange coefficient can be determined using the Sherwood number calculated for the odorant:

$$Sh_{od} = 2.0 + 0.60 \cdot Sc_{od}^{1/3} \cdot Re_{od}^{1/2} = \frac{h_{m,od} D}{K_{od}} \quad (3.26)$$

where h_m is the gas-phase exchange coefficient, D is the droplet diameter (m), and K_{od} is the odorant diffusivity (m^2/s), a constant value for a given chemical. Re_{od} is the Reynolds number for the odorant (dimensionless) and Sc_{od} is the Schmidt number for the odorant (dimensionless) defined by the following equations:

$$Re_{od} = \frac{DV_r}{\nu} \quad (3.27)$$

$$Sc_{od} = \frac{\nu}{K_{od}} \quad (3.28)$$

where V_r is the resultant velocity vector of the droplet carrying the odorant (m/s), ν is the kinematic viscosity of the odorant of at the mean temperature of the air and droplet (m^2/s).

Rearranging Equation (3.26), we obtain:

$$h_{m,od} = \frac{K_{od} Sh_{od}}{D} \quad (3.29)$$

Substituting Equation (3.29) into Equation (3.25):

$$\frac{\pi}{6} D^2 \left(3C_L \cdot \frac{dD}{dt} + D \cdot \frac{dC_L}{dt} \right) = -\pi \frac{Sh_{od} K_{od}}{D} D^2 (C_{Si} - C_G) \quad (3.30)$$

Simplifying Equation (3.30):

$$\frac{\pi}{6} D^2 \left(3C_L \cdot \frac{dD}{dt} + D \cdot \frac{dC_L}{dt} \right) = -\pi \text{Sh}_{od} K_{od} D (C_{SG} - C_G) \quad (3.31)$$

Substituting Equation (3.1) into Equation (3.30):

$$\frac{\pi}{6} D^2 \left[3C_L \cdot -2 \left(\frac{M_V}{M_m} \right) \left(\frac{K}{D} \right) \left(\frac{\rho_a}{\rho_d} \right) \left(\frac{\Delta P}{P_f} \right) \text{Sh}_w \right] + D \cdot \frac{dC_L}{dt} = -\pi \text{Sh}_{od} K_{od} D (C_{SG} - C_G) \quad (3.32)$$

In order to determine the mass concentration of odorant that escapes from the drop and travels into the air, Equation (3.32) must be solved in terms of $\frac{dC_L}{dt}$:

$$\left[3C_L \cdot -2 \left(\frac{M_V}{M_m} \right) \left(\frac{K}{D} \right) \left(\frac{\rho_a}{\rho_d} \right) \left(\frac{\Delta P}{P_f} \right) \text{Sh}_w \right] + D \cdot \frac{dC_L}{dt} = -\frac{6}{D} \text{Sh}_{od} K_{od} (C_{SG} - C_G) \quad (3.33)$$

Simplifying Equation (3.33):

$$D \cdot \frac{dC_L}{dt} = \left[-\frac{6}{D} \text{Sh}_{od} K_{od} (C_{SG} - C_G) \right] - \left[3C_L \cdot -2 \left(\frac{M_V}{M_m} \right) \left(\frac{K}{D} \right) \left(\frac{\rho_a}{\rho_d} \right) \left(\frac{\Delta P}{P_f} \right) \text{Sh}_w \right] \quad (3.34)$$

Finally, solving for $\frac{dC_L}{dt}$:

$$\frac{dC_L}{dt} = \frac{1}{D} \left[\left[-\frac{6}{D} \text{Sh}_{od} K_{od} (C_{SG} - C_G) \right] - \left[3C_L \cdot -2 \left(\frac{M_V}{M_m} \right) \left(\frac{K}{D} \right) \left(\frac{\rho_a}{\rho_d} \right) \left(\frac{\Delta P}{P_f} \right) \text{Sh}_w \right] \right] \quad (3.35)$$

Simplifying Equation (3.35):

$$\frac{dC_L}{dt} = \left[\left[-\frac{6}{D^2} \text{Sh}_{od} K_{od} (C_{SG} - C_G) \right] - \left[3C_L \cdot -2 \left(\frac{M_V}{M_m} \right) \left(\frac{K}{D^2} \right) \left(\frac{\rho_a}{\rho_d} \right) \left(\frac{\Delta P}{P_f} \right) \text{Sh}_w \right] \right] \quad (3.36)$$

Again, simplifying Equation (3.36):

$$\frac{dC_L}{dt} = \left[\left[-\frac{6}{D^2} \text{Sh}_{od} K_{od} (C_{SG} - C_G) \right] + \left[6C_L \cdot \left(\frac{M_V}{M_m} \right) \left(\frac{K}{D^2} \right) \left(\frac{\rho_a}{\rho_d} \right) \left(\frac{\Delta P}{P_f} \right) \text{Sh}_w \right] \right] \quad (3.37)$$

Method and Procedures

In order to model the droplet evaporation and simultaneous odorant release, droplet size distribution, flight trajectory, and odorant concentration rate of change must be coupled to the theoretical equation describing droplet diameter rate of change. This requires the combination of the ULLN distribution, describing droplet size frequency, with equations (3.11) through (3.13), describing droplet acceleration, equation (3.36), describing odorant concentration rate of change, and equation (3.1), describing droplet rate of evaporation. This droplet size is then coupled with the odorant concentration rate of change (equation (3.36)) to determine the total ammonia volatilization (percent).

The ULLN distribution, with parameters determined by Solomon and von Bernuth (1981) as functions of nozzle size and diameter, was used to describe drop size distribution for spray and impact sprinklers. Individual droplet trajectories and velocities are determined by numerically solving equations (3.11) through (3.13) using the Runge-Kutta-Fehlberg method explained by Gerald and Wheatly (1994). Appendix B contains a detailed explanation of the Runge-Kutta-Fehlberg method.

The initial velocity for each droplet was assumed equal to the average jet velocity (Seginer, 1965) computed using the orifice equation:

$$V = C(2gh)^{0.5} \quad (3.38)$$

where V is the velocity (m/s), C is the flow coefficient (dimensionless), and h is the head difference across the orifice (m).

Droplets were assumed to form at the nozzle, although depending on sprinkler type and pressure, the jet may be intact a short finite distance from the nozzle (von Bernuth and Gilley, 1984). The droplet diameter resulting from evaporation was

determined from equation (3.1) using a Runge-Kutta-Fehlberg method, along with the V_r calculated from the trajectory equations. The droplet diameter on the right-hand side of equation (3.1), as well as V_r , and the droplet temperature used to compute the saturated vapor pressure at the droplet surface (e_s), were averages from the previous and current time steps. It was assumed that the droplet had a uniform temperature throughout its volume (i.e. it was thoroughly mixed).

Once the droplet diameter was calculated, this value was used to determine the ammonia concentration in the liquid, C_L , at each time step, given an initial concentration. Once again, the concentration within the droplet was calculated with the Runge-Kutta-Fehlberg method (Gerald and Wheatly, 1994). The above calculations continue throughout the required time step. The conclusion of the program results in an output of final droplet diameter, water vapor lost to the atmosphere, and percent of ammonia lost to the atmosphere.

CHAPTER 4

INPUT AND OUTPUT PARAMETERS

Input Parameters

The input parameters can be divided into four categories: atmospheric characteristics, irrigation application characteristics, ammonia properties and characteristics, and simulation specific variables. Atmospheric characteristics relate to meteorological data such as temperature and relative humidity. Irrigation application characteristics describe the type of irrigation system used for application. The simulation specific variables relate to parameters that determine the beginning and end of the simulation. They include the time step specification.

Atmospheric Characteristics

The atmospheric characteristics are meteorological parameters. The atmospheric characteristic input parameters are listed in Table 4.1. TEMP_F is the average daily temperature (°F). This value is entered daily as a measured value. Typical average values for daily temperatures when irrigating swine lagoon effluent range between 16° and 38° C (61° and 101° F). The model is not limited to these ranges. These are the typical values that are found during land application. RH is the relative humidity (%). The values of relative humidity typically range between 30 and 90 percent. Again, the model is not limited by this range. These large ranges illustrate the ever-changing

atmospheric conditions and their impact on both droplet evaporation and ammonia volatilization. ELEV is the elevation of the test site (m). ELEV is used to calculate the atmospheric pressure and is therefore included as an atmospheric input parameter.

Table 4.1. Atmospheric Characteristic Input Parameters

Parameter	Description	Units
TEMPF	Average Daily Temperature	°F
RH	Relative Humidity	%
ELEV	Elevation	m

Irrigation Application Characteristics

Irrigation application characteristics refer to the type of irrigation system used to apply the lagoon effluent. The system parameters are listed in Table 4.2. NOZZ is the type of nozzle system used on the center pivot system. For this first generation model, this variable is limited to either an impact sprinkler or a low-pressure nozzle. NOZZ is used to determine the flow coefficient in the initial velocity equation for each droplet. P is the center pivot system pressure (kPa). NSPRJNK is the number of sprinklers on the center pivot system. This variable will be used in the determining downwind dispersion of ammonia. INDROP is the initial drop diameter (m). NOZZD is the diameter of the sprinkler nozzle (m). The final irrigation application input characteristic is NSAMP, the number of sampling intervals per unit time. These last three input parameters are used in determining the droplet distribution to be evaluated. The majority of the irrigation application input parameters are not used directly in the equations of Chapter 3. These input parameters are used to calculate the required variables in those equations.

Table 4.2 Irrigation Application Input Parameters

Parameter	Description	Units
NOZZ	Type of Sprinkler Used	-
P	Sprinkler Pressure	kPa
NSPRINK	Number of Sprinklers on Center Pivot	-
INDROP	Initial Drop Diameter	m
NOZZD	Nozzle Diameter	m
NSAMP	Number of Sample Intervals	-

Ammonia Properties and Characteristics

The ammonia properties and characteristics are presented in Table 4.3. DODOR is the density of the odorant (kg/m^3). In this case, it is the density of ammonia. HAMM is Henry's Law constant for ammonia (dimensionless). KODOR is the mass diffusivity of the odor vapor in the atmosphere (m^2/s). These parameters are hard-coded into the program. The input parameters are used to determine the value of the Reynolds number for the odorant, as well as the value of the Schmidt number. These input parameters are also used in determining the Sherwood number for the odorant and are directly used in determination of the odorant concentration rate of change.

Simulation Characteristics

The last type of model input is the simulation specific characteristics. The simulation specific input parameters are contained in Table 4.4. H is the iteration step size used by the program. T is the time step (s). Both of these are hard-coded into the program, but can be changed to account for error and accuracy.

Table 4.3. Ammonia Characteristic Input Parameters

Parameter	Description	Units
DODOR	Density of the Odorant	kg/m ³
HAMM	Henry's Law Constant for Ammonia	-
KODOR	Odor Diffusivity	m ² /s
INITCL	Initial Ammonia Concentration in Effluent	mg/L

Table 4.4. Simulation Characteristic Input Parameters

Parameter	Description	Units
H	Iteration Step	-
T	Time Step	s

Output Parameters

The output parameters of the model can be separated into two categories; those related to the droplet evaporation component of the model and those related to the ammonia volatilization component of the model. The model output parameters are listed in Table 4.5.

D is the final droplet diameter (mm). TOTALCL is the final ammonia concentration in the liquid (mg/L). PERC is the percent of ammonia volatilized during the entire irrigation process (%). DPEVAP is the total volume of water that evaporated during the entire irrigation process (m³).

Table 4.5. Model Output Parameters

Parameter	Description	Units
D	Final Droplet Diameter	m
TOTALCL	Final Ammonia Concentration in the Liquid	mg/L
PERC	Percent of Volatilized Ammonia	%
DPEVAP	Volume of water that Evaporated	m ³

CHAPTER 5

MODEL VALIDATION

Procedure

The objective of the model validation was to test the ability of the model to predict ammonia volatilization. An internal validation was complete for droplet evaporation and mass transfer of ammonia lost to the atmosphere. Two data sets were used to validate the overall model: Montes and Chastain (2000) and Safley et. al (1992). A brief site description, experimental parameters, and volatilization results are given for each experiment, followed by the model input parameters used for each experiment. The model validation results are presented for each set of data. A detailed sensitivity analysis is completed for the input variables in the model. A summary of the results and conclusions is followed by recommendations for further research, which concludes this chapter.

Internal Validation

An internal validation was done to determine the accuracy of the program output in comparison with data calculated using a spreadsheet for both droplet evaporation and ammonia volatilization. The internal validation is a method for checking the programming structure to ensure that the program is performing the correct calculations and returning the correct values.

The droplet evaporation was calculated using Equation 3.1 and also in spreadsheet form. The spreadsheet calculated data versus model output is found in Table 5.1. Both sets of data were calculated at various temperatures using the same required input parameters. That is, all variables except temperature were kept constant. Temperature variations were used only as a means to vary one variable to determine if the calculated data and the model predicted the same droplet evaporation. The total, mean, median, maximum, minimum and standard deviation values for the model output and calculated data are found in Table 5.2. The results of the regressions comparing observed and predicted values for droplet evaporation are contained in Table 5.3. The t-slope and t-intercept values are also found in Table 5.3. The t-tests were done with an $\alpha = 0.95$.

Table 5.1. Calculated versus Predicted Droplet Evaporation.

Temperature, F	Total Droplet Evaporation g	
	Calculated Data	Model
59	0.00209	0.00209
62.6	0.00209	0.00209
66.2	0.00209	0.00209
69.8	0.00209	0.00209
73.4	0.00209	0.00209
77	0.00209	0.00209
80.6	0.00209	0.00209
84.2	0.00209	0.00208
87.8	0.00209	0.00208
91.4	0.00208	0.00208
95	0.00208	0.00208
98.6	0.00208	0.00208
102.2	0.00208	0.00208

Table 5.2. Summary Statistics for Droplet Evaporation Validation.

	Calculated Data	Model
TOTAL	0.0271	0.0271
MEAN	0.00209	0.00209
MIN	0.00208	0.00208
MAX	0.00209	0.00209
MEDIAN	0.00209	0.00209
STD. DEV.	0.0000049	0.000049

Table 5.3. Regression Statistics for Droplet Evaporation.

	Droplet Evaporation
r^2	1
Std. Error	0.00000136
t-slope	1.089286
t-intercept	1.710882

A graph of the regression line for the calculated data versus predicted droplet evaporation is found in Figure 5.1. The r^2 value for the regression of calculated vs. predicted droplet evaporation is 1.0. The r^2 value indicates that 100% of the variation in calculated evaporation is explained by the regression line. The t-slope value leads to a “do not reject” conclusion for the hypothesis that the slope of the regression line is equal to one. The t-intercept value also leads to a “do not reject” conclusion for the hypothesis that the intercept of the regression line is zero. The r^2 value along with the t-statistics indicates that the model does an acceptable job of predicting droplet evaporation.

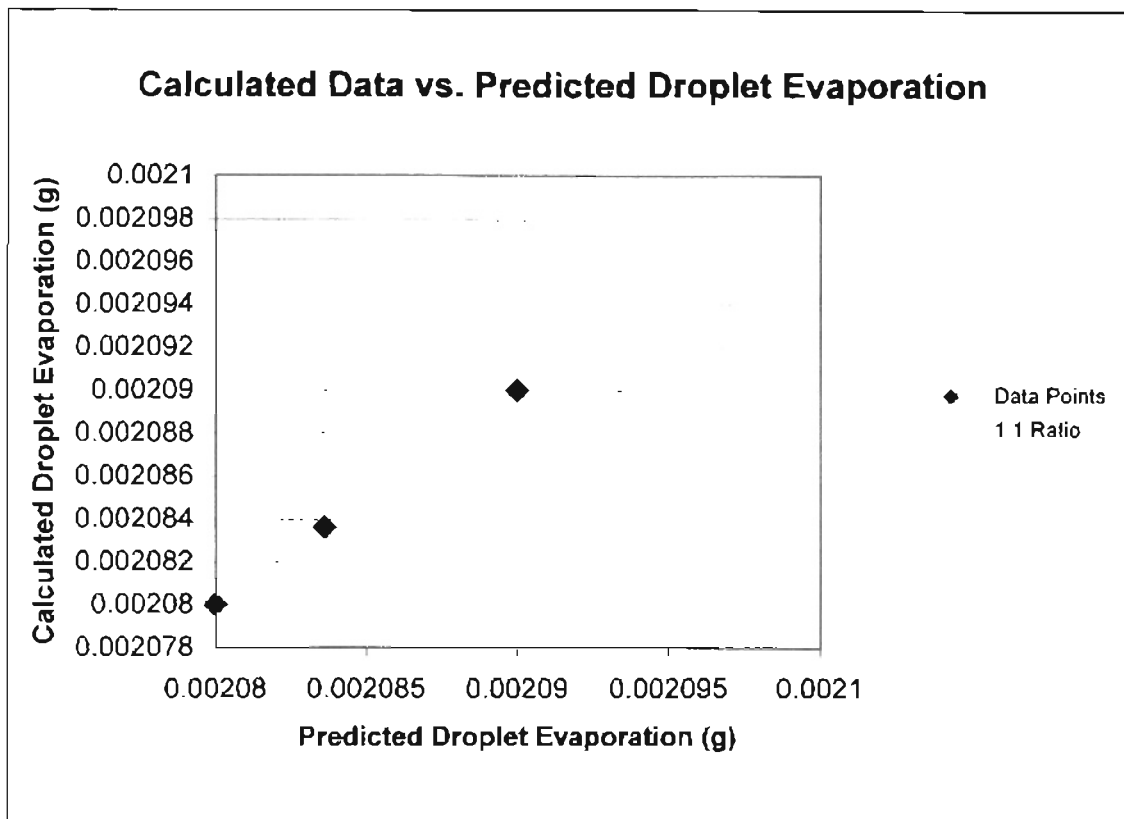


Figure 5.1. Regression of Observed vs. Predicted Droplet Evaporation for Internal Validation

The ammonia volatilization was calculated using Equation 3.17 and also in spreadsheet form. The initial droplet diameter was held constant, while the temperature was varied. All other variables were held constant. The spreadsheet calculated data versus model output is found in Table 5.4. Both sets of data were calculated using the same required input parameters. The total, mean, median, maximum, minimum and standard deviation values for the model output and calculated data are found in Table 5.5. The results of the regressions comparing observed and predicted values for ammonia volatilization are contained in Table 5.6. The t-slope and t-intercept values are also found in Table 5.6. The t-tests were done with an $\alpha = 0.95$.

Table 5.4. Calculated versus Predicted Ammonia Release.

Total Ammonia Release mg/s	
Calculated Data	Model
1.89	1.89
1.94	1.95
1.88	1.89
0.88	0.89
0.88	0.89
0.92	0.93
0.10	0.10
0.09	0.09
0.14	0.15

Table 5.5. Summary Statistics for Ammonia Release Validation.

	Calculated Data	Model
TOTAL	8.78	8.79
MEAN	0.967	0.976
MIN	0.092	0.92
MAX	1.94	1.96
MEDIAN	0.88	0.89
STD. DEV.	0.774	0.782

Table 5.6. Regression Statistics for Ammonia Release.

	Droplet Evaporation
r^2	1
Std. Error	0.00000136
t-slope	1.745884
t-intercept	-0.02635

A graph of the regression line for the calculated data versus predicted droplet evaporation is found in Figure 5.2. The r^2 value for the regression of calculated vs. predicted droplet evaporation is 1.0. The r^2 value indicates that 100% of the variation in calculated evaporation is explained by the regression line. The t-slope value leads to a “do not reject” conclusion for the hypothesis that the slope of the regression line is equal

to one. The t-intercept value also leads to a “do not reject” conclusion for the hypothesis that the intercept of the regression line is zero. The r^2 value along with the t-statistics indicates that the model does an acceptable job of predicting ammonia release.

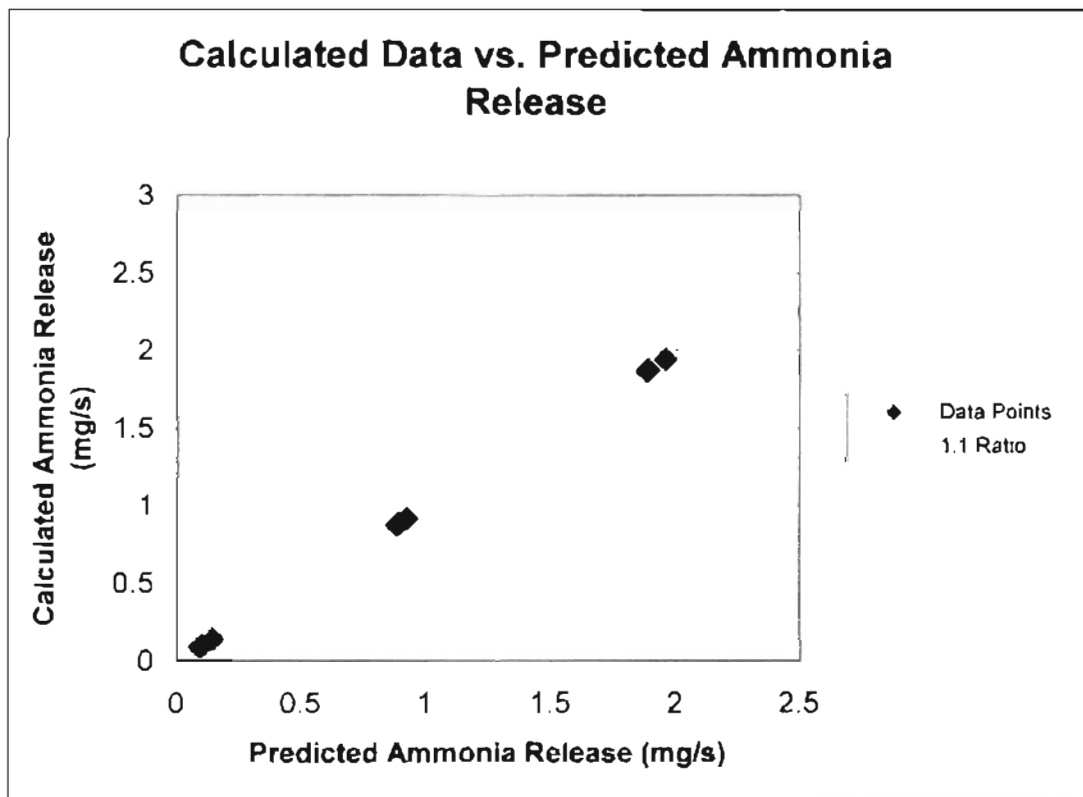


Figure 5.2. Regression of Observed vs. Predicted Ammonia Release for Internal Validation.

Site Description

Data from Montes and Chastain (2000)

The first experiment (Montes and Chastain (2000)) evaluated ammonia losses during sprinkler irrigation of swine lagoon effluent in forest and open field environments in two South Carolina locations. The 12-year-old Loblolly pine plantation (Clarendon County site) was fertilized with swine lagoon effluent to provide 67 to 134 kg of plant

available nitrogen per hectare. Rainbird 80E tough bird sprinklers with 9.5 mm nozzles were used to apply the effluent at an operating pressure of 179 kPa. The sprinklers were positioned to provide an overlap of 100%. A similar irrigation system was used to apply swine lagoon effluent to a 2-year old Sycamore and Longleaf pine plantation at the Starkey Swine Production Center at Clemson University. A 15.9 mm diameter nozzle was used on the sprinkler and the pipe diameter was 76.2 mm, with an operating pressure of 379 kPa. This site served as the open field condition since the trees were 6 meters tall or less.

Wet-bulb and dry-bulb temperatures were measured periodically during each application at each site. Average dry-bulb temperatures and relative humidity were calculated for each application. Average daily wind speed observations for the Clarendon County site were obtained from the FAA weather station located at Florence, South Carolina. Wind speed observations were obtained for the Starkey Swine Center from the FAA weather station in Anderson, South Carolina.

Lagoon nutrient content, application dates, and general environmental conditions during application are shown for the Clarendon and Starkey locations in Tables 5.7 and 5.8, respectively. A valve and a small hose were installed on the irrigation pipe, about 6 meters from the discharge of the irrigation pump. Samples of the irrigated swine effluent were collected at equal intervals during irrigation and mixed into one large container. The container was covered and remained on ice between sampling intervals. This 'irrigation' sample bottle served as a measurement of the initial ammonia concentration in the swine effluent. Eight cylindrical plastic containers were distributed on the ground in the forest and open field conditions prior to irrigation. After the application was

completed, the contents of the containers were immediately mixed together in a large sample bottle to provide the ground sample for each application. This ground sample was then immediately stored on ice and served as a measurement of the final ammonia concentration after irrigation.

The results of this study show that no differences were detected between the open field and forest environments in ammonia volatilization during sprinkler irrigation. The volatilization losses during irrigation were not significantly different from zero and should not be included in estimates of the plant available nitrogen.

Table 5.7. Nutrient Content and Environmental Conditions for the Clarendon County Site Irrigation Events (Adapted from Montes and Chastain, 2000).

Date of Application	Average Air Temperature (C)	Relative Humidity (%)	Average Wind Speed (m/s)	Characteristics of Irrigated Manure		
				TKN (mg/L)	TAN (mg/L)	Moisture (%)
07/27/1999	30	50	3.4	1149	963	99.51
07/27/1999	30	48	3.4	1054	963	99.56
07/27/1999	30	51	3.4	1041	986	99.56
11/06/1999	20	58	2.1	1066	951	99.53
11/06/1999	20	57	2.1	1040	923	99.51
11/06/1999	20	56	2.1	1014	943	99.50
03/20/1999	16	95	4.4	1403	1181	99.43
03/20/1999	16	96	4.4	1514	1325	99.50
03/20/1999	16	94	4.4	1515	1351	99.52
Average				1200	1065	99.51

Table 5.8. Nutrient Content and Environmental Conditions for the Starkey County Site Irrigation Events (Adapted from Montes and Chastain, 2000).

Date of Application	Average Air Temperature (C)	Relative Humidity (%)	Average Wind Speed (m/s)	Characteristics of Irrigated Manure		
				TKN (mg/L)	TAN (mg/L)	Moisture (%)
8/16/1999	28	58	1.9	234	189	99.86
8/16/1999	28	57	1.9	260	184	99.79
8/16/1999	28	58	1.9	234	181	99.77
8/16/1999	28	56	1.9	301	220	99.79
6/12/2000	35	35	3.4	195	154	99.95
6/12/2000	35	30	3.4	181	139	99.96
6/13/2000	33	60	3.6	185	166	99.91
6/13/2000	33	40	2.9	144	132	99.94
6/14/2000	34	40	7.1	224	200	99.94
6/14/2000	36	45	5.8	181	123	99.94
6/14/2000	36	50	4.9	240	192	99.93
6/14/2000	36	40	4.9	170	153	99.93
6/14/2000	36	30	4.9	168	124	99.95
6/15/2000	29	70	3.1	153	131	99.95
Average				205	163	99.90

Data from Safley et al (1992)

The final set of data is research completed by Safley, Barker and Westerman (1992). Irrigation experiments were conducted using a center pivot system (Valmont Model 4871) to determine the losses of nitrogen that occurs during sprinkler irrigation. The pivot was 278 m long and had five supporting towers. The sprinkler irrigation nozzles on the pivot were spaced and sized by the manufacturer to give a near-uniform application. The pivot system was used to apply liquid from an anaerobic lagoon liquid that received flushed waste from a swine farrow-to-feeder pig facility.

The six sampling stations consisted of a Taylor Instruments Model 2701 rain gauge attached to a wooden stake. The top of the rain gauge was approximately 45 cm above the ground surface. The collection funnel of this gauge has an inside diameter of approximately 9.5 cm.

Lagoon liquid samples were collected from near the irrigation pump intake approximately every 2 hours during the day for a given set of tests. Once a test was completed the amount of captured liquid was determined by reading the rain gauges at the different sampling stations. Liquid from each sampling station was collected for analysis. All liquid samples were refrigerated and transported within 24 hours to the laboratory for analysis. Samples were analyzed for total solids, ammonia nitrogen, and pH. Ammonia was determined using a salicylate reaction modified for automated procedures (Technicon, 1973; US EPA, 1979).

The pH as the applied lagoon liquid was found to increase during irrigation. Total nitrogen losses occurring during sprinkler irrigation using the center pivot were found to range from 14.9% to 43.4%. Of this amount, 53.5-100% was accounted for in volumetric loss (evaporation). Ammonia-N losses occurring during sprinkler irrigation (center pivot) were found to range from 13.9% to 37.3%. Volumetric loss of the liquid during sprinkler irrigation accounted for 62.2-100% of the ammonia-N loss. The conditions during the center pivot tests and resulting ammonia losses are listed in Table 5.9.

Site Summary

A summary of the recent studies concerning volatilization losses during the irrigation process is presented in Table 5.10. The following factors have been identified as the main sources of variation: air temperature, relative humidity, irrigation pressure, and drop diameter (Pote et al., 1980; Brunke et al., 1988; Sharpe and Harper, 1997; Montes Chastain, 2000). The summary of volatilization losses, irrigation method and ammonia concentration of the irrigate effluent for the three previously discussed experiments is found in Table 5.5.

Table 5.9. Sprinkler and Atmospheric Conditions During Center Pivot Tests (Adapted from Safley et al., 1992)

Date	Test Number	Pivot Pressure (kPa)	Dry Bulb Temp	Relative Humidity (%)	Wind Speed (km/hr)
6/23/1987	1	365	28.0	80	0-16
	2	365	28.5	72	0-18
	3	365	31.0	67	0-16
	4	365	33.0	58	0-18
7/7/1987	1	379	30.0	70	0-4
	2	379	30.0	73	0-2
	3	379	34.0	63	0-10
	4	379	30.0	65	0-21
7/15/1987	1	376	24.5	82	0-14
	2	376	24.0	82	0-9
	3	376	23.0	85	0-5
	4	376	27.0	78	0-16

Table 5.10. Recent Studies of Volatilization Losses During Sprinkler Irrigation of Liquid Swine Manure.

Volatilization Loss (%)	Irrigation Method	Ammonia Loading Rate	Source
13.9-37.3	Center Pivot	299-327 mg/L	Safley et al (1992)
Negligible	Center Pivot	163 mg/L	Montes and Chastain (2000)

Model Validation

The model validation was completed using the data from the above detailed studies. Each set of data was used as the input parameters to the model. The percent volatilization predicted by the model was compared the observed percent recorded in the two studies.

Validation using data from Montes and Chastain (2000)

The prediction model was tested and validated using the two sites, Clarendon and Starkey, examined in the paper by Montes and Chastain (2000). The model input of initial concentration and outputs of final concentration and percent of ammonia volatilization for the Clarendon site are listed in Table 5.11. The values of the observed output and the resulting predicted model output for the Clarendon site are listed in Table 5.12. The total, mean, median, maximum, minimum and standard deviation values for the model outputs for the Clarendon site are contained in Table 5.13

Table 5.11. Model Output for Clarendon Site.

Date of Application	Initial Concentration (mg/L)	Final Concentration (mg/L)	Percent Volatilization (%)
07/27/1999	963	961.1309	0.1940956
07/27/1999	963	961.056	0.201866
07/27/1999	986	984.125	0.190218
11/06/1999	951	950.1174	0.0928
11/06/1999	923	922.123	0.0950111
11/06/1999	943	942.0832	0.097223
03/20/1999	1181	1180.897	0.0087134
03/20/1999	1325	1324.908	0.0069649
03/20/1999	1351	1350.856	0.0010454

Table 5.12. Observed Versus Predicted Ammonia Volatilization for Clarendon Site.

Date of Application	Observed Percent Volatilization (%)	Predicted Model Percent Volatilization (%)
07/27/1999	0	0.1940956
07/27/1999	0	0.201866
07/27/1999	0	0.190218
11/06/1999	0	0.0928
11/06/1999	0	0.0950111
11/06/1999	0	0.097223
03/20/1999	0	0.0087134
03/20/1999	0	0.0069649
03/20/1999	0	0.0010454

Table 5.13. Summary Statistics for Model Validation from Clarendon Site.

	Percent Ammonia Volatilization (%)	
	Observed	Model
TOTAL	0	0.887937
MEAN	0	0.09866
MIN	0	0.001045
MAX	0	0.201866
MEDIAN	0	0.095011
STD DEV	0	0.082325

Comparing the total volatilization observed to the total volatilization predicted, as well as the total, mean, and maximum values, the analysis indicates that the model over predicts volatilization for this Clarendon data set during this simulation period. The maximum deviation from the predicted data, however, is only 0.2%.

The model input of initial concentration and outputs of final concentration and percent of ammonia volatilization for the Starkey site are listed in Table 5.14. The values of the observed output and the resulting predicted model output for the Starkey site are listed in Table 5.15. The total, mean, median, maximum, minimum and standard deviation values for the model outputs for the Starkey site are contained in Table 5.16.

Comparing the total volatilization observed to the total volatilization predicted, the analysis indicates that the model again over predicts volatilization for this data set during this simulation period. It also appears from the total, mean and maximum values that the model over predicts ammonia volatilization. The maximum deviation from the predicted data, however, is only 0.35%.

Table 5.14. Model Output for Starkey Site.

Date of Application	Initial Concentration (mg/L)	Final Concentration (mg/L)	Percent Volatilization (%)
8/16/1999	189	188.7364	0.1394766
8/16/1999	184	183.7372	0.1428024
8/16/1999	181	180.7475	0.1394788
8/16/1999	220	219.6785	0.1461237
6/12/2000	154	153.5157	0.3144698
6/12/2000	139	138.5293	0.3386683
6/13/2000	166	165.711	0.1741065
6/13/2000	132	131.6552	0.2611912
6/14/2000	200	199.4492	0.2753983
6/14/2000	123	122.6552	0.2803399
6/14/2000	192	191.5107	0.254846
6/14/2000	153	152.5321	0.305834
6/14/2000	124	123.5575	0.3568219
6/15/2000	131	130.8621	0.10525

Table 5.15. Observed Versus Predicted Ammonia Volatilization for the Starkey site.

Date of Application	Observed Percent Volatilization (%)	Predicted Model Percent Volatilization (%)
8/16/1999	0	0.1394766
8/16/1999	0	0.1428024
8/16/1999	0	0.1394788
8/16/1999	0	0.1461237
6/12/2000	0	0.3144698
6/12/2000	0	0.3386683
6/13/2000	0	0.1741065
6/13/2000	0	0.2611912
6/14/2000	0	0.2753983
6/14/2000	0	0.2803399
6/14/2000	0	0.254846
6/14/2000	0	0.305834
6/14/2000	0	0.3568219
6/15/2000	0	0.10525

Table 5.16. Summary Statistics for Model Validation from Starkey Site.

	Percent Ammonia Volatilization (%)	
	Observed	Model
TOTAL	0	3.23807
MEAN	0	0.231058
MIN	0	0.10525
MAX	0	0.356822
MEDIAN	0	0.258019
STD DEV	0	0.086203

Validation using data from Safley et. al (1992)

The prediction model was tested and validated using the events evaluated by Safley, Barker and Westerman (1992). The model input of initial concentration and outputs of final concentration and percent of ammonia volatilization for the site are listed in Table 5.17. The values of the observed output and the resulting predicted model output for the Claredon site are listed in Table 5.18. The total, mean, median, maximum, minimum and standard deviation values for the model outputs for the Claredon site are contained in Table 5.19.

Table 5.17. Model Output for Data from Safley et. al (1992).

Date of Application	Test Number	Initial Concentration (mg/L)	Final Concentration (mg/L)	Percent Volatilization (%)
6/23/1987	1	269	268.8112	0.070179
	2	274	273.7233	0.10099
	3	283	282.6141	0.13636
	4	279	278.4611	0.193168
7/7/1987	1	313	312.6324	0.11744
	2	307	306.6755	0.1057
	3	328	327.4115	0.17942
	4	334	333.5424	0.13701
7/15/1987	1	244	243.8732	0.051955
	2	291	290.853	0.050506
	3	296	295.8823	0.03975
	4	303	302.7787	0.07305

Table 5.18. Observed Versus Predicted Ammonia Volatilization for the Data from Safley et. al (1992).

Date of Application		Observed Percent Volatilization (%)	Predicted Model Percent Volatilization (%)
6/23/1987	1	-	0.070179
	2	27.1	0.10099
	3	17.8	0.13636
	4	25.0	0.193168
7/7/1987	1	33.3	0.11744
	2	32.2	0.1057
	3	32.7	0.17942
	4	31.9	0.13701
7/15/1987	1	37.3	0.051955
	2	23.6	0.050506
	3	13.9	0.03975
	4	15.6	0.07305

Table 5.19. Summary Statistics for Model Validation from Safley et. al (1992) Data.

	Percent Ammonia Volatilization (%)	
	Observed	Model
TOTAL	290.4	1.255528
MEAN	26.4	0.104627
MIN	13.9	0.03975
MAX	37.3	0.193168
MEDIAN	27.1	0.103345
STD DEV	7.9192	0.050239

Comparing the total volatilization observed to the total volatilization predicted, as well as the total, mean and maximum values, the analysis indicates that the model greatly over predicts volatilization for this data set during this simulation period. Again, the reasons for this over-prediction may be related to ammonia measurement. In the field study, the time between sample collection and sample analysis is not given. During this lag time, ammonia would continue to volatilize. Therefore, the field study indicates these measurements were made during irrigation, when, in reality, these rates also include volatilization at some time period after irrigation was complete. This would account for a

reported larger observed percent volatilization. Another reason for the discrepancy between the observed and predicted data could be the wind speed at the test site. This data set does not comply with the model assumption that the wind speed is less than 5 m/s. These greater wind speeds could cause significant wind drift from the test sight, resulting in larger volatilization rates.

After completing the initial evaluation of this data set, the model was optimized to predict the same volatilization rates as this data set. In order to accomplish this, however, the diffusivity parameter had to be changed to a value over 1000 times greater than the initial value. This required change is unreasonable and unrealistic. This leads to the conclusion that the model parameters are correct, and the discrepancy in the data must be due to some other phenomenon, such as the measurement method and effects of wind drift discussed previously.

Sensitivity Analysis

In order to identify the input parameters that have the most impact on model outputs, a sensitivity analysis was done. Two types of sensitivity parameters were calculated, absolute sensitivity, S , and relative sensitivity, S_r . S gives the absolute change in output for a unit change in an input parameter, while S_r gives the percent change in output for a 1% change in input parameter. Numerically these values can be calculated by (Haan, 1995):

$$S = \frac{O_2 - O_1}{P_2 - P_1} \quad (5.1)$$

$$S_r = \frac{O_2 - O_1}{P_2 - P_1} \frac{P}{O} \quad (5.2)$$

where O and P represent the particular model output and input parameters, respectively.

In this case each model input parameter, P , was increased by 10% to obtain P_2 , and decreased by 10% to obtain P_1 . The model was run once with model inputs, P , to get base values for O . The model was again run by varying one parameter at time, holding all others parameters at their base values. O_1 and O_2 values were outputs associated with P_1 and P_2 input parameters, respectively. After all of the model runs were complete, S and S_r values were computed for each output value at a particular input parameter. The sensitivity results are presented in Table 5.20.

Any parameter with an S_r value greater than or equal to 0.01 was considered to have a significant effect on the output parameters. It appears from the sensitivity analysis that the TEMPF value, air temperature, has the most effect on the volatilization of ammonia. The importance of temperature is expected because the water droplet evaporation and ammonia volatilization is dependent of the diffusion of both water molecules and ammonia away from the drop, and the transfer of heat by conduction and convection into the droplet to sustain the evaporative and volatilization processes. The effect of temperature on the volatilization process is illustrated in Figure 5.3. This is the data from the Claredon site in the paper by Montes and Chastain (2000). The data that is closely clustered together is evaluated at the same temperature. A change in temperature shows a profound change in ammonia volatilization percentage.

The sensitivity analysis also indicates which parameters have little or no effect on the output values. The sprinkler system pressure (P) appears to have not effect on the percent of ammonia volatilized. The relative humidity (RH), and initial concentration of ammonia in irrigate (INITCONC) also appear to have very little effect on the model output.

Table 5.20. Sensitivity Analysis Results

Parameter	Input Parameters			Output Parameters			Sensitivity	Relative Sensitivity
	P	P ₁	P ₂	O	O ₁	O ₂	S	S _r
P	25	22.5	27.5	0.162983	0.165996	0.159122	-0.0013749	-0.2108961
TEMPF	80	72	88	0.162983	0.129754	0.207867	0.00488203	2.39633741
RH	50	45	55	0.162983	0.179289	0.146684	-0.0032606	-1.0002786
ELEV	1000	900	1100	0.162983	0.161024	0.164981	1.9788E-05	0.12141136
INITCONC	950	855	1045	0.162983	0.162989	0.16299	6.8421E-09	3.9881E-05

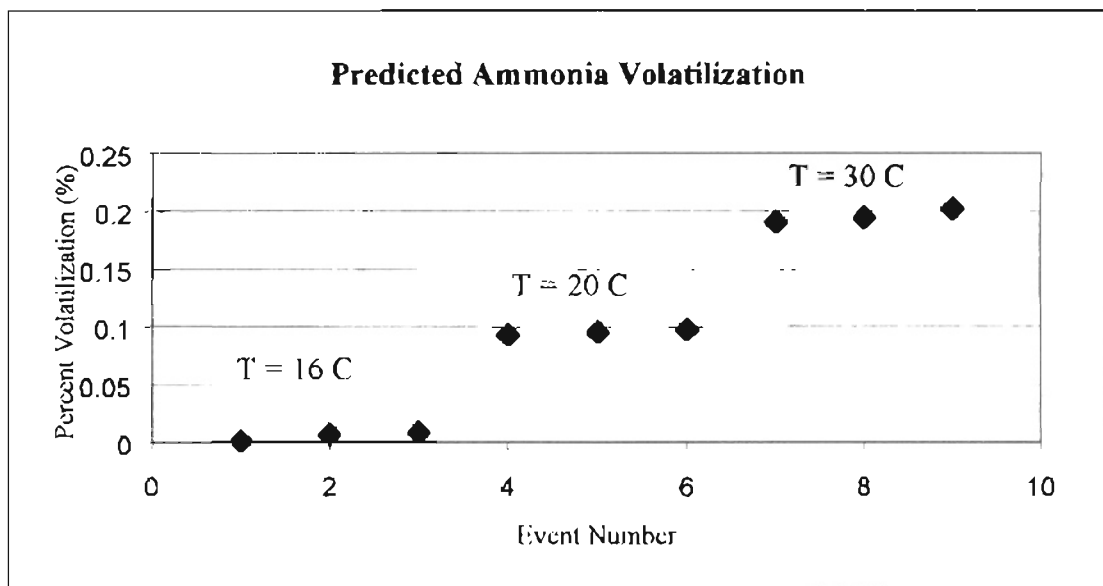


Figure 5.3. Temperature Effect on Ammonia Volatilization

Validation Results

The results from both sets of data reinforce the literature that there are many parameters that affect the rate and percent of ammonia volatilization. The following factors have been identified as the main sources of variation in the literature and reinforced in this paper: air temperature, relative humidity, and irrigation pressure (Pote

et al., 1980; Brunke et al., 1988; Sharpe and Harper, 1997; Montes Chastain, 2000). As shown in the sensitivity analysis, air temperature appears to have the most effect on ammonia volatilization, with relative humidity having a secondary effect.

When evaluating the data from Montes and Chastain (2000), the model overestimated the percentage of ammonia volatilization. Again, this could be the result of parameter problems within the model; inaccurate measurement results from the observed data, or a combination of both. The model's overestimation, however, was very small, with a maximum value of 0.3%. The conclusions made by Montes and Chastain (2000) stated that the volatilization during irrigation did not differ from zero, but were not equal to zero. These results may be due to the measurement techniques used in the study. The method may not have been able to detect a small change in concentration, as predicted by the model. This data set fit well with the required input parameters of the model. There were no assumptions as to input parameter values. Again, the volatilization dependence on temperature is well illustrated with this data set (Figure 5.3). The model does an acceptable job of predicting ammonia volatilization based on the data of Montes and Chastain (2000).

In the case of Safley, Barker and Westerman (1992), the model greatly overestimated the percentage of ammonia volatilization. Again, this could be the result of parameter problems within the model; inaccurate measurement results from the observed data, or a combination of both. The reasons for this under-prediction may be directly related to ammonia measurement. In the field study, the time between sample collection and sample analysis is given as a maximum of 24 hours. During this lag time, ammonia would continue to volatilize. Therefore, the field study indicates these measurements

were made during irrigation, when, in reality, these rates also include volatilization at some time period after irrigation was complete. This would account for a reported larger observed percent volatilization than the percent predicted by the model. Again, the data set did not comply with the model assumption that wind speeds were below the required 5 m/s. The larger wind speeds result in drift of droplets and therefore a larger volatilization rate. Although the model greatly over predicts the percent volatilization, the data does support the model's sensitivity analysis predicting that the air temperature has the greatest effect on ammonia volatilization. Increases in temperature directly produced higher volatilization percents.

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

Conclusions

This evidence indicates that the model is a fair representation of what is happening in the real world. This model does an acceptable job of predicting ammonia volatilization for the data of Montes and Chastain (2000). For the data from Safley et. al (1992), the model did not accurately predict the observed values. The data did, however, support the dependence of ammonia volatilization on air temperature. This first generation model indicates that ammonia volatilization from falling drops during irrigation may be of little importance when compared to other ammonia sources.

Recommendations for Further Research

Validating the model with only two data sets yielded limited information. It is desirable to validate the model with a variety of data sets for a variety of conditions. In particular, data sets from areas where application practices are similar under similar conditions would provide more detailed answers in the processes that are occurring. The measurement techniques also need to be replicated. The accurate measurement of ammonia during irrigation requires immediate analysis of collected samples, or a method to preserve the ammonia in the liquid.

The effect of wind speed on wind drift and ammonia volatilization needs to be further examined. The model can be modified to include droplets that would fail to fall to the ground based on the droplet size distribution and test site wind speed. The inclusion of wind drift would more accurately describe the phenomenon of ammonia volatilization during irrigation of swine lagoon effluent.

Although ammonia volatilization during irrigation is an important phenomenon, in order to accurately determine the source of ammonia from a swine production facility, ammonia volatilization after irrigation from surface ponding should be evaluated. The evapotranspiration from crop canopy and its effect on ammonia volatilization should also be studied. These components combined together should give an accurate estimate of total ammonia volatilization resulting from land application of swine lagoon effluent.

Once the entire land application process has been completed, ammonia volatilization from swine building facilities and treatment processes should be added to the model. This would allow a producer to predict ammonia volatilization and resulting mass concentration release from his or her facility at any given time. This information would prove beneficial not only to the producers, but also to neighboring communities that often complain about such odor. A producer would be able to predict the times at which ammonia levels may be high and compromise with neighboring communities regarding such issues as the time and length of land application.

There are over 160 known compounds in swine manure. It would prove beneficial to determine the volatilization rates of other compounds along with ammonia. Ammonia is a highly volatile compound and incorporating medium-range and low volatility compounds in a second-generation model would allow a more accurate

prediction of total odor generation, emission and dispersion. Validation of these model additions would play a vital role in the overall acceptance and accuracy of the second-generation model.

BIBLIOGRAPHY

- Al-Kaisi, Mahdi. 1997. Liquid Manure Application. Colorado State University Golden Plains Area Cooperative Extension. Colorado State University. <http://www.colostate.edu/Depts/CoopExt/GPA/guideln.htm>
- Al-Kaisi, Mahdi. 1998. Guidelines for Manure Land Application. Colorado State University Golden Plains Area Cooperative Extension. Colorado State University. <http://www.colostate.edu/Depts/CoopExt/GPA/manure.htm>
- ASAE. 1996. Control of Manure Odors, ASAE Standard EP379.1. ASAE. St. Joseph, MI, USA.
- Beauchamp, E.G., G.E. Kidd, and G. Thurtell. 1978. Ammonia Volatilization from Sewage Sludge Applied in the Field. *Journal of Environmental Quality* 7(1): 141-146.
- Beauchamp, E.G., G.E. Kidd, and G. Thurtell. 1982. Ammonia Volatilization from Liquid Dairy Cattle Manure in the Field. *Canadian Journal of Soil Science* 62:11-19.
- Bezdek, J.C. and K.H. Solomon. 1983. Upper Limit Lognormal Distribution for Drop Size Data. *Journal of Irrigation and Drainage Engineering* 109(1): 72-88.
- Bilanski, W.K. and E.H. Kidder. 1958. Factors that Affect the Distribution of Water from a Medium-Pressure Rotary Irrigation Sprinkler. *Transactions of the ASAE* 1(1): 19-28.
- Brunke, R., P. Alvo, P. Schuepp, and R. Gordon. 1988. Effect of Meteorological Parameters on Ammonia Loss from Manure in the Field. *Journal of Environmental Quality* 17:431-436.
- Campbell, A.J., J.A. MacLeod, and C. Stewart. 1997. Nutrient Characterization of Stored Liquid Hog Manure. *Canadian Agricultural Engineering* 39(1): 43-48.
- Campbell, Neil A. 1990. *Biology, Second Edition*. The Benjamin/Cummings Publishing Company, Inc. Fort Collins, Colorado. Pp. 1011-1044.

- Carney, P.G. and V.A. Dodd. 1989. A Comparison Between Predicted and Measured Values for the Dispersion of Malodours From Slurry. *Agricultural Engineering Research* 44:67-76.
- Chapra, Steven C. and Raymond P. Canale. 1988. *Numerical Methods for Engineers: Second Edition*. McGraw-Hill Publishing Company, New York, New York. Pp. 569-609, 611-617.
- Denmead, O.T. and M.R. Raupach. 1993. Methods for Measuring Atmospheric Gas Transport in Agricultural and Forest Systems. *Agricultural Ecosystem Effect on Trace Gases and Global Climatic Change*. ASA Special Publication no. 55, p. 19-43.
- Denmead, O.T., J.R. Simpson, and J.R. Freney. 1977. A Direct Field Measurement of Ammonia Emission After Injection of Anhydrous Ammonia. *Soil Science Society of America Journal* 41:1001-1004.
- Edling, R.J. 1985. Kinetic Energy, Evaporation, and Wind Drift of Droplets From Low Pressure Irrigation Nozzles. *Transactions of the ASAE* 28(5): 1543-1550.
- Engen, T. and G.D. Mower. 1977. Influence of Internal Factors on the Perceived Intensity and Pleasantness of Gustatory and Olfactory Stimuli. In: *The Chemical Senses and Nutrition*. M.R. Kare and O. Maller, eds. Pp. 103-121.
- Ernst, J.W. and H.F. Massey. 1960. The Effect of Several Factors on Ammonia Volatilization of Ammonia Formed from Urea in the Soil. *Soil Science Society of America Proceedings* 24:87-90.
- Evans, Robert and R.E. Sneed. 1996a. Selection and Management of Efficient Center-pivot and Linear Mover Irrigation Systems. *North Carolina Cooperative Extension Service Publication Number EBAE-91-151*. North Carolina State University.
- Evans, Robert and R.E. Sneed. 1996b. Selection and Management of Efficient Hand-Move, Solid-Set and Permanent Sprinkler Irrigation Systems. *North Carolina Cooperative Extension Service Publication Number EBAE-91-150*. North Carolina State University.
- Evans, Robert and R.E. Sneed. 1996c. Selection and Management of Efficient Self-Propelled Gun Traveler Irrigation Systems. *North Carolina Cooperative Extension Service Publication Number: EBAE-91-150*. North Carolina State University.
- Faurie, G. and R. Bardin. 1979a. La volatilization de l'ammoniac: I. Influence de la nature du sol et des composés azotés. *Annual Agronomy* 30:363-385.

- Faurie, G. and R. Bardin. 1979b. La volatilisation de l'ammoniac: II Influence des facteurs climatiques et du couvert vegetal. *Annual Agronomy* 30:502-414.
- Forsythe, George E., Michael A. Malcolm, and Cleve B. Moler. 1977. *Computer Methods for Mathematical Computations*. Prentice-Hall, Inc. Englewood Cliffs, New Jersey. Pp. 127-148.
- Fulhage, Charles D. 1993. *Gases and Odors from Swine Wastes*. University of Missouri Extension Guide Sheet G1880. Missouri Cooperative Extension Service. University of Missouri-Columbia.
- Genermont, S. and P. Cellier. 1997. A Mechanistic Model for Estimating Ammonia Volatilization from Slurry Applied to Bare Soil. *Agricultural and Forest Meteorology* 88:145-167.
- Gerald, Curtis F. and Patrick O. Wheatly. 1994. *Applied Numerical Analysis: Fifth Edition*. Addison-Wesley Publishing Company, Reading, Massachusetts. Pp. 403-409, 434, 443.
- Goering, C.E., L.E. Bode, and M.R. Gebhardt. 1972. Mathematical Modeling of Spray Droplet Deceleration and Evaporation. *Transactions of the ASAE* 15(2):220-225.
- Gordon, R., M. Leclerc, P. Schuepp, and R. Brunke. 1988. Field Estimates of Ammonia Volatilization from Swine Manure by a Simple Micrometeorological Technique. *Canadian Journal of Soil Science* 68: 369-380.
- Green, R.L. 1952. Evaluation of Air Resistance to Freely Falling Drops of Water. *Agricultural Engineering* 33(1): 28; Ammended 33(5): 286.
- Haan, C.T. 1995. "Evaluation of Uncertainty in Hydrologic and Water Quality Models." A Workshop Presented tot he South Florida Water Management District, West Palm Beach, FL.
- Hamilton, Douglas W. 1996. *What is a Waste Management System?* Oklahoma State University Extension Facts F-1734. Oklahoma Cooperative Extension Service. Oklahoma State University.
- Hargrove, W.L. 1988. Evaluation of Ammonia Volatilization in the Field. *Journal of Process Agriculture* 1:104-111.
- Hargrove, W.L. and D.E. Kissel. 1979. Ammonia Volatilization from Surface Applications of Urea in the Field and Laboratory. *Soil Science Society of America Journal* 43:359-363.

- Heber, A.J. 1997. Setbacks for Sufficient Swine Odor Dispersion and Dilution. Presented at the Livestock and Environment Symposium, University of Nebraska Cooperative Extension Service, New World Inn, Columbus, Nebraska, December 10-11.
- Hobbs, P.J., T.H. Misselbrook, and B.F. Pain. 1995. Assessment of Odours from Livestock Wastes by a Photoionization Detector, an Electronic Nose, Olfactometry, and Gas Chromatography-Mass Spectrometry. *Journal of Agricultural Engineering Research* 60:137-148.
- Hobbs, P.J., T.H. Misselbrook, and B.F. Pain. 1997. Characterisation of Odours and Emissions from Slurries Produced from Weaner Pigs Fed Dry Feed and Liquid Diets. *Journal of Science, Food and Agriculture* 73:437-446.
- Hoff, J.D., D. Nelson, and A.L. Sutton. 1981. Ammonia Volatilization from Liquid Swine Manure Applied to Cropland. *Journal of Environmental Quality* 10(1): 90-95.
- Hutchinson, G.L., R.J. Millington, and D.B. Peters. 1972. Atmospheric Ammonia: Absorption by Plant Leaves. *Science* 175:771-772.
- Jacobs, P. 1994. Odour Control Guidelines for Livestock Operators. Final Report to: Canada/Nova Scotia Agreement on the Agricultural Component of the Green Plan. 15 p.
- Jarvis, S.C. and B.F. Pain. 1990. Ammonia Volatilisation from Agricultural Land. *Proceedings of the Fertilizer Society, Peterborough, No. 298, 35 p.*
- Jensen, M.E. 1983. Design and Operation of Farm Irrigation Systems. ASAE Monograph No. 3. ASAE, 2950 Niles Road, St. Joseph, MI 49085-9659, USA.
- Johnson, Jay and Don Eckert. 1997. Best Management Practices: Land Application of Animal Manure. The Ohio State University Extension AGF-208-95. Ohio State Cooperative Extension Service. Ohio State University.
- Jongbloed, A.W. and N.P. Lenis. 1998. Environmental Concerns About Animal Manure. *Journal of Animal Science* 76:2641-2648.
- Katz, P.E. 1996. Ammoniakemissionen nach der Gullenwendung auf Grunland. These ETH Zurich, 71 p.
- Kincaid, D.C. 1989. Volumetric Water Drop Evaporation Measurement. *Transactions of the ASAE* 32(2): 925-927.
- Kincaid, D.C. and T.S. Longley. 1989. A Water Droplet Evaporation and Temperature Model. *Transactions of the ASAE* 32(2): 457-463.

- Klausner, S.D., A.C. Mathers, and A.L. Sutton. 1984. *Managing Animal Manure as a Source of Plant Nutrients*. Cooperative Extension Service of Purdue University Publication NCH-12. Purdue University.
- Kobayashi, M. and M. Kobayashi. 1995. *Waste Remediation and Treatment Using Anoxygenic Phototrophic Bacteria*. P.1269-1282. In: R.E. Blankenship et al. (ed.) *Anoxygenic Photosynthetic Bacteria*. Kluwer Academic Publ., Boston, MA
- Kohl, R.A. 1974. *Drop Size Distribution from Medium-Sized Agricultural Sprinklers*. Transactions of the ASAE 17(4): 690-693.
- Kranz, William. 1998. *Selecting Sprinkler Packages for Center Pivots*. Cooperative Extension Publication Number G88-870-A. Nebraska Cooperative Extension Service. University of Nebraska-Lincoln.
- Laws, J.O. 1941. *Measurement of Fall Velocity of Water Drops and Raindrops*. Transactions of the American Geophys. Un. 22:709-721.
- List, R.J. 1966. *Smithsonian Meteorological Tables*, Smithsonian Misc. Collections, Vol. 11. Washington DC: Smithsonian Institute.
- Lockyer, D.R. 1984. *A System for the Measurement in the Field of Losses of Ammonia Through Volatilization*. Journal of Science, Food and Agriculture 35:837-848.
- Lockyer, D.R., B.F. Pain, and J.V. Klarenbeek. 1989. *Ammonia Emissions from Cattle, Pig and Poultry Wastes Applied to Pasture*. Environmental Pollution 56:19-30.
- Mackie, Roderick I., Peter G. Stroot, and Vincent H. Varel. 1998. *Biochemical Identification and Biological Origin of Key Odor Components in Livestock Waste*. Journal of Animal Science 76:1331-1342.
- Marshall, W.R., Jr. 1954. *Atomization and Spray Drying*. Chemical Engineering Progress Monograph Series No. 2, Vol. 50. American Institute of Chemical Engineers, New York.
- McFarland, Anne and Nancy Easterling. 1995. *Odor Intensity and Offensiveness as Affected by Familiarity and Preference*. Texas Institute for Applied Environmental Research, Tarleton State University, Stephenville, Texas. 8 p.
- McLeod, A.R., M.R. Holland, P.J. Shaw, P.M. Sutherland, N.M. Darrall, and R.A. Skeffington. 1990. *Enhancement of Nitrogen Deposition to Forest Trees Exposed to Sulfur Dioxide*. Nature (London) 347:277-279.
- Minor, J. Ronald. 1995. *A Review of Literature on the Nature and Control of Odors From Pork Production Facilities*. Executive Summary for the Odor Subcommittee

of Environmental Committee of the National Pork Producers Council, Des Moines, Iowa.

- Minor, J.R. and T.E. Hazen. 1969. Ammonia and Amines: Components of Swine-Building Odor. *Transaction of the ASAE* 12(2):772-774.
- Moal, J.F., J. Martinex, F. Guiziuo, and C.M Coste. 1995. Ammonia Volatilization Following Surface-Applied Pig and Cattle Slurry in France. *Journal of Agricultural Science* 125:245-252.
- Montes, Felipe and J.P. Chastain. 2000. Ammonia Volatilization Losses During Irrigation of Liquid Manure in Commercial Forestland and Open Field Conditions. Presented at the Annual International Meeting of ASAE. Paper No. 004021. ASAE, 2950 Niles Road, St. Joseph, MI 49085-9659 USA.
- Muehling, A.J. 1969. Swine Housing and Waste Management. Department of Agricultural Engineering, College of Agriculture, University of Illinois at Champaign-Urbana.
- Mugele, R.A. and H.D. Evans. 1951. Droplet Size Distribution in Sprays. *Ind. And Engr. Chrm.* 43(6): 1317-1324.
- National Pork Producers Council (NPPC). 2000. 1999-2000 Pork Facts. Des Moines, Iowa, USA. 28 p.
- Nihlgard, B. 1985. The Ammonium Hypothesis: An Additional Explanation to the Forest Dieback in Europe. *Ambio* 14:2-6.
- Oltjen, J.W. and J.L. Beckett. 1995. Role of Ruminant Livestock in Sustainable Agricultural Systems. Presented at a Symposium title "Toward Sustainability: Animal Agriculture in the Twenty-First Centree" at the ASAS 86th Annual Meeting, Minneapolis, MN.
- Orr, C., Jr. 1966. *Particulate Technology*. The Macmillan Company, New York. 562 p.
- Pain, B.F. 1994. Odour Nuisance From Livestock Production Systems. In: *Pollution in Livestock Production Systems*, ed. I Ap Dewi, RFE CAB International, Wallingford, UK.
- Pain, B.F., V.R. Phillips, C.R. Clarkson, and J.V. Klarenbeek. 1989. Loss of Nitrogen Through Volatilization During and Following the Application of Pig or Cattle Slurry to Grassland. *Journal of Science, Food and Agriculture* 47:1-12.
- Pain, B.F., T.H. Misselbrook, C.R. Clarkson, and Y.J. Rees. 1990a. Odour and Ammonia Emissions Following the Spreading of Aerobically-Treated Pig Slurry on Grassland. *Biological Wastes* 34:259-267.

- Pain, B.F., V.R. Phillips, C.R. Clarkson, T.H. Misselbrook, Y.J. Rees, and J.W. Farrent. 1990b. Odour and Ammonia Emissions Following the Spreading of Anaerobically-Treated Pig Slurry on Grassland. *Biological Wastes* 34:149-160.
- Pain, B.F., C.R. Clarkson, V.R. Phillips, J.V. Klarenbeek, T.H. Misselbrook, and M. Bruins. 1991. Odour Emission Arising From Application of Livestock Slurries on Land: Measurements Following Spreading Using a Micrometeorological Technique and Olfactometry. *Agricultural Engineering Research* 48:101-110.
- Pote, J.W., J.R. Miner, and J.K. Koelliker. 1980. Ammonia Losses During Sprinkler Application of Animal Wastes. *Transactions of the ASAE* 23(5): 1202-1206.
- Ranz, W.E. and W.R. Marshall Jr. 1952a. Evaporation from Drops, Part I. *Chemical Engineering Progress* 48(3): 141-146.
- Ranz, W.E. and W.R. Marshall Jr. 1952b. Evaporation from Drops, Part II. *Chemical Engineering Progress* 48(4): 173-180.
- Safley, L.M., Jr., M.E. Casanda, J.W. Woodbury, and K.F. Roos. 1992a. Global Methane Emissions from Livestock and Poultry Manure. U.S. Environmental Protection Agency. Washington D.C.
- Safley, L.M., Jr., J.C. Barker, and P.W. Westerman. 1992b. Loss of Nitrogen During Sprinkler Irrigation of Swine Lagoon Liquid. *Bioresource Technology* 40:7-15.
- Schmidt, David and Larry D. Jacobsen. 1995. Odor and Odor Policy Criteria. University of Minnesota Extension Service Publication Number AEU-11. University of Minnesota Cooperative Extension Service. University Of Minnesota.
- Schmitt, Michael and George Rehm. 1998. Fertilizing Cropland With Swine Manure. University of Minnesota Extension Service Publication Number FO-5879-GO. University of Minnesota Cooperative Extension Service. University of Minnesota.
- Sharpe, R.R. and L.A. Harper. 1997. Ammonia and Nitrous Oxide Emissions from Sprinkler Irrigation Applications of Swine Effluent. *Journal of Environmental Quality* 26:1703-1706.
- Seginer, I. 1965. Tangential Velocity of Sprinkler Drops. *Transactions of the ASAE* 8(1): 90-93.
- Sievers, D.M. and E.L. Iannotti. 1982. Anaerobic Processes for Stabilization and Gas Production. In: R.J. Smith (ed.) *Research Results in Manure digestion, Runoff, Refeeding, Odors*. North Central Regional Res. Publ. 284. North Central Regional Res., Ames, IA. Pp. 1-10.

- Solomon, K.S. and R.D. von Bernuth. 1981. Droplet Size and Runoff Study, Consultant Report to Rain Bird Western Sales Corporation. VON-SOL, Claremont, CA.
- Sommer, S.G., J.E. Olesen, B.T. Christensen. 1991. Effects of Temperature, Wind Speed and Air Humidity on Ammonia Volatilization from Surface Applied Cattle Slurry. *Journal of Agricultural Science* 117:91-100.
- Smith, R.J. 1993. Dispersion of Odours From Ground Level Agricultural Sources. *Agricultural Engineering Research* 54:187-200.
- Sutton, M.A., D.S. Lee, G.J. Dollard, and D. Fowler. 1998. Atmospheric Ammonia: Emission, Deposition, and Environmental Impacts. Proceedings of the International Conference on Atmospheric Ammonia: Emissions, Deposition and Environmental Impacts. Culham, Oxford, UK. 2-4 October 1995, *Atmospheric Environment* 32(3): 269-271.
- Sweeten, J.M. 1992. Livestock and Poultry Waste Management: A National Overview. In: J. Blake et al. (ed.) *National Livestock, Poultry and Aquaculture Waste Management*. ASAE Publication 03-92. ASAE. St. Joseph, MI.
- Sweeten, John M. and J. Ronald Minor. 1993. Odor Intensities at Cattle Feedlots in Nuisance Litigation. *Bioresource Technology* 45:177-188.
- Sweeten, John M. and Maritza Rodriguez-Akabani. 1994. Approaches to Odor Measurement for Dairies and Cattle Feedlots: A State of the Art Review. Prepared for: Texas National Resource Conservation Commission, Office of Air Quality. Austin, Tx. 104 p.
- Technicon. 1973. Technicon Industrial Methods for the Examination of Water and Wastewater Treatment. *Technical Services Bulletin*. Piscataway, New Jersey.
- Terman, G.L. 1979. Volatilization Losses of Nitrogen as Ammonia from Surface Applied Fertilizers, Organic Amendments, and Crop Residues. *Advanced Agronomy* 31:189-223.
- Thompson, R.B., J.C. Ryden, and D.R. Lockyer. 1987. Fate of Nitrogen in Cattle Slurry Following Surface Application or Injection to Grassland. *Journal of Soil Science* 38:689-700.
- Thompson, A.L., D.L. Martin, J.M. Norman, J.A. Tolk, T.A. Howell, J.R. Gilley, and A.D. Schneider. 1997. Testing of a Water Loss Distribution Model for Moving Sprinkler Systems. *Transactions of the ASAE* 40(1): 81-88.
- Thompson, A.L., J.R. Gilley, and J.M. Norman. 1993a. A Sprinkler Water Droplet Evaporation and Plant Canopy Model: I. Model Development. *Transactions of the ASAE* 36(3) 735-741.

- Thompson, A.L., J.R. Gilley, and J.M. Norman. 1993b. A Sprinkler Water Droplet Evaporation and Plant Canopy Model: II. Model Application. *Transactions of the ASAE* 36(3): 743-750.
- Thompson, A.L., D.L. Martin, J.M. Norman, J.R. Gilley, and T.A. Howell. 1994. Modeling Water Losses for Moving Sprinkler Systems. ASAE Paper No., 94-2174, ASAE, St. Joseph, MI 49085.
- United States Department of Agriculture (USDA). 1996. Animal and Plant Health Inspection Service. Environmental Practices/Management by U.S. Pork Producers. Centers for Epidemiology and Animal Health, Fort Collins, Colorado, USA.
- United States Environmental Protection Agency (US EPA). 1973. Methods for Chemical Analysis of Water and Wastes, EPA 600-4-79-020. Environmental Monitoring and Support Lab, US EPA, Cincinnati, OH.
- Van Hove, L.W.A., A.J. Kooops, E.H. Adema, W.J. Vredenberg, and G.A. Pieters. 1987. Analysis of the Uptake of Atmospheric Ammonia by Leaves of *Phaseolus vulgaris*. *Atmospheric Environment* 21:1759-1763.
- von Bernouth, R.D. and J.R. Gilley. 1984. Sprinkler Droplet Size Distribution Estimation from a Single Leg Test Data. *Transactions of the ASAE* 27(5): 1435-1441.
- Wark, Kenneth, Cecil F. Warner, and Wayne T. Davis. 1998. Air Pollution: Its Origin and Control. Addison-Wesley Longman, Inc. Menlo Park, California.
- Weier, K.L., V.R. Catchpole, and L.A. Harper. 1980. An Automated Colorimetric Method for the Determination of Small Concentrations of Ammonia in Air. CSIRO Division of Tropical Crops and Pastures. *Agron. Tech. Mem.* 20.
- Westerman, P.W., J.C. Burns, L.D. King, M.R. Overcash, and R.O. Evans. 1982. Swine Lagoon Effluent Applied to Coastal Bermuda Grass. Final Report of the EPA Project R-804608 USEPA.
- Williams, C. Mike, James C. Barker, Robert W. Bottcher, David F. Caldwell, John J. Classen, Kenneth L. Esbenshade, Thomas J. Hoban, Frank J. Humenik, Patrick Knowlson, Kurt Edward Parbst, Susan S. Schiffman, Philip W. Westerman, and Kelly D. Zering. 1998. Control of Odor Emissions from Animal Operations: A Report from the Board of Governors of the University of North Carolina. North Carolina Agricultural Research Service, College of Agriculture and Life Sciences, North Carolina State University.

- Williamson, Robert E. and E. Dale Threadgill. 1974. A Simulation for the Dynamics of Evaporating Spray Droplets in Agricultural Spraying. *Transactions of the ASAE* 17(2): 254-261.
- Wilson, J.D., G.W. Thurtell, G.E. Kidd, and E.G. Beauchamp. 1981. Estimation of the Rate of Gaseous Mass Transfer From a Surface Source Plot to the Atmosphere. *Atmospheric Environment* 16(8): 1861-1867.
- Yonts, C. Dean, Norman L. Klocke, William L. Kranz, Derrel L. Martin, and Kelly Wertz. 1997a. Water Loss From Above-Canopy and In-Canopy Sprinklers. Cooperative Extension Publication G97-1328-A. Nebraska Cooperative Extension Service. University of Nebraska-Lincoln.
- Yonts, C. Dean, Norman L. Klocke, William L. Kranz, Derrel L. Martin, and Kelly Wertz. 1997b. Application Uniformity of In-Canopy Srinklers. Cooperative Extension Publication G97-1328-A. Nebraska Cooperative Extension Service. University of Nebraska-Lincoln.
- Zahn, J.A., J.L. Hatfield, Y.S. Do, A.A. DiSpirito, K.A. Laird, and R.L. Pfeiffer. 1997. Characterization of Volatile Organic Emissions and Wastes from a Swine Production Facility. *Journal of Environmental Quality* 26:1687-1696

APPENDICIES

APPENDIX A

AMMONIA VOLATILIZATION FORTRAN CODE

```
C PROGRAM LANDAPP - 5/1/01
C
C*****
C
C PROGRAM LANDAPP
C
C
C*** PROGRAM DESCRIPTION
C
C This program will predict the generation rate and mass
C concentrations of ammonia released during the land
C application of swine lagoon effluent. The program requires
C user input parameters relating to irrigation application
C methods, atmospheric conditions and characteristics, ammonia
C properties and simulation specific variables. The program
C then calculates the resulting water droplet evaporation and
C volatilization of ammonia. The output parameters include
C initial and final droplet diameters, total effluent ir-
C rigated, initial ammonia concentration, and concentration of
C ammonia volatilization.
C
C*** GLOSSARY OF VARIABLES
C
C T = Time, seconds
C H = Step size used in time iteration loop
C ZDOT = Dummy variables used in Subroutine RK45TRAJ
C NEQN = Number of equations to be solved, 1 in this case
C VZ = Velocity of droplets, m/s, in z-direction
C VZNEW = Velocity of droplets, m/s, in z-direction, calculated by
C subroutine
C ERROR = The error calculated in Subroutine RK45TRAJ
C NITER = The number of iterations the DO LOOP will run
C C = coefficient dependent upon type of sprinkler system used
C CL = The initial ammonia concentration in the liquid in
C one nozzle or sprinkler, mg/L
```

```

C TOTALCL = The total concentration of ammonia in the entire volume
C   of effluent irrigate, mg/L
C NOZZ = Type of nozzle used, impact or spray
C NOZZD = Diameter of the nozzle used, m
C NSPRIN = Number of sprinklers on the pivot system
C NSAMP = Number of droplet diameters per nozzle which will be
C   evaluated
C   P = Sprinkler pressure, psi
C MPRESS = Sprinkler pressure, kPa
C DELTAD = Change in diameter used in the droplet distribution, m
C MIND = Minimum droplet diameter, m
C   D = Droplet Diameter, m
C PERC = Percent of ammonia volatilized during irrigation, %
C TEMPF = Temperature of the air, F
C TEMPK = Temperature of the air, K
C TEMPC = Temperature of the air, C
C TEMPWM = Wet bulb temperature of the air, F
C   RH = Relative Humidity, %
C VISC = Viscosity of the water,
C ADENS = Density of the air, kg/m^3
C DRDENS = Density of the droplet, kg/m^3
C KDROP = Diffusivity of the water droplet, m^2/s
C   RE = Reynold's number for the drop, dimensionless
C SCDROP = Schmidt's number for the drop, dimensionless
C   SH = Sherwood number for the drop, dimensionless
C ELEV = Elevation of the test site, m
C   PA = Atmospheric pressure, atm
C   MV = Molecular weight of the diffusing water vapor, g/mole
C   MA = Mean molecular weight of the gas mixture, g/mole
C NEWDROP = New droplet diameter, m
C   D = Droplet diameter, m
C CONST = Dummy variable used in this subroutine
C   PV = Saturated vapor pressure of droplet at droplet
C   temperature, mb
C   PS = Vapor pressure of ambient air, mb
C
C*** SUBROUTINES CALLED
C
C   SUBROUTINE RK45TRAJ
C   SUBROUTINE RK45DROP
C   SUBROUTINE RK45CONC
C
C*** DECLARATION OF VARIABLES

REAL T, H, C, P, MPRES
REAL VZ(1), VZNEW(1), ERROR(1), ZDOT(1), TOTALCL

```



```

INTEGER NITER, NOZZ, NSPRINK, NSAMP
COMMON MIND, PERC, HAMM, NEWDROP(1)
C
REAL TEMPF, TEMPK, VISC, ADENS, DRDENS, KDROP, RE, SC, SHODOR
REAL INDROP(1), ELEV, PA, MV, MA, PV, PS
REAL CONST, DDOT(1)
C
REAL VISODOR, KODOR, REODOR, SCODOR
REAL NEWDROP, INITCONC(1), CONST2, CDOT(1), NEWCL(1)
C
C   An output file is opened to store results
C
OPEN(UNIT = 10, FILE='LANDAPP.OUT', STATUS = 'UNKNOWN')
C
C   The following lines of the program allow the user to dictate
C   the system pressure.
C
PRINT*, 'INPUT SPRINKLER PRESSURE (psi) '
READ*, P
MPRES = P*6.895001
C
C   The following lines of the program allow the user to dictate
C   the type of nozzle system used, either spray or impact
C
PRINT*, 'PLEASE DICTATE TYPE OF NOZZLE USED '
1 PRINT*, 'ENTER 1 FOR IMPACT SPRINKLER, 2 FOR SPRAY NOZZLE '
READ*, NOZZ
IF (NOZZ.EQ.1) THEN
  C = 0.98
C   DM = 46.79*(N**(0.37))*(P**(-0.39))
ELSEIF (NOZZ.EQ.2) THEN
  C = 0.65
C   DM = 16.18*(N**(0.87))*(P**(-0.3))
ENDIF
C
C   The following lines of the program calculate the initial value
C   of the droplet velocity in the z-direction.
C
VZ(1) = C*(2*9.81*MPRES/9.790399)**0.5
VZNEW(1) = 0
C
C   The next line calculate the droplet distribution used in the
C   program.
C
PRINT*, 'ENTER THE NUMBER OF DROPLET DIAMETERS TO BE TESTED '
READ*, NSAMP

```

```

PRINT*, 'ENTER THE MINIMUM DROP DIAMETER '
READ*, INDROP(1)
C
DELTAD = (0.006-INDROP(1))/NSAMP
C   The next lines in this subroutine prompts the user to
C   enter the ambient air temperature (F) and the relative
C   humidity. It also converts the temperature to the required
C   units.
C
      PRINT*, 'ENTER THE TEMPERATURE (F) '
      READ*, TEMPF
      PRINT*, 'ENTER THE RELATIVE HUMIDITY (%) '
      READ*, RH
      TEMPK = (TEMPF - 32)*5/9 + 273

C
C   The next lines of this subroutine calculate the viscosity,
C   air density, and droplet density.

VISC = 0.0000002*TEMPK**3.0-0.0006*TEMPK**2.0 + 0.759*TEMPK+0.9122
ADENS = 364.39*TEMPK**(-1.0073)
DRDENS = 1000/(0.000004*TEMPK**2-0.0021*TEMPK+1.271)

C
C   The next print statement prompts the used to enter the
C   elevation of the test site in question (m).
C
      PRINT*, 'ENTER THE ELEVATION OF THE TEST SITE (m)'
      READ*, ELEV

C
C   The next line calculates the atmospheric pressure.
C
      PA = 101.3*(1-0.00002258*ELEV)**5.255

C
C   The following line calculates the diffusivity of the
C   droplet.
C
      KDROP = (101.3/PA)*8.8*10**(-10)*TEMPK**(1.81)
      KDROP = 0.0000286
      IF (KDROP.EQ.0)THEN
          GOTO 100
      ENDIF

C
C   The user is prompted to enter the initial concentration
C   of ammonia in the irrigated effluent.
C

```

```
PRINT*, 'ENTER INITIAL AMMONIA CONCENTRATION IN THE EFFLUENT'  
READ*, INITCONC(1)
```

C

C The next two lines involve declaration of the step size and
C the number of iterations required by the program.

C

```
H = 0.1  
NITER = 3
```

C

C A double-loop is performed to determine the distance traveled,
C evaporation of the droplets and volatilization of the
C respective odorant

C

```
DO 2 D = INDROP(1), 0.006, DELTAD
```

```
DO 3 T = 0.0, NITER, H
```

```
CALL RK45TRAJ(T, H, 1, VZ, VZNEW, ERROR, ZDOT)
```

C

C The next lines of this subroutine calculate the Reynold's
C number, Schmidt number, and Sherwood number for the water
C droplet.

C

```
RE = INDROP(1)*VZNEW(1)/VISC  
SC = VISC/KDROP  
SHDROP = 2.0 + 0.60*SC**(0.333)*RE**(0.5)
```

C

C The following are entered as hard code into the program:
C Mean molecular weight of the gas mixture (air) and the
C molecular weight of the diffusing water vapor.

C

```
MV = 18.01  
MA = 29
```

C

C The next few lines of the subroutine calculate the
C saturated vapor pressure of the droplet at the droplet
C temperature and the vapor pressure of the ambient air.

C

```
PV = ((164.8 + TEMPF)/157)**8  
PS = (RH*PV)/100
```

C

C The next line of the program combines the above equations
C into a dummy constant for ease of programming and computer
C computation time.

C

```

CONST = -2*(MV/MA)*KDROP*(ADENS/DRDENS)*((PV-PS)/PA)*SHDROP
C
C   The subroutine RK45DROP is now called to determine the change
C   in droplet diameter at each droplet size and at each time
C   step.
C
      CALL RK45DROP(H, I, INDROP,NEWDROP,ERROR, DDOT,CONST)
C
C   The subroutine RK45DROP returns a value for the new droplet
C   diameter.
C
      KODOR = 3000*SQRT(0.09)
      VISODOR = VISC
      REODOR = (NEWDROP(1)*VZNEW(1))/VISODOR
      SCODOR = VISODOR/KODOR
      SHODOR = 2.0 + 0.60*SCODOR**(1/3)*REODOR**(0.5)
      HAMM = 4*10**(-7)/0.024
C
C   The next line of the program combines the above equations
C   into a dummy constant for ease of programming and computer
C   computation time.
C
      CONST2 = -2*SHODOR*KODOR/(NEWDROP(1)**2)
C
C   The subroutine RK45CONC is now called to determine the change
C   in ammonia concentration at each droplet size and at each time
C   step.
C
      CALL RK45CONC(H,I, INITCONC, NEWCL, ERROR, CDOT, CONST,
CONST2,
      &NEWDROP)

3   CONTINUE

C   TOTALCL = INITCONC(1)-NEWCL(1)
C
2   CONTINUE
C
C   The next lines of the program calculate the total concentration
C   of ammonia in the liquid, based on the concentration in 1
C   nozzle and the total number of heads on the pivot.
C
PRINT*, 'ENTER NUMBER OF SPRINKLER HEADS ON THE PIVOT '
READ*, NSPRINK
TOTALCL = NSPRINK*NEWCL(1)*NSAMP

```

```

    PERC = (INITCONC(1)-NEWCL(1))*100/INITCONC(1)
    PRINT*, INITCONC(1), NEWCL(1), PERC
C
  100 END
C
C   This is the end of the main program. The following subroutines
C   are used to calculate the droplet evaporation and odorant
C   volatilization.
C
C*****
C
C   SUBROUTINE TRAJFUNC(T, VZ, ZDOT)
C
C*** SUBROUTINE DESCRIPTION
C
C   This subroutine is called by the Runge-Kutta-Fehlberg sub-
C   routine (RK45TRAJ). It is used to solve for the velocity
C   of the the droplets in the z-direction using the differential
C   equations for acceleration (Equation 3.13 in Chapter 3).
C
C*** GLOSSARY OF VARIABLES
C
C   ZDOT = Dummy variable
C   T = Time, seconds
C   VZ = Droplet velocity in the z-direction, m/s
C
C*** SUBROUTINES CALLED
C
C   NONE
C
C*** DECLARATION OF VARIABLES
C
C   REAL VZ(1), ZDOT(1)
C
C   The following command calcualtes the velocity of the droplets
C   in the z-direction using ballistics equations
C
C   ZDOT(1) = (-0.25)*(VZ(1)**2) - (9.8)
C   RETURN
C   END
C
C*****
C
C   SUBROUTINE RK45TRAJ(T, H, NEQN, VZ, VZNEW, ERROR, ZDOT)
C
C*** SUBROUTINE DESCRIPTION

```

```

C
C   This subroutine is the Runge-Kutta-Fehlberg method used to
C   solve a differential equation
C
C*** GLOSSARY OF VARIABLES
C
C   T = Time, seconds
C   H = Step Size, dimensionless
C   NEQN = Number of equations, 1 in this case
C   VZ = Velocity of the droplets in the z-direction, m/s
C   VZNEW = New velocity calculated using Runge-Kutta, m/s
C   ERROR = Error related to Runge-Kutta-Fehlberg Method
C   ZDOT = Dummy variable used in numerical method
C   ZHAT = Dummy variable used in calculatin the error
C
C*** SUBROUTINES CALLED
C
C   SUBROUTINE TRAJFUNC
C
C*** DECLARATION OF VARIABLES
C
REAL ERROR(1), ZHAT(4), H, T
REAL VZNEW(1), ZDOT(1), VZ(1)
REAL K1(1), K2(1), K3(1), K4(1), K5(1), K6(1)

CALL TRAJFUNC(T, VZ, ZDOT)
DO 10 I = 1, NEQN
  K1(I) = H*ZDOT(I)
  VZNEW(I) = VZ(I) + K1(I)/4
10 CONTINUE

CALL TRAJFUNC(T+H/4, VZNEW, ZDOT)
DO 15 I = 1, NEQN
  K2(I) = H*ZDOT(I)
  VZNEW(I) = VZ(I) + 3*K1(I)/32 + 9*K2(I)/32
15 CONTINUE

CALL TRAJFUNC(T+3*H/8, VZNEW, ZDOT)
DO 20 I = 1, NEQN
  K3(I) = H*ZDOT(I)
  VZNEW(I) = VZ(I) + 1932*K1(I)/2197 - 7200*K2(I)/2197
&          + 7296*K3(I)/2197
20 CONTINUE

CALL TRAJFUNC(T+12*H/13, VZNEW, ZDOT)
DO 25 I = 1, NEQN

```

```

      K4(I) = H*ZDOT(I)
      VZNEW(I) = VZ(I) + 439*K1(I)/216 - 8*K2(I) + 3680*K3(I)/513
&
      - 845*K4(I)/4104
25 CONTINUE

      CALL TRAJFUNC(T+H, VZNEW, ZDOT)
      DO 30 I = 1, NEQN
      K5(I) = H*ZDOT(I)
      VZNEW(I) = VZ(I) - 8*K1(I) + 2*K2(I) - 3544*K3(I)/2565
&
      + 1859*K4(I)/4104 - 11*K5(I)/40
30 CONTINUE

      CALL TRAJFUNC(T+H/2, VZNEW, ZDOT)
      DO 35 I = 1, NEQN
      K6(I) = H*ZDOT(I)
35 CONTINUE

      DO 40 I = 1, NEQN
      ZHAT(I) = VZ(I) + 25*K1(I)/216 + 1408*K3(I)/2565 +
&
      2197*K4(I)/4104 - K5(I)/5
40 CONTINUE

      DO 45 I = 1, NEQN
      VZNEW(I) = VZ(I) + 16*K1(I)/135 + 6656*K3(I)/12825 +
&
      28561*K4(I)/56430 - 9*K5(I)/50 + 2*K6(I)/55
45 CONTINUE

      DO 50 I = 1, NEQN
      ERROR(I) = ZHAT(I) - VZNEW(I)
50 CONTINUE
      END
C
C   This is the end of the RK45TRAJ subroutine.
C
C*****
C
C   SUBROUTINE RK45DROP(H, NEQN, Y, YNEW, ERROR, DDOT, CONST)
C
C*** SUBROUTINE DESCRIPTION
C
C   This subroutine is the Runge-Kutta-Fehlberg method used to
C   solve a differential equation.
C
C*** GLOSSARY OF VARIABLES
C
C   T = Time, s

```

```

C   H = Step size, dimensionless
C   NEQN = Number of equations, in this case, 1
C   Y = Initial drop diameter, m
C   YNEW = New drop diameter calculated by the subroutine, m
C   ERROR = Error related the the Runge-Kutta-Fehlberg method
C   DDOT = Dummy variable used in this numerical method
C   CONST = Constant used in subroutine DROPLET and transferred
C           to this subroutine
C
C*** SUBROUTINES CALLED
C
C   SUBROUTINE DROPFUNC
C
C*** DECLARATION OF VARIABLES
C
REAL ERROR(*), YHAT(4), H
REAL YNEW(*), DDOT(1), Y(*)
REAL K1(1), K2(1), K3(1), K4(1), K5(1), K6(1)

CALL DROPFUNC(Y, DDOT, CONST)
DO 10 I = 1, NEQN
  K1(I) = H*DDOT(I)
  YNEW(I) = Y(I) + K1(I)/4
10 CONTINUE

CALL DROPFUNC(YNEW, DDOT, CONST)
DO 15 I = 1, NEQN
  K2(I) = H*DDOT(I)
  YNEW(I) = Y(I) + 3*K1(I)/32 + 9*K2(I)/32
15 CONTINUE

CALL DROPFUNC(YNEW, DDOT, CONST)
DO 20 I = 1, NEQN
  K3(I) = H*DDOT(I)
  YNEW(I) = Y(I) + 1932*K1(I)/2197 - 7200*K2(I)/2197
&          + 7296*K3(I)/2197
20 CONTINUE

CALL DROPFUNC(YNEW, DDOT, CONST)
DO 25 I = 1, NEQN
  K4(I) = H*DDOT(I)
  YNEW(I) = Y(I) + 439*K1(I)/216 - 8*K2(I) + 3680*K3(I)/513
&          - 845*K4(I)/4104
25 CONTINUE

CALL DROPFUNC(YNEW, DDOT, CONST)

```



```

DO 30 I = 1, NEQN
  K5(I) = H*DDOT(I)
  YNEW(I) = Y(I) - 8*K1(I) + 2*K2(I) - 3544*K3(I)/2565
&          + 1859*K4(I)/4104 - 11*K5(I)/40
30 CONTINUE

```

```

CALL DROPFUNC(YNEW, DDOT, CONST)
DO 35 I = 1, NEQN
  K6(I) = H*DDOT(I)
35 CONTINUE

```

```

DO 40 I = 1, NEQN
  YHAT(I) = Y(I) + 25*K1(I)/216 + 1408*K3(I)/2565 +
&          2197*K4(I)/4104 - K5(I)/5
40 CONTINUE

```

```

DO 45 I = 1, NEQN
  YNEW(I) = Y(I) + 16*K1(I)/135 + 6656*K3(I)/12825 +
&          28561*K4(I)/56430 - 9*K5(I)/50 + 2*K6(I)/55
45 CONTINUE

```

```

DO 50 I = 1, NEQN
  ERROR(I) = YHAT(I) - YNEW(I)
50 CONTINUE

```

```

C   Y(1) = YNEW(1)
C   END

```

```

C
C   This is the end of the RK45DROP subroutine. It returns the
C   new droplet diameter to the droplet subroutine.
C

```

```

C*****
C

```

```

C   SUBROUTINE DROPFUNC(Y,DDOT, CONST)
C

```

```

C*** SUBROUTINE DESCRIPTION
C

```

```

C   This subroutine is called by the Runge-Kutta-Fehlberg sub-
C   routine (RK45TRAJ). It is used to solve for the change in
C   droplet diameter (Equation 3.1 in Chapter 3).
C

```

```

C*** GLOSSARY OF VARIABLES
C

```

```

C   T = Time, s
C   Y = Droplet Diameter,m
C   DDOT = Dummy variable used by the subroutine

```

```

C  CONST = Dummy constant used by the subroutine
C
C*** SUBROUTINES CALLED
C
C  NONE
C
C*** DECLARATION OF VARIABLES
C
C  REAL Y(1), DDOT(1), CONST
C
C  The next lines of this subroutine calculate the change in
C  droplet diameter (Equation 3.1).
C
C  DDOT(1) = CONST/Y(1)
C  RETURN
C  END
C
C  This is the end of subroutine DROPFUNC
C
C*****
C
C  SUBROUTINE RK45CONC (H,NEQN, Y, YNEW, ERROR, CDOT, CONST,
C  &CONST2, NEWDROP)
C
C*** SUBROUTINE DESCRIPTION
C
C  This subroutine is the Runge-Kutta-Fehlberg method used to
C  solve a differential equation.
C
C*** GLOSSARY OF VARIABLES
C
C  T = Time, s
C  H = Step size, dimensionless
C  NEQN = Number of equations, in this case, 1
C  Y = Initial concentration of ammonia, mg/L
C  YNEW = New droplet ammonia concentration calculated by the
C  subroutine, mg/L
C  ERROR = Error related the the Runge-Kutta-Fehlberg method
C  CDOT = Dummy variable used in this numerical method
C  CONST = Constant
C  CONST2 = Constant
C
C*** SUBROUTINES CALLED
C
C  SUBROUTINE CONCFUNC
C

```

C*** DECLARATION OF VARIABLES

C

REAL ERROR(1), YHAT(4), H, CONST, CONST2
REAL YNEW(1), CDOT(1), Y(1), NEWDROP(1)
REAL K1(1), K2(1), K3(1), K4(1), K5(1), K6(1)

CALL CONCFUNC(Y, CDOT, CONST, CONST2, NEWDROP)
DO 10 I = 1, NEQN
 K1(I) = H*CDOT(I)
 YNEW(I) = Y(I) + K1(I)/4
10 CONTINUE

CALL CONCFUNC(YNEW, CDOT, CONST, CONST2, NEWDROP)
DO 15 I = 1, NEQN
 K2(I) = H*CDOT(I)
 YNEW(I) = Y(I) + 3*K1(I)/32 + 9*K2(I)/32
15 CONTINUE

CALL CONCFUNC(YNEW, CDOT, CONST, CONST2, NEWDROP)
DO 20 I = 1, NEQN
 K3(I) = H*CDOT(I)
 YNEW(I) = Y(I) + 1932*K1(I)/2197 - 7200*K2(I)/2197
& + 7296*K3(I)/2197
20 CONTINUE

CALL CONCFUNC(YNEW, CDOT, CONST, CONST2, NEWDROP)
DO 25 I = 1, NEQN
 K4(I) = H*CDOT(I)
 YNEW(I) = Y(I) + 439*K1(I)/216 - 8*K2(I) + 3680*K3(I)/513
& - 845*K4(I)/4104
25 CONTINUE

CALL CONCFUNC(YNEW, CDOT, CONST, CONST2, NEWDROP)
DO 30 I = 1, NEQN
 K5(I) = H*CDOT(I)
 YNEW(I) = Y(I) - 8*K1(I) + 2*K2(I) - 3544*K3(I)/2565
& + 1859*K4(I)/4104 - 11*K5(I)/40
30 CONTINUE

CALL CONCFUNC(YNEW, CDOT, CONST, CONST2, NEWDROP)
DO 35 I = 1, NEQN
 K6(I) = H*CDOT(I)
35 CONTINUE

DO 40 I = 1, NEQN
 YHAT(I) = Y(I) + 25*K1(I)/216 + 1408*K3(I)/2565 +

```

&          2197*K4(I)/4104 - K5(I)/5
40 CONTINUE

      DO 45 I = 1, NEQN
        YNEW(I) = Y(I) + 16*K1(I)/135 + 6656*K3(I)/12825 +
&          28561*K4(I)/56430 - 9*K5(I)/50 + 2*K6(I)/55
45 CONTINUE

      DO 50 I = 1, NEQN
        ERROR(I) = YHAT(I) - YNEW(I)
50 CONTINUE

C   Y(1) = YNEW(1)
      END
C
C   This is the end of the RK45CONC subroutine. It returns the
C   new droplet ammonia concentration to the main program.
C
C*****
C
      SUBROUTINE CONCFUNC(Y,CDOT, CONST, CONST2, NEWDROP)
C
C*** SUBROUTINE DESCRIPTION
C
C   This subroutine is called by the Runge-Kutta-Fehlberg subroutine
C   (RK45CONC). It is used to solve the change in concentration
C   with time equation (Equation 3.33 in Chapter 3).
C
C*** GLOSSARY OF VARIABLES
C
C   T = Time, s
C   CONST = Dummy variable used in this subroutine
C   SHODOR = Sherwood number for the odorant, dimensionless
C   NEWDROP = New droplet diameter, m
C   KODOR = Odor diffusivity, m2/s
C   CDOT = Dummy variable used in this subroutine
C   CONST2 = Dummy variable used in this subroutine
C
C*** SUBROUTINES CALLED
C
C   NONE
C
C*** DECLARATION OF VARIABLES
C
      REAL CONST, CONST2, NEWDROP(1), CDOT(1), HAMM, Y(1)
C

```

```

C   The next lines of this subroutine calculate the change in
C   ammonia concentration in the liquid (Equation 3.33).
C
  HAMM = 4*10**(-7)/0.024
  CDOT(1) = CONST2*HAMM*Y(1) - (-2)*Y(1)*CONST/(NEWDROP(1)**2)
  RETURN
  END
C
C   This is the end of subroutine CONCFUNC.
C
C*****
C
C***** END OF LANDAPP MODEL *****
20*****
C

```

APPENDIX B

RUNGE-KUTTA-FEHLBERG NUMERICAL METHOD DESCRIPTION

There are many different step-by-step methods for numerically solving ordinary differential equations. Each of these methods falls into one of four general categories: Taylor series methods, Runge-Kutta methods, Multistep methods, and Extrapolation methods.

The Runge-Kutta method, named after two German mathematicians, is designed to approximate the Taylor series methods without requiring explicit definitions of, or evaluations of, derivatives beyond the first. They developed algorithms that solve a differential equation efficiently and yet are the equivalent of approximating the exact solution by matching the first n terms of the Taylor series expansion.

To impart some idea of how the Runge-Kutta methods are developed, the derivation of a simple second-order is presented here. The increment to the y is a weighted average of two estimates of the increment, which is called k_1 and k_2 . Thus for the equation $dy/dx = f(x, y)$,

$$\begin{aligned}y_{n+1} &= y_n + ak_1 + bk_2, \\k_1 &= h \cdot f(x_n, y_n), \\k_2 &= h \cdot f(x_n + \alpha h, y_n + \beta k_1).\end{aligned}\tag{B.1}$$

The values of k_1 and k_2 can be considered estimates of the change in y when x advances by h , because they are the product of the change in x and a value for the slope

of the curve, dy/dx . The problem is to devise a scheme of choosing the four parameters, a , b , α , and β . These are estimated by making the above equations agree as well as possible with the Taylor-series expansion, in which the y -derivatives are written in terms of f , from $dy/dx = f(x, y)$,

$$y_{n+1} = y_n + h \cdot f(x_n, y_n) + \frac{h^2}{2} \cdot f'(x_n, y_n) + \dots \quad (\text{B.2})$$

An equivalent form, since $df/dx = f_x + f_y dy/dx = f_x + f_y f$, is

$$y_{n+1} = y_n + h \cdot f_n + h^2 \left(\frac{1}{2} f_x + \frac{1}{2} f_y f \right)_n \quad (\text{B.3})$$

Substituting the definitions of k_1 and k_2

$$y_{n+1} = y_n + ah \cdot f(x_n, y_n) + bh \cdot f[x_n + \alpha h, y_n + \beta h \cdot f(x_n, y_n)]. \quad (\text{B.4})$$

Expanding the last term of the previous equation in a Taylor series in term of x_n, y_n , remembering that f is a function of two variables, retaining only first derivative terms:

$$f[x_n + \alpha h, y_n + \beta h \cdot f(x_n, y_n)] = (f + f_x \alpha h + f_y \beta h f)_n \quad (\text{B.5})$$

On the right side of Equations (B.3) and (B.5) f and its partial derivatives are all to be evaluated at (x_n, y_n) .

Substituting from Equation (B.5) into Equation (B.4):

$$y_{n+1} = y_n + ah \cdot f_n + bh(f + f_x \alpha h + f_y \beta h f)_n, \quad (\text{B.6})$$

or, rearranging,

$$y_{n+1} = y_n + (a+b)h \cdot f_n + h^2 (\alpha b f_x + \beta b f_y f)_n \quad (\text{B.7})$$

Equation (B.7) will be identical to Equation (B.3) if

$$\begin{aligned} a + b &= 1, \\ \alpha b &= \frac{1}{2}, \\ \beta b &= \frac{1}{2} \end{aligned} \quad (\text{B.8})$$

Note that only three equations need to be satisfied by the four unknowns. One value may be chosen arbitrarily (with minor restrictions); hence there is a complete set of second-order methods.

Fourth-order Runge-Kutta methods are most widely used and are derived in a similar fashion. The classical fourth-order Runge-Kutta method is given by

$$y_{n+1} = y_n + \frac{1}{6}(k_0 + 2k_1 + 2k_2 + k_3)$$

where

$$\begin{aligned} k_0 &= hf(y_n, t_n) \\ k_1 &= hf\left(y_n + \frac{1}{2}k_0, t_n + \frac{h}{2}\right) \\ k_2 &= hf\left(y_n + \frac{1}{2}k_1, t_n + \frac{h}{2}\right) \\ k_3 &= hf(y_n + k_2, t_n + h) \end{aligned}$$

Notice that four evaluations of the function $f(y, t)$ are required for each step.

As $h \rightarrow 0$, the classical fourth-order Runge-Kutta method agrees with the Taylor series asymptotically through terms of order h^4 . However, no estimate of the local discretization error is readily available to help pick the step size. A modern modification

of the Runge-Kutta method, the Runge-Kutta-Fehlberg method, includes this step size control.

The basis for the Runge-Kutta-Fehlberg scheme is to compute two Runge-Kutta estimates for the new value of \hat{y}_{n+1} but of different orders of errors. This, instead of comparing estimates of y_{n+1} for h and $h/2$, comparisons between the estimates \hat{y}_{n+1} and y_{n+1} are completed using fourth- and fifth-order Runge-Kutta formulas. Moreover, both equations make use of the same k 's; only six function evaluations are needed.

The Runge-Kutta-Fehlberg method requires six function evaluations per step. Four of these function values are combined with one set of coefficients to produce a fourth-order method, and all six values are combined with another set of coefficients to produce a fifth-order method. Comparison of the two values yields an error estimate that is used for step size control. An algorithm for the Runge-Kutta-Fehlberg method is shown in Figure B-1.

The Runge-Kutta-Fehlberg method is primarily designed to solve non-stiff (DEFINITION) and mildly stiff differential equations when derivative evaluations are inexpensive. The method integrates a system of NEQN first order ordinary differential equations of the form

$$\frac{DY(I)}{DT} = f(T, Y(1), Y(2), \dots, Y(NEQN))$$

This Runge-Kutta-Fehlberg method is called a single-step method because it uses only the information from the last step computed. In this it has the ability to perform the next step with a different step size and are ideal for beginning the solution where only the initial conditions are available.

$$\begin{aligned}
k_1 &= h \cdot f(x_n, y_n), \\
k_2 &= h \cdot f\left(x_n + \frac{h}{4}, y_n + \frac{k_1}{4}\right), \\
k_3 &= h \cdot f\left(x_n + \frac{3h}{8}, y_n + \frac{3k_1}{32} + \frac{9k_2}{32}\right), \\
k_4 &= h \cdot f\left(x_n + \frac{12h}{13}, y_n + \frac{1932k_1}{2197} - \frac{7200k_2}{2197} + \frac{7296k_3}{2197}\right), \\
k_5 &= h \cdot f\left(x_n + h, y_n + \frac{439k_1}{216} - 8k_2 + \frac{3680k_3}{513} - \frac{845k_4}{4104}\right), \\
k_6 &= h \cdot f\left(x_n + \frac{h}{2}, y_n - \frac{8k_1}{27} + 2k_2 - \frac{3544k_3}{2565} + \frac{1859k_4}{4104} - \frac{11k_5}{40}\right); \\
\hat{y}_{n+1} &= y_n + \left(\frac{25k_1}{216} + \frac{1408k_3}{2565} + \frac{2197k_4}{4104} - \frac{k_5}{5}\right) \\
y_{n+1} &= y_n + \left(\frac{16k_1}{135} + \frac{6656k_3}{12825} + \frac{28561k_4}{56430} - \frac{9k_5}{50} + \frac{2k_6}{55}\right) \\
\text{Error, } E &= \frac{k_1}{360} - \frac{128k_3}{4275} - \frac{2197k_4}{75240} + \frac{k_5}{50} + \frac{2k_6}{55}
\end{aligned}$$

Figure B.1. An Algorithm for the Runge-Kutta-Fehlberg Method (Adapted from Gerald and Wheatly, 1994).

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