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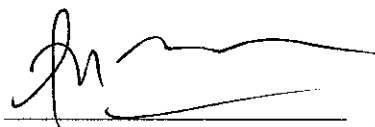
**Development of Toxic Effect Risk Model For Inherent Safety Design**

by

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## CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

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KHADEEJA BINTI SHARIFF

## ABSTRACT

Safety and environmental risk assessments are done in parallel or when the design stage of the process plant is almost completed. Analysis of safety conducted at the last stage exposes the plant to various hazards. The objective of this project is to develop a model to predict the concentration levels and toxic effect of accidental gaseous release as an inherent safety approach to process plant design. For this simulation, the author develops a two-dimensional Gaussian plume model into Microsoft Excel Worksheet applications. The Gaussian model developed predicts concentrations from one point source at ground level to determine the effect of toxic releases to receptors close to the ground (people, plants and animals). Input data requirements for this model include the physical properties of the gaseous component such as its density, temperature, specific heat and its volumetric flowrate. The model takes into account atmospheric and meteorological conditions, requiring data input such as the ambient temperature, wind velocity, wind stability category and the area class. The author simulated the model hypothetically on two industrial toxic releases, Ammonia ( $\text{NH}_3$ ), a gas lighter than air and Sulfur Dioxide ( $\text{SO}_2$ ), a dense gas. The distance of rupture from ground level, the diameter of the rupture and the time of exposure are set similar for both simulations to compare the effects of dense gas toxic releases with that of light gases. Results showed that both gases have an almost similar peak concentration of 70.34 ppm for  $\text{NH}_3$  and 69.98 ppm for  $\text{SO}_2$ . As the toxic cloud moves further downwind, the concentration of  $\text{NH}_3$  disperses faster than that of  $\text{SO}_2$ . The difference in this is the factor of buoyancy flux.  $\text{NH}_3$  produces a positive buoyancy flux. Since  $\text{SO}_2$  is a dense gas, the plume tends to slump and spread out in thick clouds rather than float buoyantly into the air. For  $\text{SO}_2$ , plume rise is small, producing a negative plume rise. Approaching 100km downwind, the difference in concentrations of  $\text{SO}_2$  and  $\text{NH}_3$  increases twice as much. Although the peak concentrations are almost similar, the extent of risk exposure differs greatly. Probit values for  $\text{NH}_3$  ranges from -50.26 to -17.19 while the Probit range for  $\text{SO}_2$  is from -20.71 to -3.37. This measurement of the probability of death shows 60-80% higher Probit values of  $\text{SO}_2$  as compared to  $\text{NH}_3$ . Results prove that denser gas has a higher adverse effect than lighter gas. For this

simulation, both gases do not reach the IDLH limits (Immediately Dangerous to Life and Health) but the produced concentrations can cause dizziness, disorientation and restricted visual. The author also modeled the toxic release of  $\text{NH}_3$  on different wind stability conditions, permitting to Pasquill's wind stability category. Results show that unstable wind conditions (wind stability category A) give lower levels of concentration (peak concentration 13 ppm) as compared to the toxic release under stable wind conditions (wind stability category F) where peak concentrations mounted to 1,023 ppm.

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## ABBREVIATIONS AND NOMENCLATURES

$c$	concentration level of toxic release ( $\text{mmg/m}^3$ )
$C_{p_a}$	specific heat of air ( $\text{kJ/kmol.K}$ )
$C_{p_s}$	specific heat of gaseous toxic release ( $\text{kJ/kmol.K}$ )
$d_s$	diameter of vessel rupture or leak (m)
$F_b$	buoyancy flux ( $\text{m}^4/\text{s}^3$ )
$g$	gravity acceleration ( $\text{m/s}^2$ )
$h_s$	point of toxic release from ground level (m)
$\Delta h$	plume rise (m)
$h_e$	effective plume rise (m)
$M_a$	MW of air ( $\text{g/gmol}$ )
$M_s$	MW of gaseous toxic release ( $\text{g/gmol}$ )
$P_a$	atmospheric pressure (atm)
$P_s$	pressure of toxic release (atm)
$Q$	emission rate of toxic release ( $\text{g/s}$ )
$T$	duration of toxic release (s)
$T_s$	temperature of gaseous release (K)
$T_a$	atmospheric temperature (K)
$u$	average wind velocity (m/s)
$V_s$	velocity of gaseous toxic release (m/s)
$x$	distance in the x-direction (m)
$y$	distance in the y-direction (m)
$z$	distance in the z-direction (m)
$\rho_a$	density of air ( $\text{kg/m}^3$ )
$\rho_s$	density of gaseous toxic release ( $\text{kg/m}^3$ )
$\sigma_y$	lateral dispersion coefficient (m)
$\sigma_z$	vertical dispersion coefficient (m)

# CHAPTER 1

## INTRODUCTION

### 1.1 BACKGROUND

The design of a chemical process plant undergoes a sequence of phases, beginning with feasibility studies, selection of materials and technology, detail engineering, construction and lastly commissioning. Various tools such as computer software are utilized in the designing stage. These tools aid the engineers to best design a process plant with good optimization of process conditions.

The aim of detailed engineering for a process plant is to create a process plant that is safe, environmentally friendly and uncomplicated operability wise (Heikkila, 1999). Above all that, the main aim of a process plant in the first place is to ensure profitability besides catering for demands and needs. Since designing of a plant is primarily economic-driven, the process designs at times overlook safety and environmental concerns. Engineers and technologists are aware of the importance of conducting safety and environmental risk analysis during the design of a plant but it is often not integrated into the early design phases.

Among the hazard exposure in a chemical process plant is the release of toxic substances from vessels or storage tanks. Toxic releases contaminate the atmosphere and create various forms of impact or injuries. The impact varies according to the extent of contaminant; the higher the concentration of toxic releases, the higher the risk of injury. This emission must be accounted for, even at the design stage to minimize, if possible eliminate the risk and consequences of air pollution. The minor injuries for toxic releases would be dizziness and short of breath, while the extreme injury would be death. Following this, emergency response plans can be properly identified according to the extent of toxic release from the source point.

A significant case to relate to is an accidental toxic gas release from a Union Carbide chemical plant in Bhopal in India that happened back in 1984. That incident which could have easily been avoided killed 2,500 people. Although the gas releases could not be predicted, preventive measures such as evacuation of nearby areas could have been taken to avoid the probability of deaths. Another incident relating to toxic release is one that occurred in a South African fertilizer plant in 1973. The ammonia released due to storage vessel failure caused the deaths of 18 people. Correct emergency responses could have been taken to prevent these deaths if the extent of contaminant can be traced.

Many studies and models have been developed to predict the effect of the contaminant. These models act as justifications to the importance of integrating safety analysis into the preliminary design phases. This is the concept of inherent safety design; utilizing tools and technology as a safety approach to eliminate possibilities of accidents or mishaps.

## **1.2 PROBLEM STATEMENT**

### **1.2.1 Problem Identification**

Safety and environmental risk assessments are commonly done in parallel or when the design stage of the process plant is almost completed. Analysis of safety conducted at the last stage exposes the plant to various hazards. One hazard not to be overlooked is the risk effect of toxic substances leaking from storage facilities or vessels. Therefore, it is a crucial and valuable practice to estimate the risk of toxic release during the designing stage to minimize risk exposures to the plant.

### **1.2.2 Significance of the Project**

With the prediction of toxic release concentrations to the surrounding, preventive measures can be planned ahead to counter for any incidents that might occur resulting from a vessel or storage leak or failure. Following the predicted concentrations, the extent of exposure to the toxic release can be defined into several categories to relate the hazard

exposure to its level of concentration. Since the study is on gaseous toxic releases, an air dispersion model is used.

## **1.3 OBJECTIVES AND SCOPE OF STUDY**

### **1.3.1 Relevancy of the Project**

The toxic effect risk model developed by the author serves to predict concentration levels of gaseous releases to the atmosphere due to vessel or storage leaks or failures. With this prediction, the extent of injury can be pre-determined in the case of an incident occurring. The model runs on specific parameters inputs by the user. User input requirements are physical properties and conditions of the toxic release, vessel or storage tank design specifications and also the atmospheric conditions. These data inputs are required to produce an output that closely models a gaseous toxic release to the atmosphere.

### **1.3.2 Scope of Study**

This model predicts the effect of gaseous toxic releases from vessels or storage tanks to the atmosphere. The author develops an air dispersion Gaussian plume model into the Microsoft Excel worksheet to first determine concentration levels of contaminants from the source point of toxic release into the atmosphere.

However, measurement of toxic effect releases is not only dependent on the concentration levels but also the duration of exposure to the release. Therefore, the model incorporates this prediction of concentrations levels with the probability of death. This is done through Probit (probability of death) calculations, a measurement relating to the probability of death based on the concentration levels and also the period of time the toxic is released to the atmosphere.

## **CHAPTER 2**

### **LITERATURE REVIEW AND THEORY**

#### **2.1 Safety and Hazards**

Safety can be defined as a concept covering hazard identification, risk assessment and accident prevention. Apart from prioritizing to achieve profit margins, safety in plant operations ranks just as important. This is because an unsafe plant cannot be profitable due to losses of throughput and production and also capital (Heikkila, 1999).

Hazard is a condition with the potential of causing an injury or damage due to exposed risks regardless it being predicted or unpredicted (Heinrich, 1968). Risk is a measurement of the possibility of loss, involving two measurable parameters, consequences and probability. Safety-wise, the main purpose of process plant design is to minimize the total process risk which is the product of the possibility of an incident to occur and the consequences of the incident. Some events are more likely to occur than others and the probability and consequences need to be identified to categorize the extent of safety a certain process is in.

Therefore, the logical approach to safety is to identify hazards and analyzing them, if possible eliminating them or prevent the consequences to take place. The relationship between identifying hazards and eliminating them at an early stage is the concept of inherent safety.

#### **2.2 Inherent Safety**

There have been several safety analysis methods readily available and widely used. These analyses use different tools and standards so the results vary from one analysis to another. Different safety methods are used for different stages of process development, design and operation.



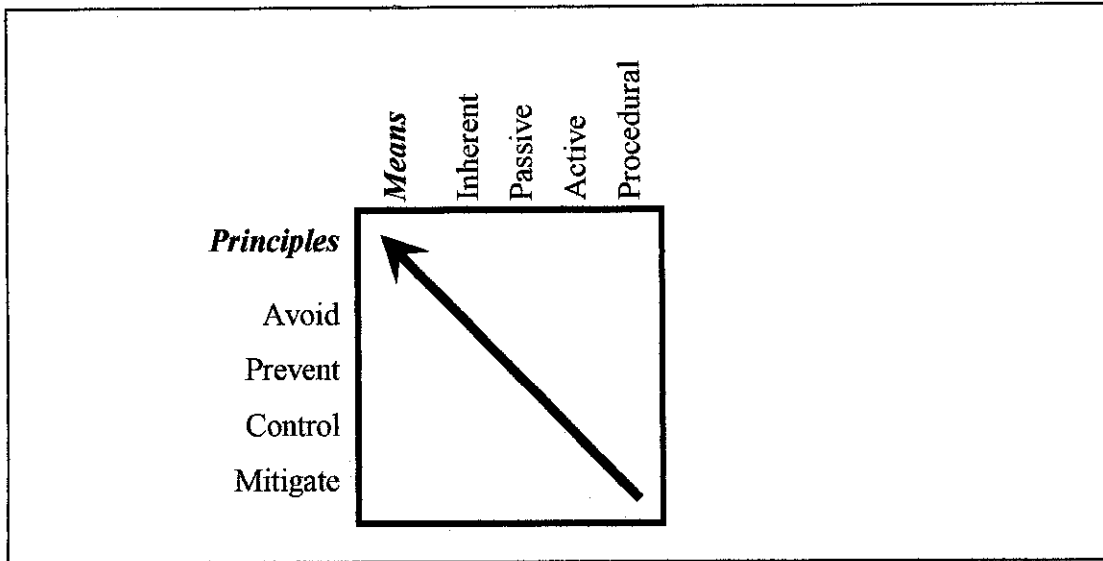
Among the commonly used safety analyses in the process industry are the DOW Fire and Explosion Hazard Index and the Mond Index (Heikkila, 1999). These two are rapid-hazard assessments of fire and explosion for use in chemical plants during process and plant development stage. Another widely used analysis is the Hazard and Operability Analysis (HAZOP) but this analysis is not done during the conceptual design stage, only when the process design is complete or when there are disturbances in the plant operation.

Inherent safety is a concept in which the evaluation of safety is done to minimize or eliminate the risk and exposures to accidents by utilizing specific tools and technology. It aims to remove the hazards out of a process rather than using controls or mitigation steps to overcome a hazard itself. These tools predict the possibility of an accident and evaluate the risks exposed leading to consequences if an accident were to happen. This is a measure to minimize hazards instead of investing on 'added-on' safeguard management controls that can be costly to provide and maintain (Heikkila, 1999).

Inherent safety can be combined with more traditional passive, active and procedural approaches to provide defence in depth by addressing hazard elimination/avoidance, prevention, control and mitigation ([www.aeatech.com](http://www.aeatech.com)).

Chemical process risk management can be categorized into four categories (Hendershot, 1997):

- Inherent - Eliminating hazards in the conceptual stage by assessing risks of process conditions
- Passive - Minimizing the hazards by process equipment and design features by reducing the frequency of consequences and potential hazards
- Active - Using engineering controls and safety shutdown systems, as a response or feedback towards an unpredicted or accidental incident
- Procedural - Using operating procedures, regular and routine administrative checks as an approach to continuous effort to minimize risks



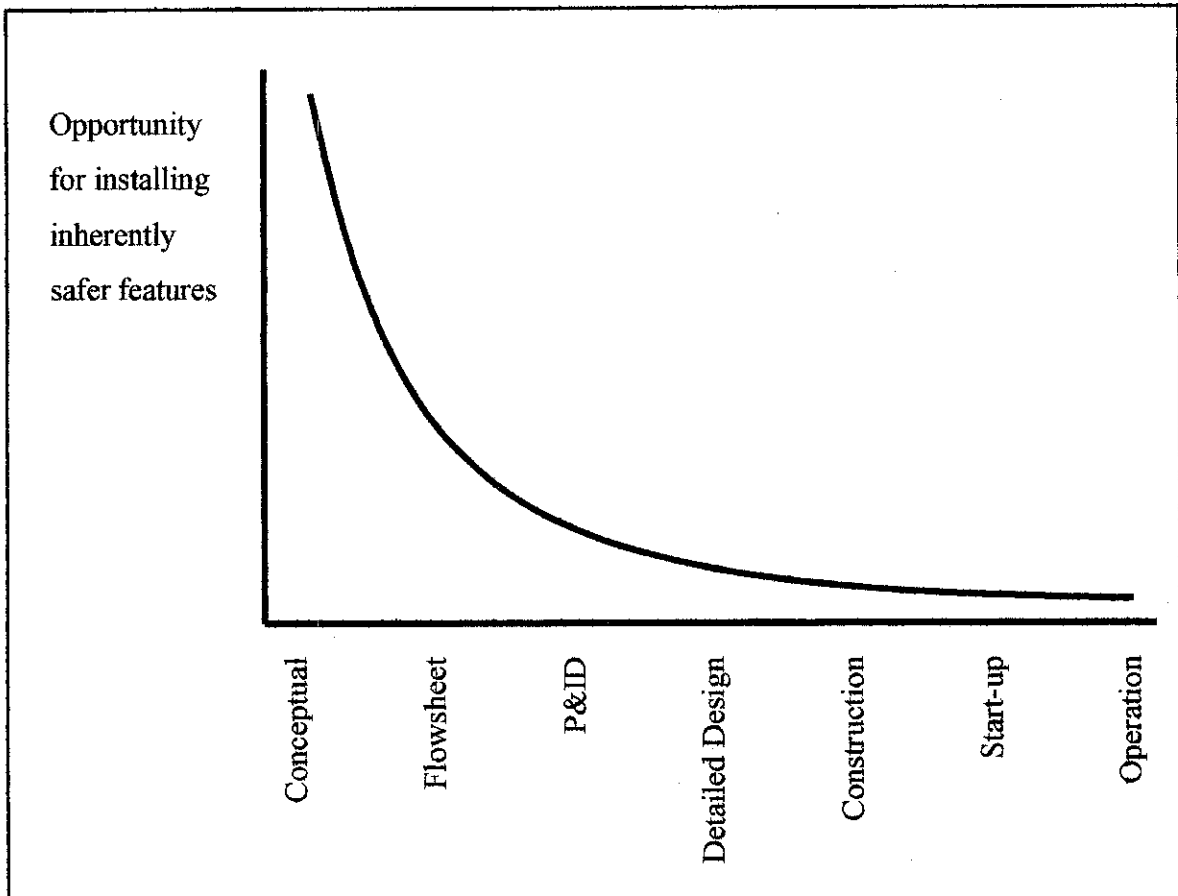
**Figure 2.1 Defenses in Depth**

(Sources taken from AEA Technology website)

Referring to Figure 2.1, the aim of the inherent safety approach is to manage the hazards in the upper left of the paradigm rather than in the lower right hand corner ([www.aeatech.com](http://www.aeatech.com)). If the possibility of reducing a hazard cannot be accomplished, then the approach of managing the hazards correctly must be taken into care (Ragan, 2002). Procedural measures of mitigating an action are seen as the last option to managing a hazard. This option is clearly a right move when actions to control or prevent the hazard from happening fail. Above all, it can be clearly visualized that the first principal here is the inherent approach, which can clearly avoid a mishap or incident altogether and minimize the need to control or mitigate the situation further on.

With the inherent safety approach, the possibility of disturbing the design process at a later stage decreases as the process design moves further into detail engineering. The

more extensive the process design is, the more expensive it is to make modifications or to bear the loss later on during plant operations.



**Figure 2.2** Inherently Safer features become harder to install as a project progresses

(Kletz, 1991)

Figure 2.2 shows a high opportunity for installing inherently safer features during the conceptual stage as being compared to the operational stage. The early stages of process design are where the inherent safety approach should be widely practiced. The expenses of doing modifications during the end stages of process design (from detailed design to

operation) can be costly and proves to be wasteful if the opportunity to identify hazards at an earlier stage is not fully utilized.

### **2.3 Air Pollution and Toxic Releases**

One of the major problems as we approach the 21<sup>st</sup> century is the increase of airborne contaminants into our atmosphere. Air pollutants range from solid and liquid (fine particles or aerosols) to gaseous forms. Pollutants are classified according to its origin, compositions, chemical properties, physiological effects, location or even legislation. Also, pollutants can be described as natural or man-made, particulate or gaseous and primary or secondary (Hunter and Oyama, 2000).

Deaves et. al. (2001) citing on toxic release

Several low boiling point materials are stored in closed vessels at ambient temperature, using their own vapor pressure to maintain a liquid state. These materials are often toxic, flammable or both and thus any uncontrolled release can have potentially disastrous consequences. (p. 1)

Toxicity is described as a property of a substance that injures life and beings or exposes an injury to health when it is being introduced into a living organism's system. Toxic hazard exposure is dependent on the duration of exposure and the concentration of the toxic released.

Toxic releases either in gaseous, liquid or solid form enters the body either by inhalation and ingestion (nose and mouth) or by external contact (skin). Usually, gases, vapors, fumes and dust are inhaled while liquids and solids are ingested (Plees, 1995). External contact of toxic release through the skin can occur at the same time of inhaling, through the linings of the eyes, mouth and throat and urinary tract. The amount of toxic entering the body depends on the amount inhaled or ingested by the body itself, but is also dependant of the concentration of pollutant surrounding the body and the toxicity of the materials itself.

Hepatotoxic agents (e.g., carbon tetrachloride) affect the liver; nephrotoxic agents (e.g., halogenated hydrocarbons) affect the kidneys while neurotoxic agents (e.g., methanol and benzene) affect the nervous system (Hunter and Oyama, 2000).

The most common term to classify the extent of toxicity is the Threshold Limit Value (TLV), which is defined as the concentration of the toxic in air that can be inhaled without harmful effect for five consecutive 8-hour working days. For emergency planning, legislations have been set to protect or serve as a warning to people, using LC50 and LD50 for toxicity. LD50 is defined as the dose administered orally or by skin contact that would cause the deaths of 50% of the test group sample within an observation period of 14 days. LC50 on the other hand is the concentration in air in which exposure to the material in 24 hours or less causes 50% deaths in a test group.

Probit is a term describing the probability of death, given by the equation (Plees, 1995)

$$Pr = A + B \ln (c^n t)$$

where

c = concentration of toxic gas (ppm)

t = duration of exposure (min)

A, B and n are constants for it's a particular material and its equations are available for a number of common toxic gases in industrials. Probit equations vary for different materials and the more toxic the gas is by character; the higher the values of constants B and n.

With the increasing number of operating chemical plants around the world, accidental releases of material to the atmosphere has struck an interest throughout. There are two types of accidental release. Catastrophic ruptures of pipelines or vessels can produce a release lasting from a few seconds to a few minutes. Leaks of gases or liquids from seals, pipe joints and valves starts slowly and increase in size. Another is a high-pressure

release of gases or liquids from pressure relief valves that might last from 10 minutes to half an hour. This is described as a small continuous release (Schnell and Dey, 1999).

#### 2.4 Gaussian Air Dispersion Model

Noonan (1999) states that: “Dispersion model may be used to assess a population’s risk of exposure to air pollution from a local source or sources, when the prime interest is in the region close to the source” (p.1).

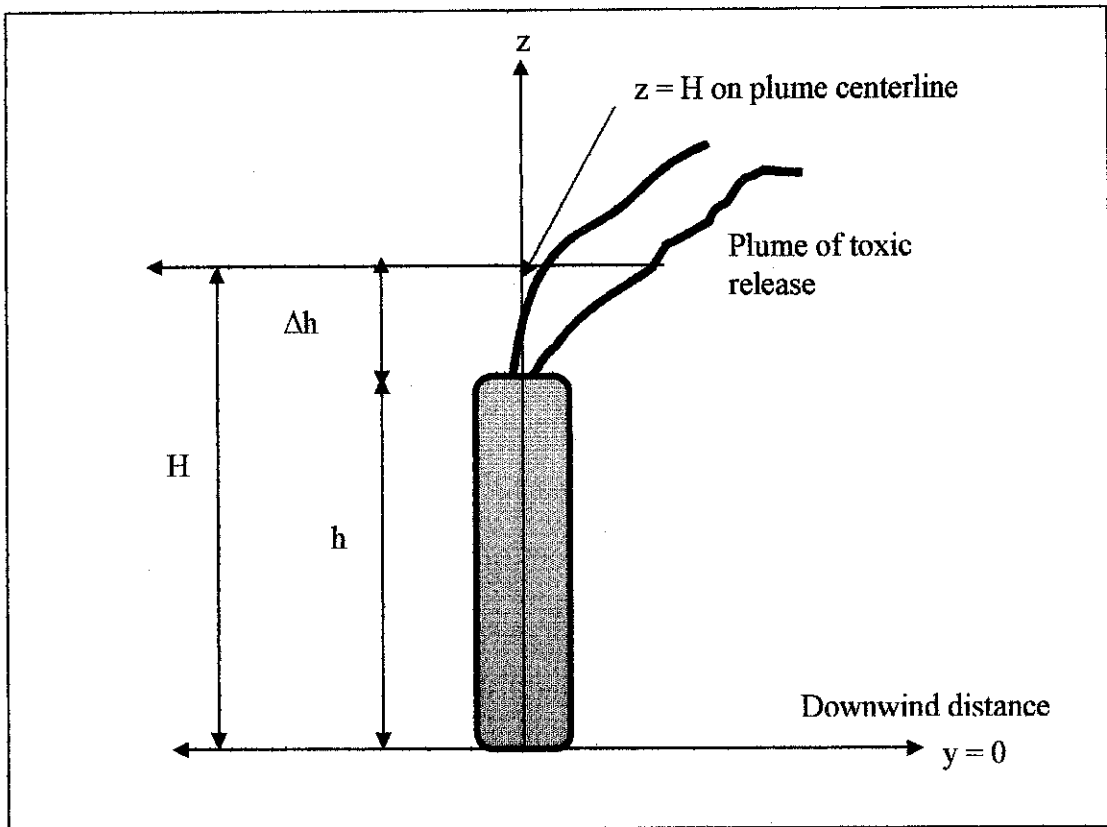
The traditional approach to predicting pollutant dispersion in the atmosphere is the use of Gaussian plume models (Kim, 2002). The Gaussian plume model is the most common air pollution model based on a simple formula describing three dimensional concentration field generated by a point source under stationary meteorological and emission conditions. The Gaussian models are based on steady state assumptions, and they require the flow to be in a homogenous and stationary turbulence state (Zannetti, 1990).

For a 2-dimensional spreading (see Figure 2.3), the plume is assumed to be emitted from a point with coordinates (0, H), where H is called the effective height. This effective height is the sum of the physical height (h); the height of the vessel from ground level and the plume rise (h).

The Gaussian plume derivation is as follows (De Nevers, 2000):

$$(\text{Accumulation rate}) = \sum (\text{all flow rates in}) - \sum (\text{all flow rates out}) \quad (2.0)$$

$$\text{Accumulation rate} = \frac{\partial (cV)}{\partial t} = V \frac{\partial c}{\partial t} = \Delta x \Delta y \Delta z \frac{\partial c}{\partial t} \quad (2.1)$$



**Figure 2.3** Two-dimensional air dispersion

The flux of material being mixed across any surface is given by (De Nevers, 2000):

$$\text{Flux} = (\text{time rate of mass flow per unit area}) = -K \frac{\partial c}{\partial n} \quad (2.2)$$

where  $c$  = concentration

$n$  = distance in the direction considered either  $x$ ,  $y$  or  $z$

$K$  = turbulent dispersion coefficient

The dimension of this flux is mass/time.area meaning that it has the same units for molecular diffusivity giving it the same form as being mass molecular diffusion. The turbulent dispersion coefficient, K is often called the eddy diffusivity (De Nevers, 2000).

$$\text{Net flow in the } x \text{ direction} = (-K \frac{\partial c}{\partial x})_{|x} - (-K \frac{\partial c}{\partial x})_{|x+\Delta x} \quad (2.3)$$

$$\text{Net flow in the } y \text{ direction} = (-K \frac{\partial c}{\partial y})_{|y} - (-K \frac{\partial c}{\partial y})_{|y+\Delta y} \quad (2.4)$$

$$\text{Net flow in the } z \text{ direction} = (-K \frac{\partial c}{\partial z})_{|z} - (-K \frac{\partial c}{\partial z})_{|z+\Delta z} \quad (2.5)$$

Substituting Eqs. (2.1), (2.3), (2.4) and (2.5) into Eq. (2.0) and dividing both sides by  $\Delta x \Delta y \Delta z$ ,

$$\begin{aligned} \frac{\partial c}{\partial t} = & \frac{(-K \frac{\partial c}{\partial x})_{|x} - (-K \frac{\partial c}{\partial x})_{|x+\Delta x}}{\Delta x} + \frac{(-K \frac{\partial c}{\partial y})_{|y} - (-K \frac{\partial c}{\partial y})_{|y+\Delta y}}{\Delta y} \\ & + \frac{(-K \frac{\partial c}{\partial z})_{|z} - (-K \frac{\partial c}{\partial z})_{|z+\Delta z}}{\Delta z} \end{aligned} \quad (2.6)$$

But  $\lim_{\Delta x \rightarrow 0}$ ,  $\lim_{\Delta y \rightarrow 0}$  and  $\lim_{\Delta z \rightarrow 0}$

$$\frac{\partial c}{\partial t} = K \frac{\partial^2 c}{\partial x^2} + K \frac{\partial^2 c}{\partial y^2} + K \frac{\partial^2 c}{\partial z^2} \quad (2.7)$$



The resulting concentration for two dimensional spreading is (Zannetti, 1990)

$$c = \frac{Q}{2 \Pi \sigma_y \sigma_z u} \exp [-1/2 (y/\sigma_y)^2 ] \exp [-1/2 (h_e - z/\sigma_z)^2 ] \quad (2.8)$$

in which  $u$  is the average horizontal wind speed,  $h_e$  is the effective emission height and  $\sigma_y$  and  $\sigma_z$  are lateral and vertical dispersion coefficients respectively.

Equation (2.8) illustrates several relationships between the concentrations and the parameters, which must be satisfied by all plume models:

- 1) The mean concentration is inversely proportional to the mean wind speed
- 2) The mean concentration is directly proportional to the release rate
- 3) The mean concentration is inversely proportional to the cross sectional area

The concentration of emission from the point of release takes into account the wind speed, height of the point of release, the area of point of release, the gaseous emission rate, the velocity of the gas released, the temperature of the gas released, the ambient temperature as well as the atmospheric stability conditions (Tirabassi, 2003).

Assumptions included in equations expressed are (Abdul Wahab):

- 1) inert passive pollutants
- 2) no gravity fallout
- 3) perfect reflection of the plume at underlying surface
- 4) a non-zero wind speed

The atmospheric stability conditions are based on Pasquill's wind stability category, which defines the air characteristics. The stability of the atmosphere is its tendency to resist or enhance vertical motion or alternatively to suppress existing turbulence (Essa et.

al, 2002). Wind stability is dependant on night or day and the wind speed. Below is the key to stability categories:

**Table 2.1** Key Stability Categories

Surface wind speed (at 10m above ground) m/s	Day Incoming solar radiation			Night	
	Strong	Moderate	Slight	Thinly overcast	Clear
0-2	A	A-B	B	-	-
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

The corresponding stability categories are as in Table 2.2 in the following page.

**Table 2.2 Pasquill's Wind Stability Category**

Wind Category	Condition
A	Very unstable
B	Unstable
C	Moderately unstable
D	Neutral
E	Moderately stable
F	Very stable

Pasquill's wind stability determines the dispersion coefficients  $\sigma_y$  and  $\sigma_z$ . The coefficients can be obtained graphically (Appendix B) or by calculating dispersion coefficients with formula recommended by Briggs.

## CHAPTER 3

### METHODOLOGY

The author developed the toxic effect risk model by carrying out the following steps:

**Step 1: Model development**

**Step 2: Simulation**

#### **3.1 Step 1: Model development**

In the first development step, the author builds the model by defining appropriate parameters required for users to input into the Excel worksheet. The author used a two-dimensional Gaussian air dispersion model, developing formulas by Briggs. The aim of the model is to generate a graph (output) that shows the concentration level of toxic releases at different distances from the source point of release. Subsequently, the concentration levels will define the risk of the concentration levels, citing the risk exposure in terms of probability of death (Probit).

To do this, various parameters and conditions are verified to be entered by the user into the Excel worksheet. The parameters are

#### *Gaseous Release*

- Name of component
- Molecular weight,  $M_s$  in kg/kgmol
- Specific heat,  $C_{p_s}$  in kJ/kmol.K
- Density,  $\rho_s$  in kg/m<sup>3</sup>
- Temperature,  $T_s$  in Kelvin
- Pressure,  $P_s$  in atm
- Flowrate,  $q$  in m<sup>3</sup>/s
- Distance of leak/rupture from ground level,  $h_s$  in meters

- Diameter of leak/rupture,  $d_s$  in meters
- Duration of exposure,  $t$  in seconds

*Atmospheric conditions*

- Molecular weight of air,  $M_a$  in kg/kgmol
- Density of air,  $\rho_a$  in  $\text{kg/m}^3$
- Ambient temperature,  $T_a$  in Kelvin
- Specific heat of air,  $C_{p_a}$  in  $\text{kJ/kmol.K}$
- Wind velocity,  $\bar{u}$  in  $\text{m/s}$
- Wind stability (Pasquill Stability A-F)
- Condition of area (urban or country)

From the inputs above, the model calculates,

$$\text{Rate of toxic release } Q_s = \frac{\text{Flowrate, } Q}{\text{Density, } \rho_s} \quad \text{in g/s} \quad (3.1)$$

$$\text{Gas exit velocity, } V_s = \frac{\text{Flowrate, } Q}{\text{Area of leak, } A} \quad \text{in m/s} \quad (3.2)$$

Gases possess positive buoyancy if they are lighter than air. The plume has a momentum due to the velocity as well as buoyancy [3]. This flux buoyancy is defined by

$$\text{Flux buoyancy, } F_b = \frac{\rho_s}{\rho_a} g V_s \frac{d_s^2}{4} [ (1 - M_s/M_a) + (\rho_a/\rho_s - 1) (C_{p_s}/C_{p_a}) ] \quad \text{in m}^4/\text{sec}^3 \quad (3.3)$$

The density difference is due to the higher than ambient temperature in the plume. This higher temperature causes the plume to be buoyant. This phenomenon is called the plume rise [3]. To account for this, the plume rise is calculated by,

$$x^* = 14 (Fb)^{0.625} \quad \text{when } Fb < 55 \quad (3.4)$$

$$x^* = 34 (Fb)^{0.4} \quad \text{when } Fb \geq 55 \quad (3.5)$$

where  $3.5x^*$  is the distance at which the plume rise terminates at.

From Eq. (3.2), the final plume rise is

$$\Delta h = 1.60 \frac{(Fb)^{1/3}}{\bar{u}} (3.5x^*)^{2/3} \quad (3.6)$$

Equation (3.6) however applies to gases that have lower density than that of air. For dense gas releases, the model predicts the following for  $\Delta h$ ,

$$\Delta h/d_s = 1.32 (V_s/u)^{1/3} (\rho_s/\rho_a)^{1/3} \left[ \frac{V_s^2 \rho_s}{d_s g (\rho_s - \rho_a)} \right]^{1/3} \quad (3.7)$$

The effect of the plume rise on the point source of release is the summation of  $H$  and  $\Delta h$ .

$$H = h_s + \Delta h \quad (3.8)$$

For wind stability, the user has to determine the wind condition during the time of the release and state the stability according to Pasquill type A-F.

Based on these wind stabilities, the lateral and vertical dispersion is determined. These coefficients are also dependent on rural or countryside areas.

**Table 3.1** Formulas recommended by Briggs for open country conditions (Schnelle et. al)

Pasquill Type	$\sigma_y$ (m)	$\sigma_z$ (m)
A	$0.22x (1+0.0001x)^{-0.5}$	$0.20x$
B	$0.16x (1+0.0001x)^{-0.5}$	$0.12x$
C	$0.11x (1+0.0001x)^{-0.5}$	$0.08x (1+0.0002x)^{-0.5}$
D	$0.08x (1+0.0001x)^{-0.5}$	$0.06x (1+0.00015x)^{-0.5}$
E	$0.06x (1+0.0001x)^{-0.5}$	$0.03x (1+0.0003x)^{-1}$
F	$0.04x (1+0.0001x)^{-0.5}$	$0.016x (1+0.0003x)^{-1}$

**Table 3.2** Formulas recommended by Briggs for urban area conditions (Schnelle et. al)

Pasquill Type	$\sigma_y$ (m)	$\sigma_z$ (m)
A-B	$0.32x (1+0.0004x)^{-0.5}$	$0.24x (1+0.001x)^{-0.5}$
C	$0.22x (1+0.0004x)^{-0.5}$	$0.20x$
D	$0.16x (1+0.0004x)^{-0.5}$	$0.014x (1+0.0003x)^{-0.5}$
E-F	$0.11x (1+0.0004x)^{-0.5}$	$0.08x (1+0.00015x)^{-0.5}$

The lateral and vertical dispersion coefficients can also be determined from graphs in Appendix B.

### 3.2 Step 2: Simulation

Once all this parameter required are entered into the worksheet, the model generates a concentration-distance graph based on the following equation for a two-dimensional dispersion:

$$c = \frac{Q}{2 \Pi \sigma_y \sigma_z u} \exp [-1/2 (y/\sigma_y)^2 ] \exp [-1/2 (h_e - z/\sigma_z)^2 ] \quad (3.9)$$

$z = 0$ , taking ground level as (0,0) with  $y$  as the downwind distance in the  $y$ -direction and  $z$  as the vertical distance.

The concentration values are then used to define the probit parameter,

$$Pr = A + B \ln (c^R t) \quad (3.10)$$

The probit equation parameters for this model are available for the following materials (Refer Appendix C).



## CHAPTER 4 RESULTS AND DISCUSSION

### 4.1 DATA REQUIREMENTS

#### 4.1.1 Data Input

Input data for this toxic-effect risk model comprises of two sets; one is the input data of the toxic gaseous release and the other is the input data of atmospheric and meteorological conditions. Sets of input data required are as below:

Data of Gaseous Toxic Release:

1. Name of component (chosen from a list of 22 available components)
2. Molecular Weight,  $M_s$  (kg/kgmol)
3. Density,  $\rho_s$  ( $\text{kg/m}^3$ )
4. Specific Heat,  $C_{p_s}$  (kJ/kmol.K)
5. Temperature,  $T_s$  (K)
6. Pressure,  $P_s$  (atm)
7. Flowrate,  $q_s$  ( $\text{m}^3/\text{s}$ )
8. Distance from ground-level,  $h_s$  (m)
9. Diameter of rupture,  $d_s$  (m)
10. Duration of Exposure,  $t$  (s)

Data of Atmospheric and Meteorological conditions:

1. Molecular Weight,  $M_a$  (kg/kgmol)
2. Density,  $\rho_a$  ( $\text{kg/m}^3$ )
3. Specific Heat,  $C_{p_a}$  (kJ/kmol.K)
4. Ambient Temperature,  $T_a$  (K)
5. Wind velocity,  $\bar{u}$  (m/s)
6. Wind Stability category (A-F, chosen based on Pasquill wind stability table)
7. Area class (chosen either urban or country)

#### 4.1.2. Data Output

Calculated data:

1. Rate of toxic release,  $Q$  (g/s)
2. Gas exit velocity,  $V_s$  (m/s)
3. Flux buoyancy,  $F_b$  ( $m^4/s^3$ )
4. Distance at which plume rise effect terminates,  $x^*$  (m)
5. Plume rise,  $\Delta h$  (m)
6. Plume effect,  $H$  (m)

#### 4.2 RESULTS

The model was first tested on Ammonia ( $NH_3$ ) and Sulfur Dioxide ( $SO_2$ ), two components differing in density. The two components were tested with the same atmospheric and meteorological conditions and duration of exposure. Subsequently, the model was tested on  $NH_3$  to observe the effects of various wind stability on toxic releases.

##### 4.2.1. Ammonia ( $NH_3$ )

Data of Gaseous Toxic Release:

1. Name of component = 4 ( $NH_3$ )
2.  $M_s = 17.03$  kg/kgmol
3.  $\rho_s = 1.4045$  kg/ $m^3$
4.  $C_{p_s} = 0.1442$  kJ/kmol.K
5.  $T_s = 300$  K
6.  $P_s = 1.63$  atm
7.  $q_s = 11.05$   $m^3/s$
8.  $h_s = 15$  m
9.  $d_s = 0.01$  m
10.  $t = 300$  s

Data of Atmospheric and Meteorological conditions:

1.  $M_a = 29.0 \text{ kg/kgmol}$
2.  $\rho_a = 2.2640 \text{ kg/m}^3$
3.  $C_{p_a} = 0.038 \text{ kJ/kmol.K}$
4.  $T_a = 303 \text{ K}$
5.  $\bar{u} = 3 \text{ m/s}$
6. Wind Category = C
7. Area class = c (country)

#### 4.2.2. Sulfur Dioxide

Data of Gaseous Toxic Release:

1. Name of component = 21 ( $\text{SO}_2$ )
2.  $M_s = 64.06 \text{ kg/kgmol}$
3.  $\rho_s = 11.56 \text{ kg/m}^3$
4.  $C_{p_s} = 32.82 \text{ kJ/kmol.K}$
5.  $T_s = 300 \text{ K}$
6.  $P_s = 4.16 \text{ atm}$
7.  $q_s = 0.865 \text{ m}^3/\text{s}$
8.  $h_s = 15 \text{ m}$
9.  $d_s = 0.01 \text{ m}$
10.  $t = 300 \text{ s}$

Data of Atmospheric and Meteorological conditions:

1.  $M_a = 29.0 \text{ kg/kgmol}$
2.  $\rho_a = 2.2640 \text{ kg/m}^3$
3.  $C_{p_a} = 0.038 \text{ kJ/kmol.K}$
4.  $T_a = 303 \text{ K}$
5.  $\bar{u} = 3 \text{ m/s}$

- 6. Wind Category = C
- 7. Area class = c (country)

**Table 4.1** Results of NH<sub>3</sub> concentration and Probit values

Downwind distance (km)	Concentration (ppm)	Probit values
0.00	0.0000	0.00
0.30	70.2837	-17.19
0.50	26.0241	-20.86
0.80	10.5873	-24.19
1.20	4.9543	-27.00
1.80	2.3669	-29.73
3.00	0.9701	-33.03
6.00	0.3155	-37.19
10.00	0.1483	-39.98
14.00	0.0933	-41.70
16.00	0.0781	-42.35
18.00	0.0671	-42.92
20.00	0.0586	-43.42
22.00	0.0520	-43.86
25.00	0.0444	-44.45
30.00	0.0356	-45.26
40.00	0.0254	-46.52
60.00	0.0160	-48.21
85.00	0.0110	-49.62
100.00	0.0092	-50.27

**Table 4.2 SO<sub>2</sub> concentration and Probit values**

Downwind distance (km)	Concentration (ppm)	Probit values
0.00	0.0000	0.00
0.30	69.9843	-3.37
0.50	25.9133	-5.46
0.80	10.5422	-7.34
1.20	4.9361	-8.94
1.80	2.4198	-10.43
3.00	1.1742	-11.95
6.00	0.4995	-13.75
10.00	0.2616	-15.11
14.00	0.1714	-15.99
16.00	0.1453	-16.34
18.00	0.1258	-16.64
20.00	0.1108	-16.91
22.00	0.0988	-17.15
25.00	0.0849	-17.47
30.00	0.0686	-17.92
40.00	0.0493	-18.61
60.00	0.0315	-19.55
85.00	0.0216	-20.35
100.00	0.0182	-20.71

### 4.2.3. Effect of Wind Stability on NH<sub>3</sub> concentrations

The effect of wind stability (Pasquill wind stability A-F) on concentrations and Probit values of NH<sub>3</sub> was tested with this model. Parameter inputs remain the same, but the wind stability is varied. Results are tabulated as below:

**Table 4.3** Wind Stability effects on concentration of NH<sub>3</sub>

Downwind Distance (km)	Wind Stability					
	A	B	C	D	E	F
0.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.30	13.6650	31.3153	70.3427	150.8255	364.0482	1023.7026
0.50	4.9669	11.3824	26.0460	60.2265	139.6071	392.5735
0.80	1.9677	4.5093	10.5962	26.7520	59.6358	167.6942
1.20	0.8905	2.0409	4.9584	13.6596	29.6030	83.2424
1.80	0.4062	0.9311	2.3689	7.1632	15.2920	42.9999
3.00	0.1535	0.3518	0.9709	3.3000	7.1289	20.0455
6.00	0.0425	0.0976	0.3158	1.2341	2.9137	8.1924
10.00	0.0171	0.0393	0.1484	0.6283	1.6752	4.7099
14.00	0.0095	0.0219	0.0933	0.4117	1.2171	3.4217
16.00	0.0076	0.0175	0.0782	0.3498	1.0818	3.0411
18.00	0.0062	0.0143	0.0671	0.3035	0.9787	2.7513
20.00	0.0052	0.0120	0.0587	0.2677	0.8975	2.5229
22.00	0.0044	0.0103	0.0520	0.2393	0.8317	2.3379
25.00	0.0036	0.0083	0.0444	0.2063	0.7533	2.1174
30.00	0.0026	0.0062	0.0356	0.1674	0.6579	1.8491
40.00	0.0016	0.0039	0.0254	0.1212	0.5378	1.5113
60.00	0.0008	0.0020	0.0161	0.0778	0.4132	1.1608
85.00	0.0005	0.0012	0.0110	0.0537	0.3344	0.9391
100.00	0.0004	0.0009	0.0092	0.0452	0.3041	0.8536

## 4.3 DISCUSSION

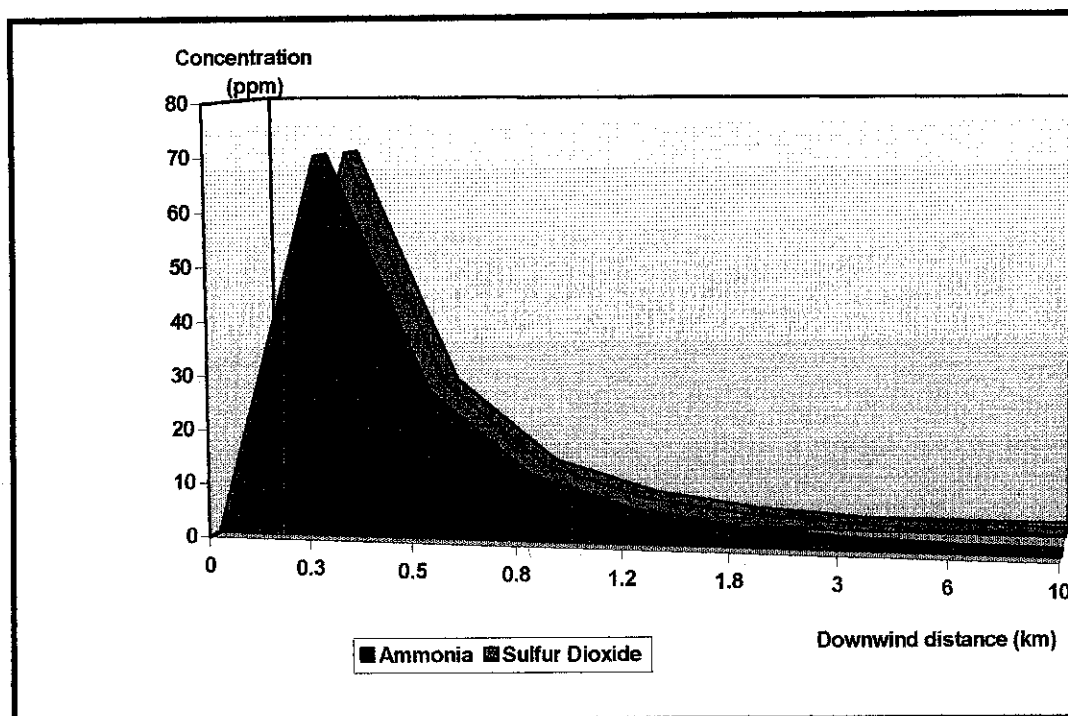
### 4.3.1. 2-Dimensional Gaussian Model

Trial runs for  $\text{NH}_3$  and  $\text{SO}_2$  are done in a two-dimensional modeling. Since this model is to predict concentrations at ground level to determine its effect on receptors close to ground (people, plants and animals), the vertical distance  $z$  is set to zero.

### 4.3.2. Comparison of concentration levels between $\text{NH}_3$ and $\text{SO}_2$

Two different components in gaseous form were tested with this model to determine the concentration levels at distances from the point of source to 100 km downwind. Ammonia ( $\text{NH}_3$ ) and Sulfur Dioxide ( $\text{SO}_2$ ) are both toxic materials from industrials that pose great hazards if it were released into the atmosphere. Ammonia in gaseous form is lighter than air ( $\rho = 1.4045 \text{ kg/m}^3$ ) while Sulfur Dioxide ( $\rho = 11.56 \text{ kg/m}^3$ ) is a heavy gas; its density is higher than air. The model is simulated for both toxic materials with the same rate of toxic release,  $Q$  in g/s, also for the atmospheric and meteorological conditions.

The comparison of output of concentration levels against the distance downwind is shown Figure 4.1 in the following page.



**Figure 4.1** Graph of comparison between concentrations of  $\text{NH}_3$  and  $\text{SO}_2$

Based on calculated results, both toxic materials give almost similar concentrations, with the highest peak concentrations reaching 70.34 ppm for  $\text{NH}_3$  and 69.98 ppm for  $\text{SO}_2$  respectively, occurring at a downwind distance of 0.3 km. Plumes rise buoyantly due to the fact that they are hotter than the surrounding air and also because they are released in an upward motion, having a vertical velocity. As they mix with the surrounding air, it loses velocity and they level off when they reach ambient temperature. However, the plume rise is also dependent on the density of the gases. Here, gases lighter than air like  $\text{NH}_3$  has a positive buoyancy flux, indicating that the plume is fluffy and almost weightless, and produces a larger plume rise than that of  $\text{SO}_2$ . Gases that are denser than air have a tendency to slump and spread out in thick clouds rather than float buoyantly



into the air. Due to this, the plume rise is small, in this case producing a negative plume rise, indicating that the cloud release is heavy and slumps at a level much lower compared to that of the lighter gas. The differences in plume rise for both these gases are because of the initial buoyancy and momentum of the release.

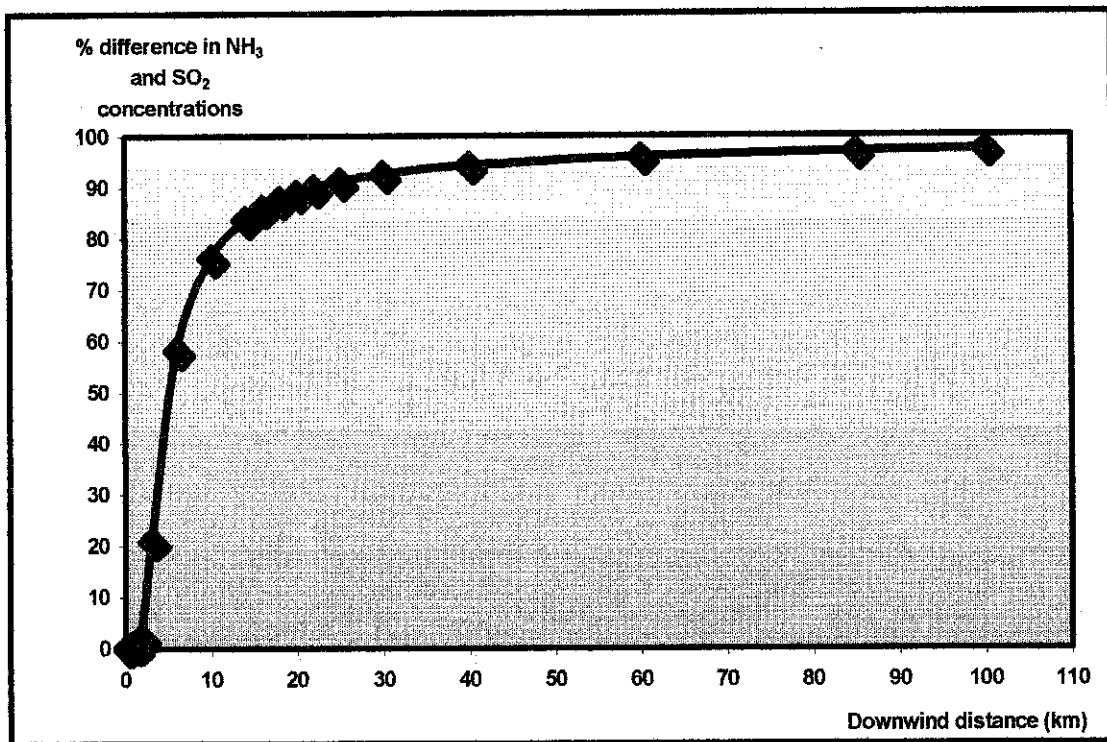


Figure 4.2 Graph of percentage difference between concentrations of NH<sub>3</sub> and SO<sub>2</sub>

Although the plume rise for NH<sub>3</sub> is higher than that of SO<sub>2</sub>, the concentration levels of these two pollutants are almost similar. The difference of concentration levels between NH<sub>3</sub> and SO<sub>2</sub> is minimal at the peak points, but as the toxic cloud moves further downwind, the difference in concentration levels start to increase. This is due to the fact that SO<sub>2</sub> is a much denser gas than NH<sub>3</sub>. At the same point downwind where the lighter gas starts to rise buoyantly, the denser gas starts plumes downwards. Therefore, the

difference in concentration between SO<sub>2</sub> and NH<sub>3</sub> increases as it approaches 100 km downwind. Figure 4.2 above illustrates this.

### 4.3.3 Comparison of Probit values between NH<sub>3</sub> and SO<sub>2</sub>

Probit values measure the probability of death when exposed to a certain concentration with a function of its time exposure.

The Probit equation for NH<sub>3</sub> is

$$\text{Pr} = -35.9 + 1.85 \ln (c^2t) \quad (4.1)$$

The Probit equation for SO<sub>2</sub> is

$$\text{Pr} = -1.22 + \ln (c^{2.4}t) \quad (4.2)$$

As explained, the concentration of NH<sub>3</sub> and SO<sub>2</sub> at the same distance in the y-direction is almost similar, but the extent of danger exposed by each of these two toxic materials can be seen through its Probit values. The basic understanding to relate the danger of a certain toxic materials with its Probit values is that the higher the Probit values, the higher it is the risk of exposure.

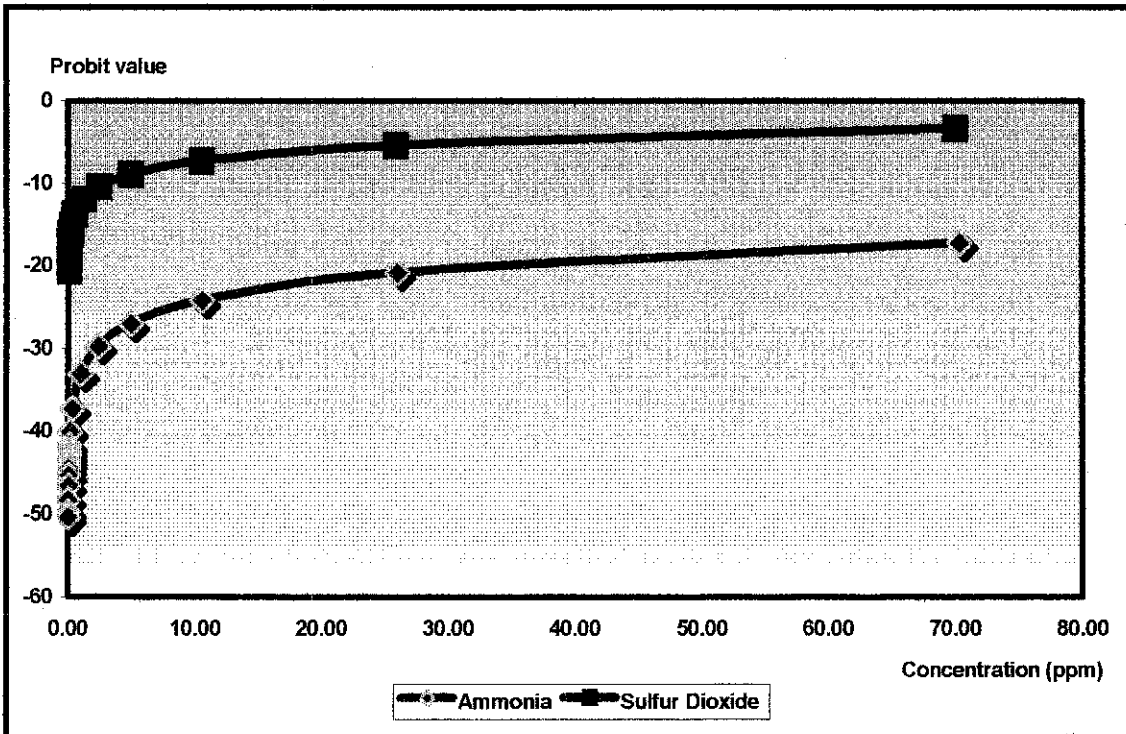


Figure 4.3 Graph of Probit values against concentrations of NH<sub>3</sub> and SO<sub>2</sub>

From Figure 4.3, the Probit values for NH<sub>3</sub> ranges from -50.26 to -17.19 while the Probit range for SO<sub>2</sub> is from -20.71 to -3.37. Probit values for SO<sub>2</sub> are 60-80% higher than NH<sub>3</sub>. This shows that SO<sub>2</sub> releases expose a higher exposure risk, even at almost similar concentrations with NH<sub>3</sub>.

Based on the concentration levels and the Probit values, the extent of injury caused or the appropriate action to be taken can be identified. These values responses to how much damage or injury the toxic release can cause if an accident were to occur. ILDH values (Immediately Dangerous to Life and Health) for NH<sub>3</sub> is 300 ppm while for SO<sub>2</sub> is 100 ppm, indicating that it takes a smaller volume concentration of SO<sub>2</sub> to exposure great

danger to life than  $\text{NH}_3$  ([www.aiche.com](http://www.aiche.com)). At 70 ppm of  $\text{SO}_2$ , a person exposed to this toxic will experience disorientation, dizziness and restricted visual. Exposure to 70 ppm of  $\text{NH}_3$  causes nausea and headache and ([www.cdc.gov](http://www.cdc.gov)).

#### **4.3.4 Effect of wind stability on toxic releases**

With this model, the effects of wind stability on the concentration and Probit values of  $\text{NH}_3$  were studied. The Pasquill wind stability category classifies the condition of the atmosphere, measuring the meteorology of air to certain degrees of stability. Although the categories are subjected to one's definition of air stability, Pasquill's categorizing of wind stability shows a clear and concise effect of the condition of atmosphere on toxic releases.

Pasquill's wind stability categorizes wind category A as very unstable, B as unstable, C as moderately unstable, D as neutral, E moderately stable and F as stable. The results show the highest concentration if an  $\text{NH}_3$  were to release in a stable wind condition (F). During steady wind, there is no turbulence or eddy current to carry the molecules of toxic gases higher or further into the atmosphere. The molecules itself have momentum to rise, but the rate of transfer between the gases and the air molecules are low. This relates to the dispersion coefficients,  $\sigma_y$  and  $\sigma_z$ , the primary functions of the wind stability. Dispersion coefficients are transport coefficients in which determine the lateral and vertical spreading of the molecules. Therefore, the more unstable the atmospheric conditions, the easier it is for gases to diffuse into the atmosphere. Figure 4.4 shows the relevancy of the wind stability to the concentration of the toxic release.

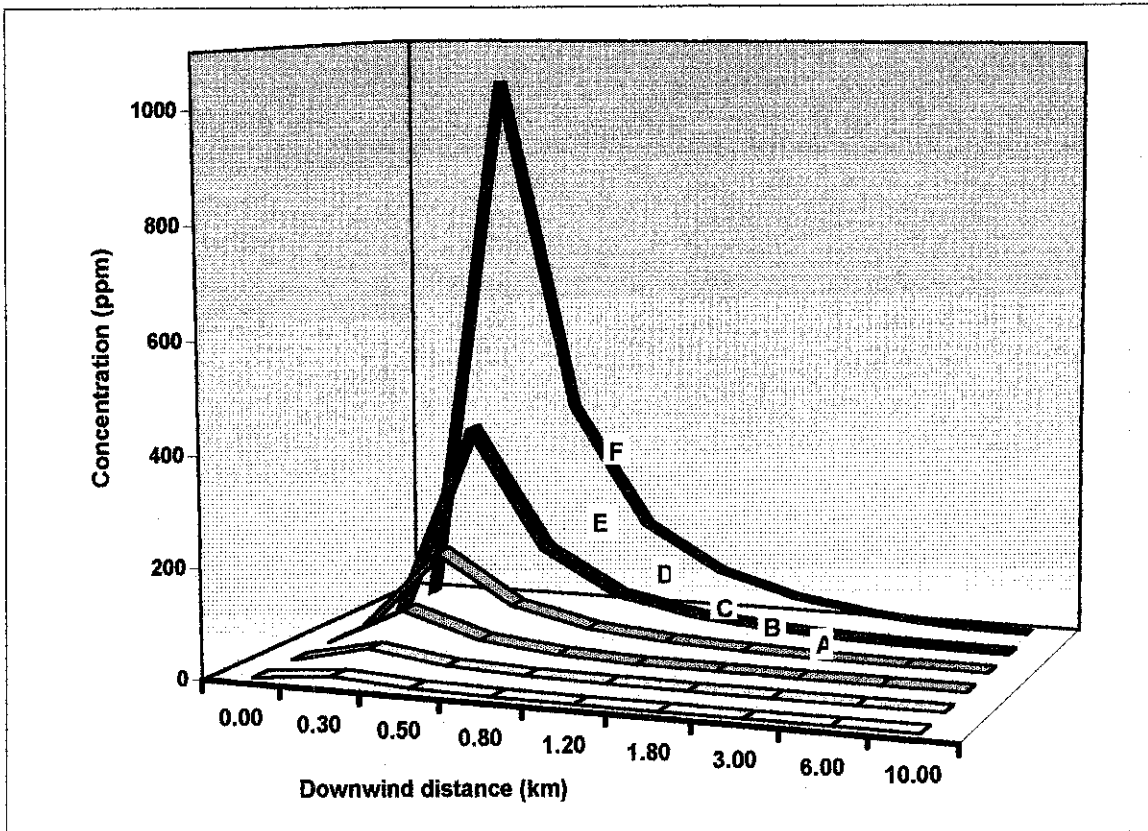


Figure 4.4 Effects of wind stability on concentrations of  $\text{NH}_3$

Concentrations of  $\text{NH}_3$  can go up to 1,023 ppm during stable wind conditions as compared to only 13 ppm, indicating that meteorological factors highly affects dispersion of gases into the atmosphere. The plume rise of the gaseous release is also dependant on the wind conditions. Plume rise has an inverse relationship with wind velocity, at which when the wind is stable, the air velocity is low and the plume rise is high. During unstable conditions (wind category A), the peak concentration of  $\text{NH}_3$  is very low, at 13 ppm. This is a clear explanation of the relationship between dispersion coefficients, wind speed, plume rise and the concentration of the gas. Unstable wind conditions have a high wind velocity; in which it has higher lateral and vertical dispersion coefficients, allowing the gas molecules to disperse easily into the atmosphere.

## CHAPTER 5

### CONCLUSION AND RECOMMENDATIONS

#### 5.1 Conclusion

The toxic effect risk model developed for inherent safety design is an effective tool that can be used to carefully predict the concentration levels of gaseous toxic releases into the atmosphere. Following that, the risk and consequences of this toxic release can be prevented or eliminated at an early stage by determining the extent risk involved.

From the study, the Gaussian air dispersion model clearly simulates the accidental toxic release from vessels and storage tanks by predicting the toxic level of concentration at different distances from the point source of pollution. Variable inputs required from the user are properties of the gaseous release and atmospheric and meteorological conditions. The output from this is a concentration-distance graph and a Probit-concentration graph.

The model tested on two different materials,  $\text{NH}_3$  and  $\text{SO}_2$  produced results showing almost similar concentrations for both gases. The peak concentration for  $\text{NH}_3$  and  $\text{SO}_2$  were 70.28 ppm and 70.32 ppm respectively. Since  $\text{NH}_3$  is a lighter gas than air, the plume rise is higher than  $\text{SO}_2$ ; heavier gases form thicker clouds and slump towards the ground with respect to time. The probit values for  $\text{SO}_2$  are much higher than the values for  $\text{NH}_3$  although at almost similar peak concentrations. This shows that  $\text{SO}_2$  has 60-80% greater risk of exposure than the toxic release of  $\text{NH}_3$ . At the concentrations obtained, both toxic releases exposes minimal hazard to the human body.

Wind stability strongly affects the concentration of pollutants downwind. During unstable wind (Pasquill wind stability A), the concentration level of  $\text{NH}_3$  downwind is comparatively low (peak concentration 13ppm) as that during stable wind (Pasquill wind stability F) which gives a much higher concentration level (peak concentration 1,023 ppm). The more stable the condition of the wind, the higher the level of concentration downwind due to the inability of the gas molecules to disperse easily into the atmosphere.

## **5.2 Recommendations**

For further development, specific references to relate the Probit equations to the extent of injury could be expanded to correctly define certain ranges of Probit values with its consequences and risk exposures. Most of the guidelines relating the exposure levels of injury to the concentration of toxic materials do not have a sharp dividing line to clearly define levels of dangerous or potentially hazardous. The extent and injury effect of toxic materials to human life is very subjective and is dependant upon many factors- the toxic material, the receptor and its surroundings. Threshold values are guidelines to determine toxicity of a substance, but many other factors also have to be taken into account.

Another expansion to this model is to include the variable of time into the dispersion model. The concentration calculated for this model assumes the duration of time of release is small since the model serves for the purpose of instantaneous gas release. Hence, the time exposure is negligible here. Besides determining the concentration of the gases at distances downwind, it should also determine concentration levels at specific interval times.

## CHAPTER 6

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## **APPENDIX A**

## Toxic Effect Risk Model for Gaseous Releases

Enter the following inputs:

### Gaseous Release

Name of component  
 Molecular weight  
 Density  
 Specific heat  
 Temperature  
 Pressure  
 Flowrate  
 Distance of leak/rupture from ground level  
 Diameter of leak/rupture  
 Duration of exposure


kg/kgmol  
 kg/m<sup>3</sup>  
 kJ/kgmol.K  
 K  
 atm  
 m<sup>3</sup>/s  
 m  
 m  
 s

### Atmospheric conditions

Molecular weight of air  
 Density of air  
 Specific heat of air  
 Ambient temperature  
 Wind velocity  
 Wind stability (A-F)  
 Condition of area (U=Urban, C=Country)


kg/kgmol  
 kg/m<sup>3</sup>  
 kJ/kgmol.K  
 K  
 m/s

### Calculated values

Rate of toxic release  
 Stack gas exit velocity  
 Flux buoyancy  
 x\*  
 Plume rise  
 Plume effect


g/s  
 m/s  
 m<sup>4</sup>/s<sup>3</sup>  
 m  
 m  
 m

Probit equation parameters:

Row	Component		MW	A	B	n
1	Acrolein	C3H4O	56.060	-9.931	2.05	1.00
2	Acrylonitrile	C3H3N	53.064	-29.42	3.01	1.43
3	Allyl Alcohol	C3H6O	58.080	-4.22	1.00	1.00
4	Ammonia	H3N	17.030	-36.9	1.85	2.00
5	Benzene	C6H6	78.110	-109.78	5.30	2.00
6	Bromine	Br2	159.800	-9.04	0.92	2.00
7	Carbon Disulfide	CS2	76.130	-48.56	4.20	1.00
8	Carbon monoxide	CO	28.010	-37.98	3.70	1.00
9	Carbon Tetrachloride	CCl4	153.840	-6.29	0.41	2.50
10	Chlorine	Cl2	70.905	-8.29	0.92	2.00
11	Ethylene Oxide	C2H4O	44.050	-6.19	1.00	1.00
12	Hydrogen Chloride	HCl	36.461	-16.85	2.00	1.00
13	Hydrogen Cyanide	HCN	27.026	-29.42	3.01	1.43
14	Hydrogen Sulfide	H2S	34.082	-31.42	3.01	1.43
15	Methyl Bromide	CH3Br	94.939	-56.81	5.27	1.00
16	Methyl Isocyanate	C2H3NO	57.052	-5.642	1.64	0.66
17	Nitrogen Dioxide	NO2	46.006	-13.79	1.40	2.00
18	Phosgene	CCl2O	98.920	-19.27	3.89	1.00
19	Phosphine	H3P	33.998	-2.25	1.00	1.00
20	Propylene Oxide	C3H6O	58.060	-7.415	0.51	2.00
21	Sulfur Dioxide	SO2	64.065	-15.67	2.10	1.00
22	Toluene	C7H8	92.130	6.794	0.41	2.60

## Toxic Effect Risk Model for Gaseous Releases

Enter the following inputs:

### Gaseous Release

Name of component	4	
Molecular weight	17.03	kg/kgmol
Density	1.4045	kg/m <sup>3</sup>
Specific heat	0.1442	kJ/kmol.K
Temperature	370	K
Pressure	1.63	atm
Flowrate	7.16	m <sup>3</sup> /s
Distance of leak/rupture from ground level	15.00	m
Diameter of leak/rupture	0.01	m
Duration of exposure	300	s

### Atmospheric conditions

Molecular weight of air	29.000	kg/kgmol
Density of air	2.2640	kg/m <sup>3</sup>
Specific heat of air	0.0038	kJ/kmol.K
Ambient temperature	303	K
Wind velocity	3	m/s
Wind stability (A-F)	c	
Condition of area (U=Urban, C=Country)	c	

### Calculated values

Rate of toxic release	10,050.60	g/s
Gas exit velocity	63,272.93	m/s
Flux buoyancy	2,163,237.1941	m <sup>4</sup> /s <sup>3</sup>
x*	11,628.4164	m
Plume rise	81,612.9708	m
Plume effect	81,627.9708	m

**Estimated Concentration of Ground-Level Toxic Release (ppm)  
on Plume Centerline at Selected Distances (m) from point source**

Downwind distance (km)	Estimated concentration (ppm)	Probit
0.00	0.0000	0.00
0.30	70.3427	-17.19
0.50	26.0460	-20.86
0.80	10.5982	-24.19
1.20	4.9584	-27.00
1.80	2.3689	-29.73
3.00	0.9709	-33.03
6.00	0.3158	-37.19
10.00	0.1484	-39.98
14.00	0.0933	-41.70
16.00	0.0782	-42.35
18.00	0.0671	-42.92
20.00	0.0587	-43.42
22.00	0.0520	-43.86
25.00	0.0444	-44.44
30.00	0.0356	-45.26
40.00	0.0254	-46.51
60.00	0.0161	-48.21
85.00	0.0110	-49.62
100.00	0.0092	-50.27

**Toxic Effect Risk Model for Gaseous Releases**

Enter the following inputs:

**Gaseous Release**

Name of component	21	
Molecular weight	64.065	kg/kgmol
Density	9.4966	kg/m <sup>3</sup>
Specific heat	0.9390	kJ/kmol.K
Temperature	370	K
Pressure	1.77	atm
Flowrate	1.06	m <sup>3</sup> /s
Distance of leak/rupture from ground level	30.00	m
Diameter of leak/rupture	0.01	m
Duration of exposure	300	s

**Atmospheric conditions**

Molecular weight of air	29.000	kg/kgmol
Density of air	2.2640	kg/m <sup>3</sup>
Specific heat of air	0.0038	kJ/kmol.K
Ambient temperature	303	K
Wind velocity	3	m/s
Wind stability (A-F)	c	
Condition of area (U=Urban, C=Country)	c	

**Calculated values**

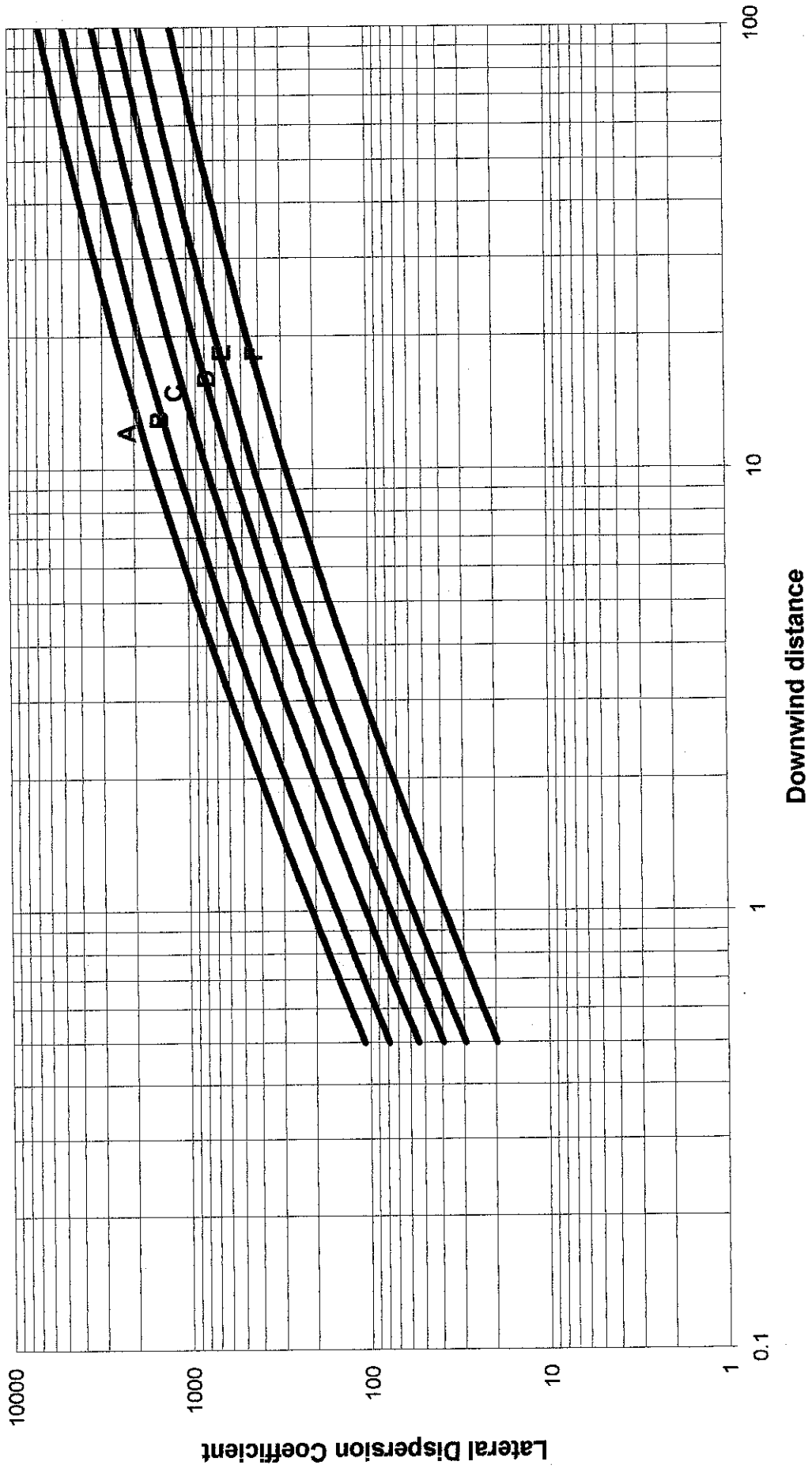
Rate of toxic release	10,047.40	g/s
Stack gas exit velocity	9,354.77	m/s
Flux buoyancy		m <sup>4</sup> /s <sup>3</sup>
x*		m
Plume rise	370.2142	m
Plume effect	400.2142	m

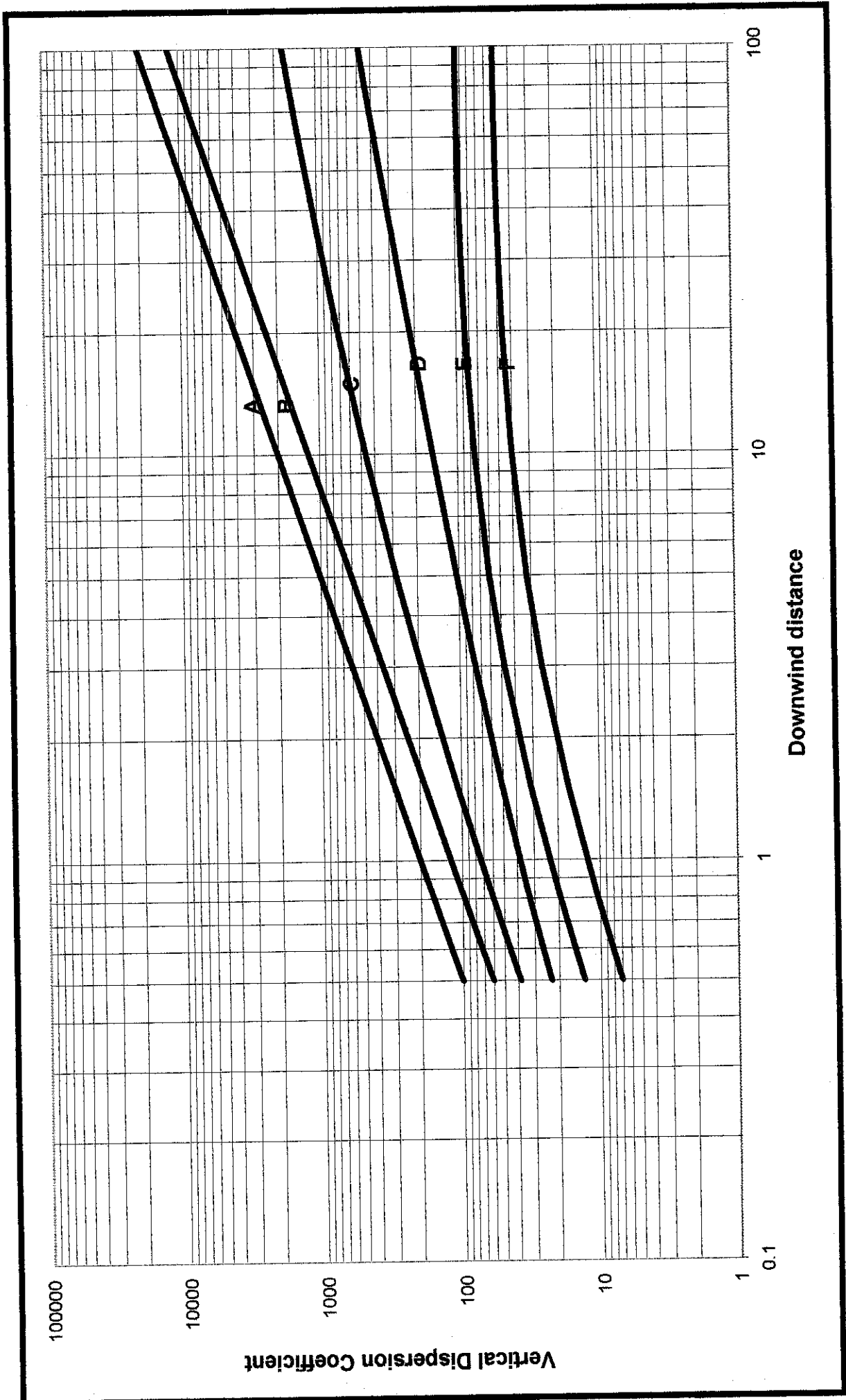
**Estimated Concentration of Ground-Level Toxic Release (ppm)  
on Plume Centerline at Selected Distances (m) from point source**

Downwind distance (km)	Estimated concentration (ppm)	Probit
0.00	0.0000	0.0000
0.30	70.3203	-3.3588
0.50	26.0377	-5.4451
0.80	10.5928	-7.3338
1.20	4.9570	-8.9285
1.80	2.3806	-10.4688
3.00	1.0755	-12.1373
6.00	0.4626	-13.9091
10.00	0.2503	-15.1990
14.00	0.1665	-16.0544
16.00	0.1419	-16.3914
18.00	0.1233	-16.6865
20.00	0.1088	-16.9485
22.00	0.0973	-17.1839
25.00	0.0838	-17.4970
30.00	0.0679	-17.9381
40.00	0.0491	-18.8211
60.00	0.0314	-19.5590
85.00	0.0216	-20.3452
100.00	0.0182	-20.7070



## **APPENDIX B**



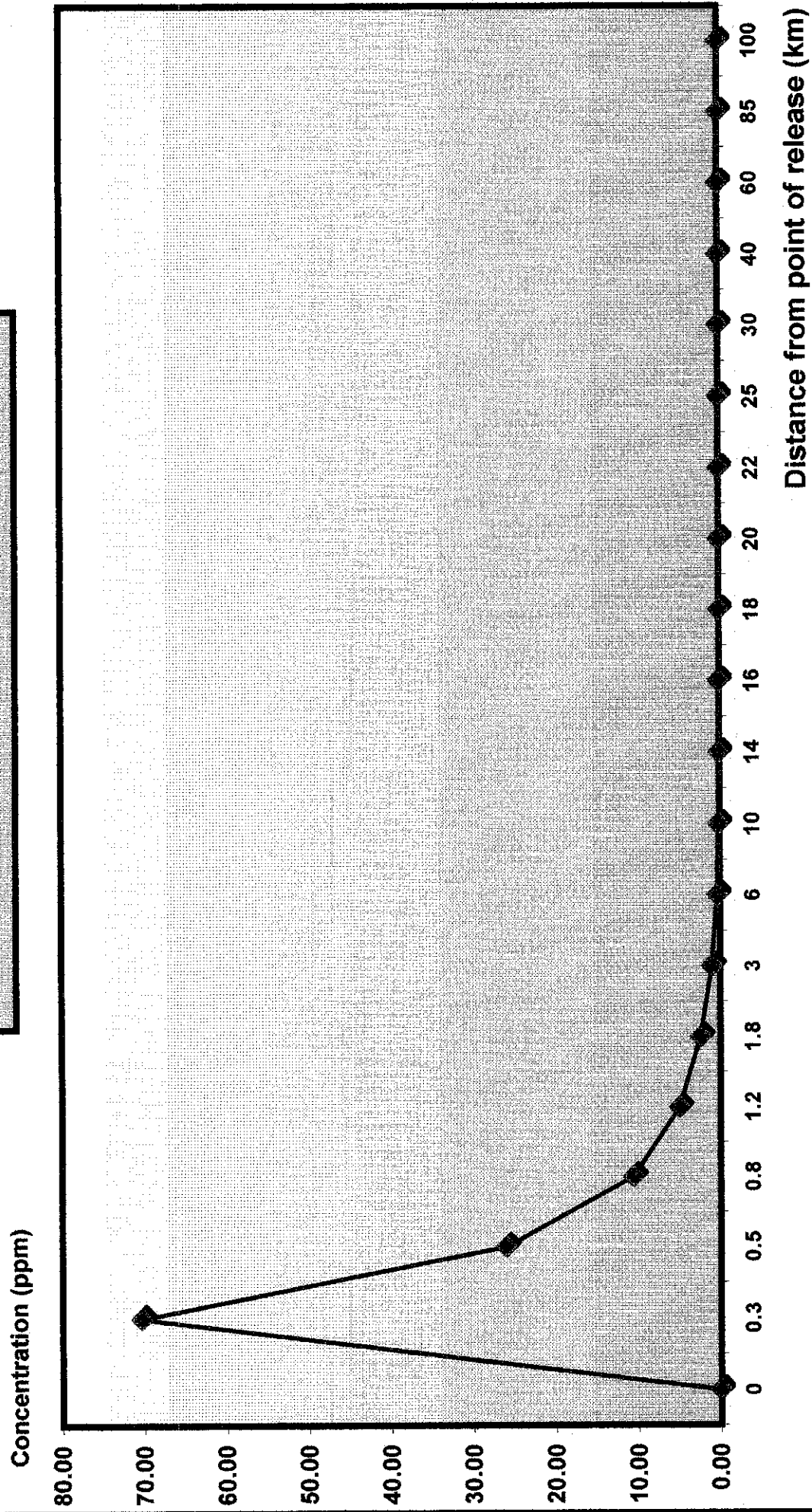


## **APPENDIX C**

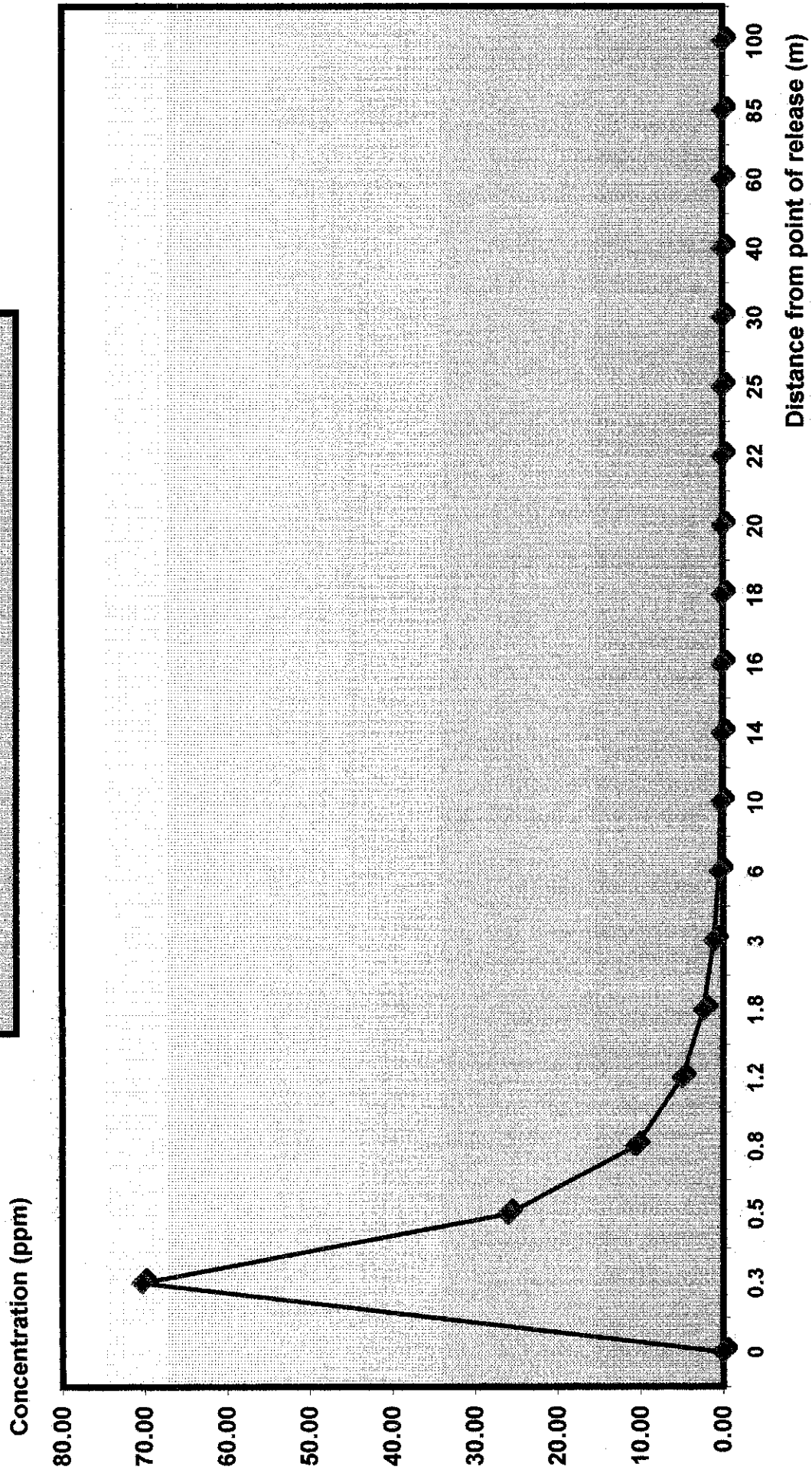
Component	Formula	Molecular weight (kg/kmol)	A	B	n
Acrolein	C <sub>3</sub> H <sub>4</sub> O	56.060	-9.931	2.05	1.00
Acrylonitrile	C <sub>3</sub> H <sub>3</sub> N	53.064	-29.42	3.01	1.43
Allyl Alcohol	C <sub>3</sub> H <sub>6</sub> O	58.080	-4.22	1.00	1.00
Ammonia	H <sub>3</sub> N	17.030	-35.9	1.85	2.00
Benzene	C <sub>6</sub> H <sub>6</sub>	78.110	-109.78	5.30	2.00
Bromine	Br <sub>2</sub>	159.800	-9.04	0.92	2.00
Carbon Disulfide	CS <sub>2</sub>	76.130	-46.56	4.20	1.00
Carbon monoxide	CO	28.010	-37.98	3.70	1.00
Carbon Tetrachloride	CCl <sub>4</sub>	153.840	-6.29	0.41	2.50
Chlorine	Cl <sub>2</sub>	70.905	-8.29	0.92	2.00
Ethylene Oxide	C <sub>2</sub> H <sub>4</sub> O	44.050	-6.19	1.00	1.00
Hydrogen Chloride	HCl	36.461	-16.85	2.00	1.00
Hydrogen Cyanide	HCN	27.026	-29.42	3.01	1.43
Hydrogen Sulfide	H <sub>2</sub> S	34.082	-31.42	3.01	1.43
Methyl Bromide	CH <sub>3</sub> Br	94.939	-56.81	5.27	1.00
Methyl Isocyanate	C <sub>2</sub> H <sub>3</sub> NO	57.052	-5.642	1.64	0.65
Nitrogen Dioxide	NO <sub>2</sub>	46.006	-13.79	1.40	2.00
Phosgene	CCl <sub>2</sub> O	98.920	-19.27	3.69	1.00
Phosphine	H <sub>3</sub> P	33.998	-2.25	1.00	1.00
Propylene Oxide	C <sub>3</sub> H <sub>6</sub> O	58.060	-7.415	0.51	2.00
Sulfur Dioxide	SO <sub>2</sub>	64.065	-15.67	2.10	1.00
Toluene	C <sub>7</sub> H <sub>8</sub>	92.130	6.794	0.41	2.50

## **APPENDIX D**

Concentration of NH<sub>3</sub> vs Downwind distance



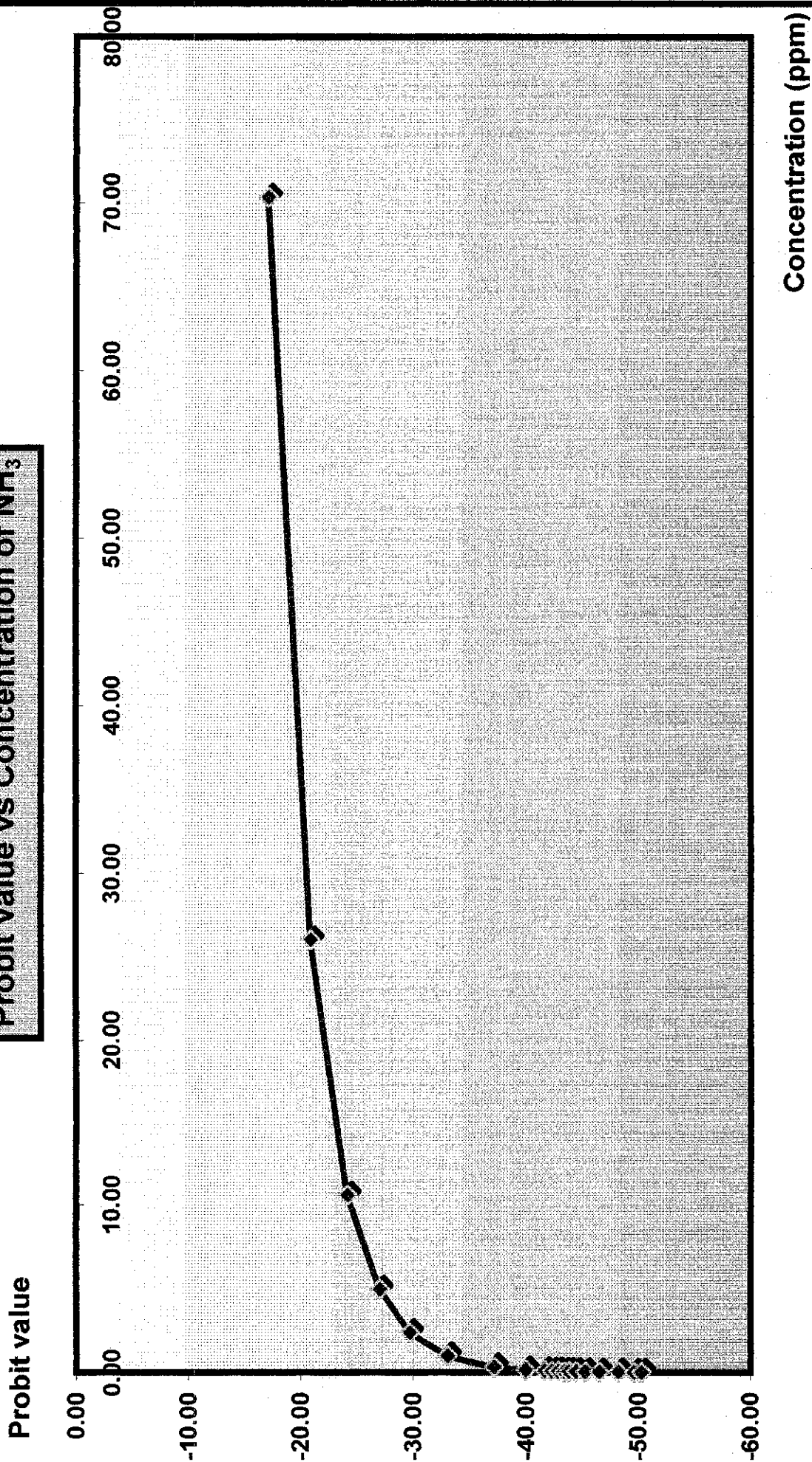
### Concentration of SO<sub>2</sub> vs Downwind distance



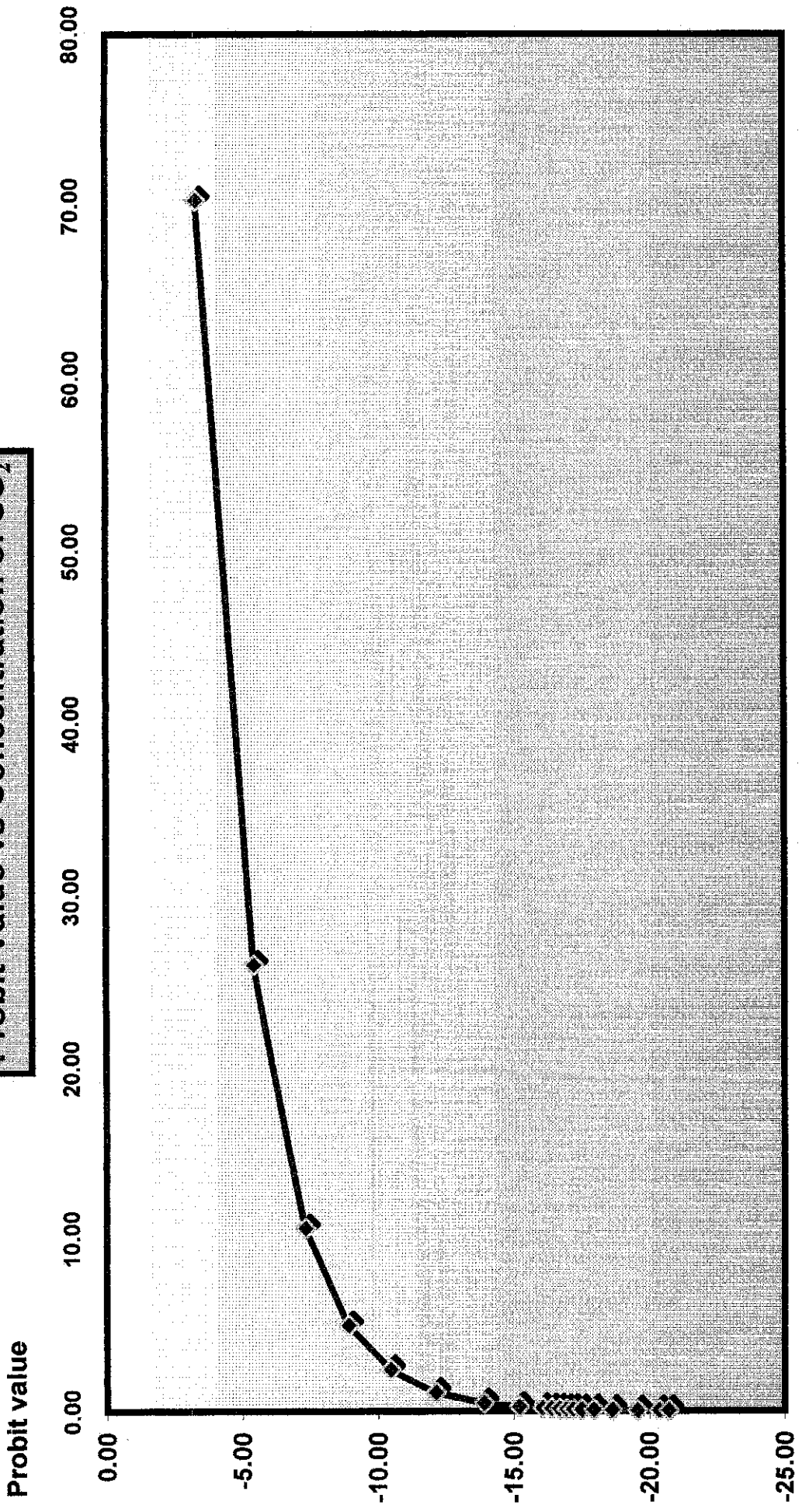


## **APPENDIX E**

Probit value vs Concentration of  $\text{NH}_3$



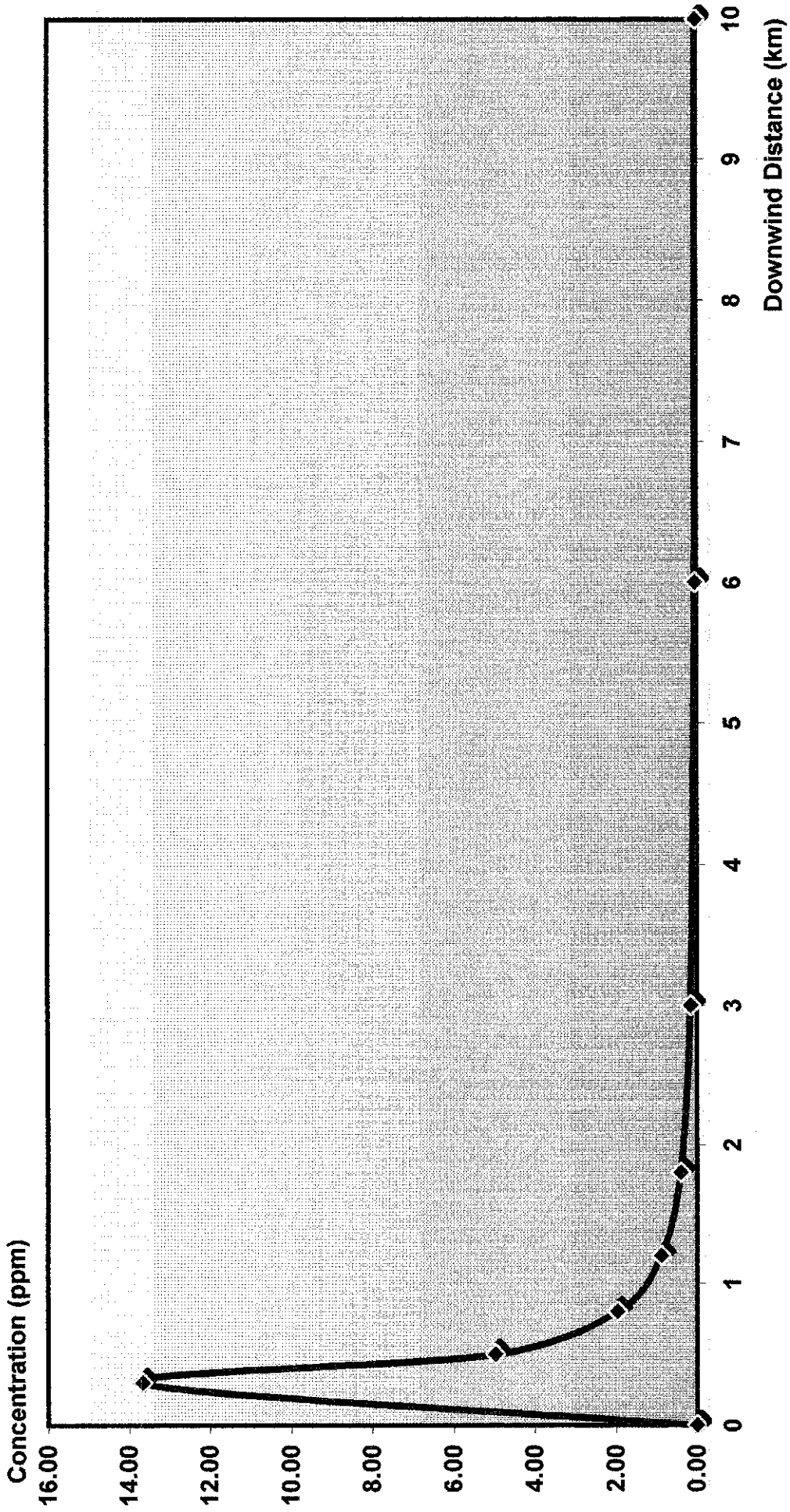
Probit Value vs Concentration of SO<sub>2</sub>



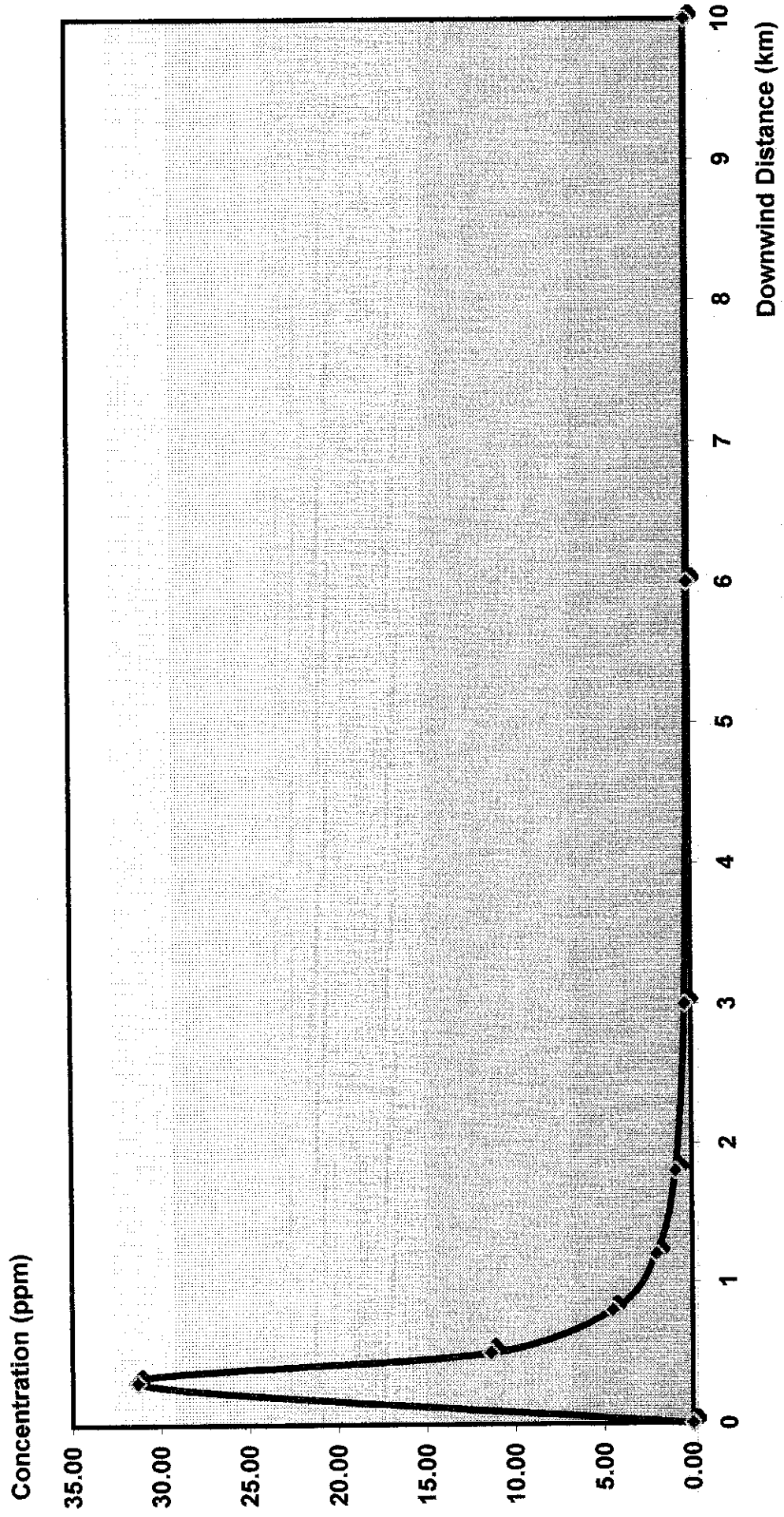
Concentration (ppm)

**APPENDIX F**

Graph of NH<sub>3</sub> Concentration vs Downwind Distance at Wind Stability A

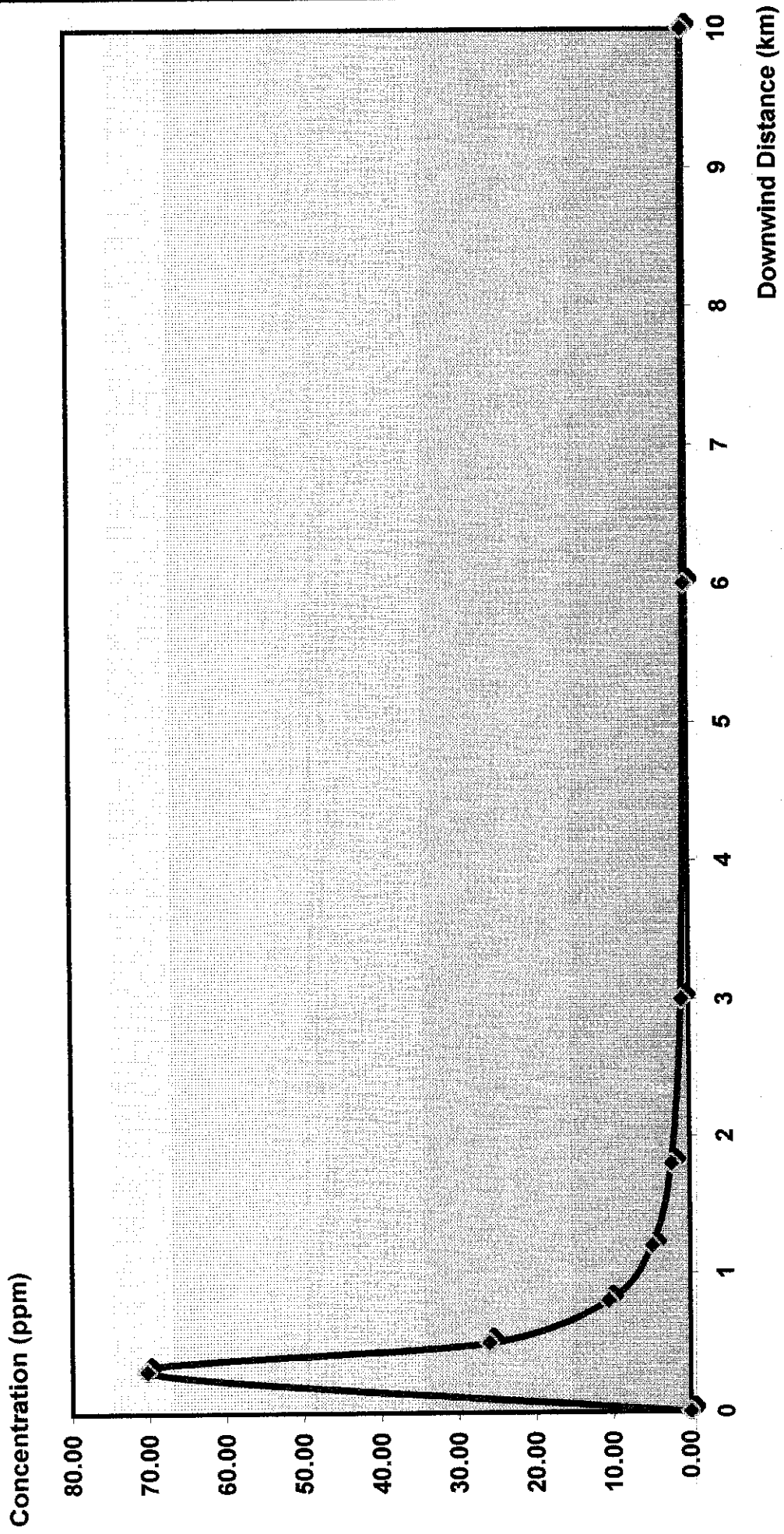


**Graph of NH<sub>3</sub> Concentration vs Downwind Distance at Wind Stability B**

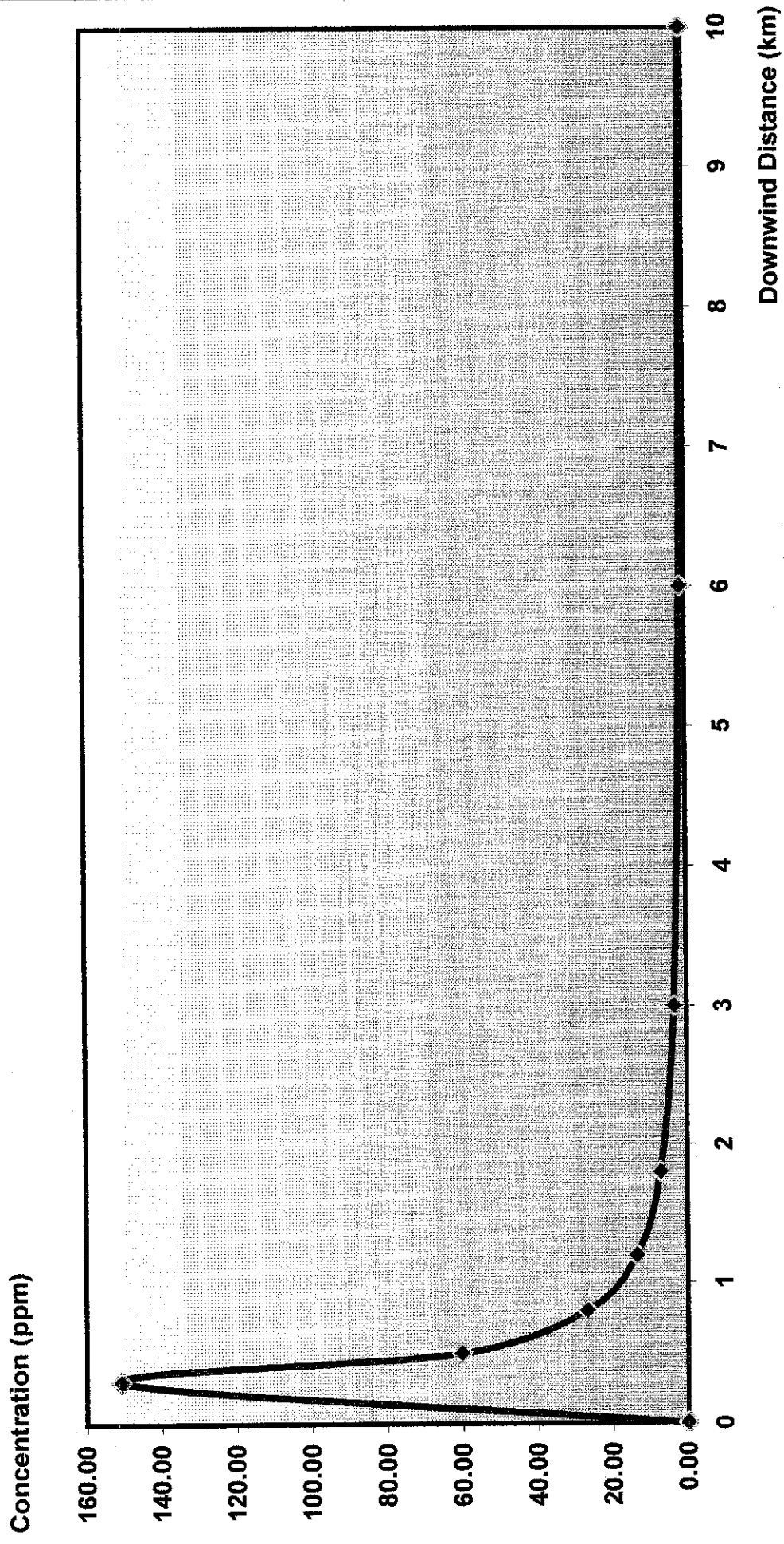




Graph of NH<sub>3</sub> Concentration vs Downwind Distance at Wind Stability C

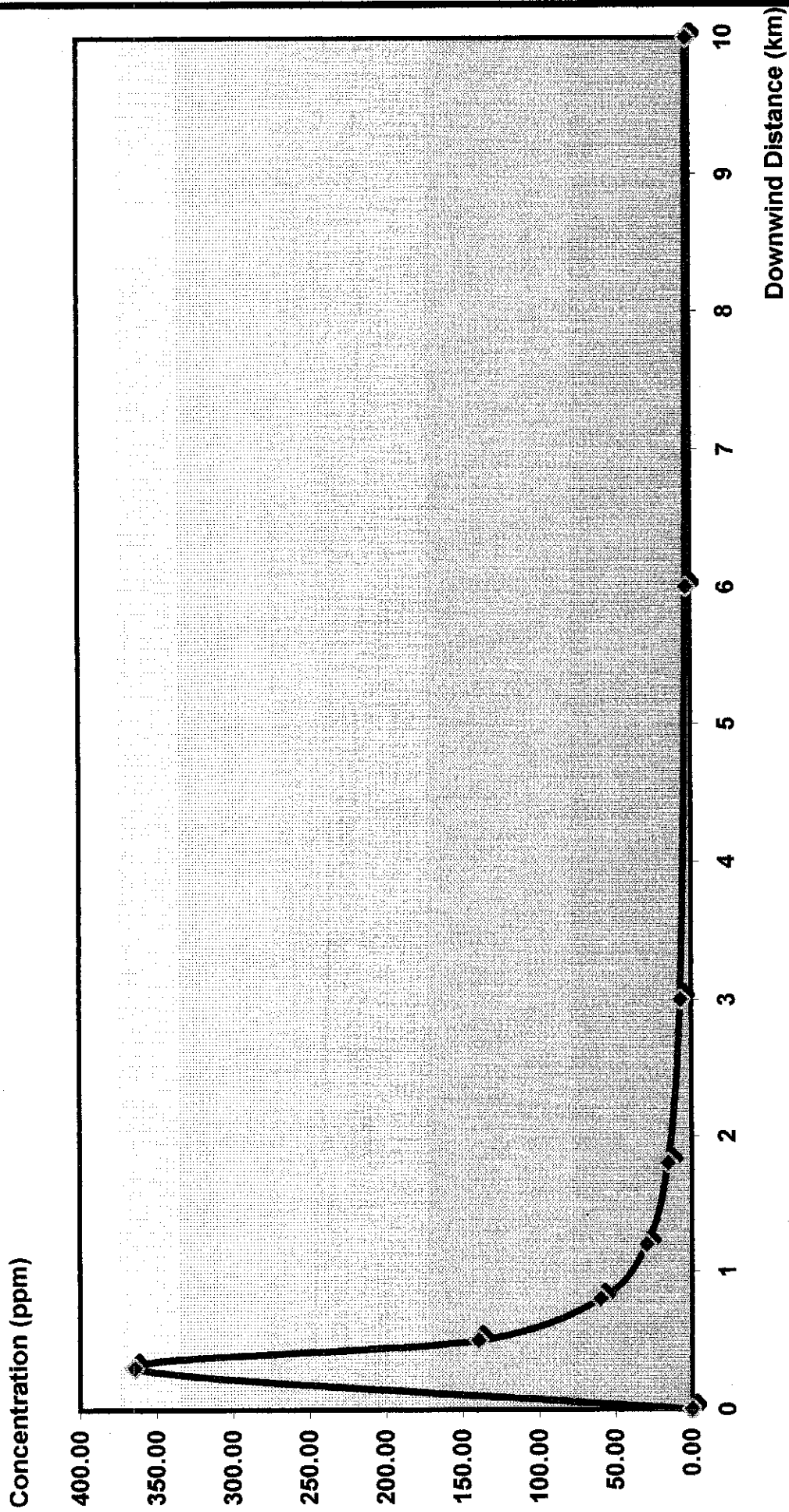


Graph of  $\text{NH}_3$  Concentration vs Downwind Distance at Wind Stability D

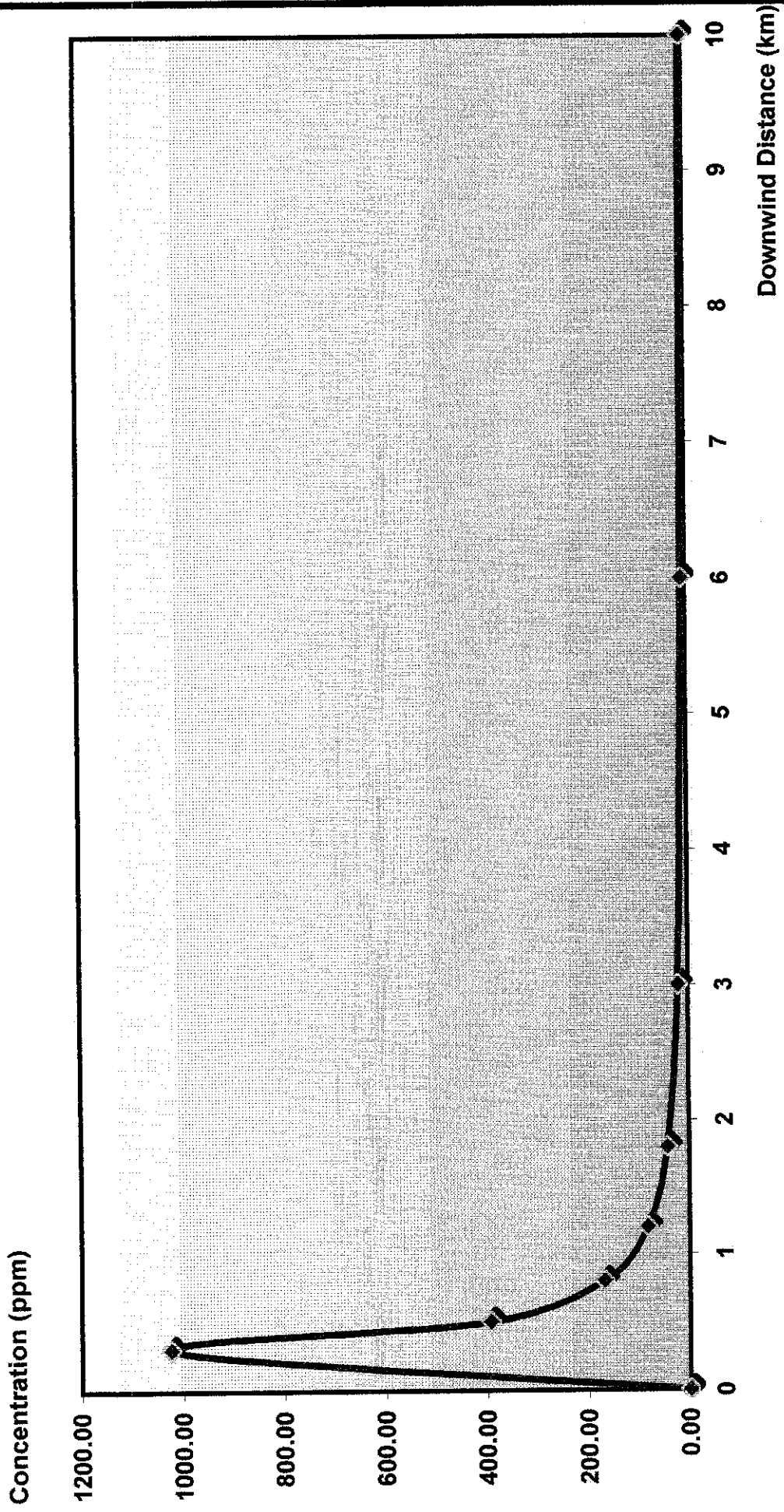




Graph of NH<sub>3</sub> Concentration vs Downwind Distance at Wind Stability E

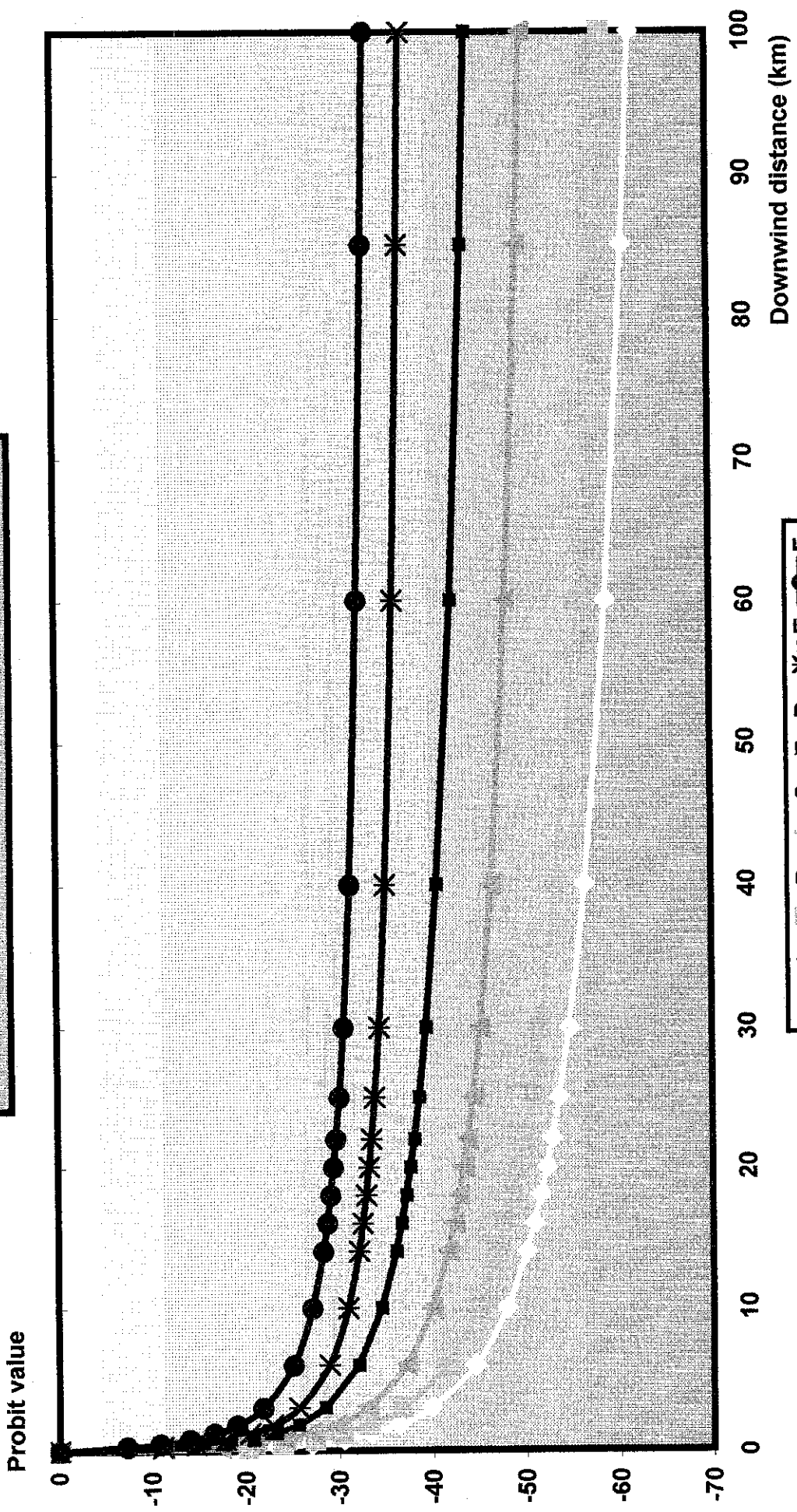


Graph of NH<sub>3</sub> Concentration vs Downwind Distance at Wind Stability F



## **APPENDIX G**

Probit values of NH<sub>3</sub> at various Wind Stabilities



A B C D E F