



**Department of Fire Safety Engineering**  
Lund Institute of Technology  
Lund University

# Project II

Uncertainty analysis of a sub-scenario from an accident with  
hazardous material

Tsukuba, Japan

1998

Björn Hedskog  
Fredrik Ryber

Institutionen för Brandteknik  
Lunds Tekniska Högskola  
Lunds Universitet  
Box 118  
221 00 Lund

Department of Fire Safety Engineering  
Institute of Technology  
University of Lund  
Box 118  
S - 210 00 Lund  
SWEDEN

## “Uncertainty analysis of a sub-scenario from an accident with hazardous material”

by

Björn Hedskog  
Fredrik Ryber

Tsukuba, Japan  
1998

### **Abstract**

In this report a scenario containing dangerous material in the Tretorn area in Helsingborg, Sweden is evaluated. The risk analysis is based on simulations in the computer program @Risk. (English)

### **Keywords:**

Uncertainty analysis, hazardous material, @Risk

## Summary

This report is an uncertainty analysis of a sub-scenario from an accident with hazardous material in the Tretorn area in Helsingborg, Sweden and is based on the report "Risktänkande i Tretorns området". To do the uncertainty analysis the computer program @Risk and the formulas for the Gaussian atmospheric discharge are used.

The result from the report is that the "wind velocity" and the "hole cross-sectional area" are the parameters, which have the largest influence on the safety distance and should therefore be determined with high accuracy.

The individual risk is presented as risk contours and the societal risk is presented as Frequency-Number curves. The result of these presentations is that the risk is too high compared to international recommendations.

## Table of contents

|  |    |
|--|----|
| <b>Introduction</b> .....  | 5  |
| <b>1. Description of scenario</b> .....                                  | 6  |
| <b>2. Uncertainty analysis of calculations of the consequences</b> ..... | 6  |
| <b>2.1 Input data</b> .....  | 6  |
| <b>2.1.1 Used formulas</b> .....   | 6  |
| <b>2.1.2 The distributions of the parameters</b> .....                   | 8  |
| <b>2.2 Results</b> .....   | 9  |
| <b>2.3 Correlation</b> .....   | 11 |
| <b>3. Risk evaluation</b> .....  | 12 |
| <b>3.1 Individual risk</b> .....   | 12 |
| <b>3.2 Societal risk</b> .....   | 13 |
| <b>4. Conclusions</b> .....  | 15 |
| <b>References</b> .....  | 16 |

*The following report is made in the education. The objective has been training in solving problems and methodology. The quality of the conclusions and the result has not been controlled in a way it has to be done for quality control. The report should therefor be used with great cautions. The one who uses the result in any situation is responsible for that himself.*

## **Introduction**

This report has been made as a part of the course “Risk Management II”, Department of Fire Safety Engineering, Lund Institute of Technology, Lund University. This report is an uncertainty analysis of a scenario containing hazardous material in the Tretorn area in Helsingborg, Sweden and is based on the report ”Risktänkande i Tretorns området” ref./1/.

The objective of this report is to investigate how uncertainties in input data affect the results in the calculation of consequences i.e. number of affected people. In order to do the uncertainty analysis the computer program @Risk, ref./2/ is used. The calculation models that have been used for the analysis are designed for calculations by hand. The result of the report will be a more accurate value for the safety distance than presented in ref./1/. The individual risk is presented as risk contours and the societal risk is presented as a Frequency-Number (F-N) curve.

### *Limitations*

In this report a number of limitations has been made. The population densities and some of the values of probabilities are rough estimates.

Assumptions in the calculations:

- The probability of an accident with condensed chlorine is taken from ref./1/ and is not examined further
- Chlorine is a heavy gas but when it will behave as a light gas at a relatively short distance from the source, the used calculation model is for light gases (Gaussian atmospheric dispersion model)
- It is assumed that all the liquid chlorine flashes (i.e. the fraction of liquid flash to vapor is 100 %)
- The distributions for the parameters is rough estimates and some parameters are assumed to be constant
- One of the results of the report is how different input data affect the output. This gives an indication of what parameters that are the most important and where more effort has to be done. In this report, the most important parameters have been defined but no further actions are taken to improve the results.

## 1. Description of scenario

The Tretorn area is a central part of the city of Helsingborg, Sweden, and is an attractive expansion area where many new activities like shopping center, university and residents are planned to be built. The scenario is an accident with a discharge of chlorine, Cl<sub>2</sub>, at a shunting yard, close to the Tretorn area. The analyzed sub-scenarios are discharges from the tank, either from the liquid phase or the vapor phase. No other sub-scenarios are analyzed. For a description and further details see Hedskog et. al. ref./1/.

## 2. Uncertainty analysis of calculations of the consequences

The uncertainty analysis is made with the computer program @Risk. The uncertainties in the results are calculated from a number of numerical calculations where the distributions of the input data are defined. In this report "Monte Carlo- simulations" is used. For every simulation one value of each input parameter is chosen and used in a defined formula. By doing this a number of times, in this report 10 000, the result will be a distribution of the output data.

### 2.1 Input data

The formulas used to determine the safety distance in the report "Risktänkande i Tretorns området" is based on the Gaussian atmospheric dispersion model i.e. a disperse model for light gases. The used criterion to obtain the safety distance was the concentration 100 ppm. However, in this uncertainty analysis the concentration will be the LC50 value, which is a more realistic and more accepted value. To be able to use the computer program @Risk an analytical formula had to be expressed for the safety distance. The formulas presented in this chapter and which lead to a final expression for the safety distance are taken from ref./3/.

#### 2.1.1 Used formulas

The first step is to derive an expression for the LC50 concentration. This value equals the concentration of the substance that causes 50% deaths of the exposed people during a time t. The expression for the LC50-concentration is obtained from the Probit function:

$$Pr = -8.29 + 0,92 * \ln(C^2 * t) \Rightarrow C_{LC50} = \sqrt{\frac{e^{(5+8.29)/0.92}}{t}} \quad \text{equation (1)}$$

*Pr = a probit function connected to how many of the exposed people that dies. Pr = 5 equals to 50% of the exposed people dies i.e. the concentration when Pr = 5 equals LC50.*

*t = time of exposition [minutes]*

*C = the concentration of the substance [ppm]*

*C<sub>LC50</sub> = the concentration of the substance which equals to 50 % deaths of the exposed people [ppm].*

When this concentration is defined, the next step is to define a formula, which calculates the safety distance. To do this, the mass flow out of the tank is needed. In the studied scenario two different types of leakage have been examined. Either the damage is done in the part of the tank where the chlorine is in vapor phase or where the chlorine is in the liquid phase. Therefore, two types of discharge are possible with different consequences and to take the two outcomes into account two different equations have to be used.

The first equation describes the mass flow when there is a liquid discharge.

$$G_L = C_D A \rho \left[ \frac{2(p - p_a)}{\rho} \right]^{(1/2)} \quad \text{equation (2)}$$

$G_L$  = liquid discharge rate [kg/s],  $C_D$  = discharge coefficient,  $A$  = hole cross-sectional area [ $m^2$ ],  $p$  = tank pressure [Pa],  $p_a$  = atmospheric pressure [Pa],  $\rho$  = substance density [ $kg/m^3$ ]

When there is a liquid discharge of chlorine, all the discharged chlorine will not evaporate immediately. Some quantity of the liquid will form a pool, which then evaporates. According to ref./3/ almost 100% of the discharged volume evaporates immediately and therefore, all the discharged chlorine is assumed to evaporate.

The second equation describes the mass flow when there is a vapor discharge.

$$G_V = C_D A p \left[ \frac{\gamma M}{RT} \left( \frac{2}{\gamma + 1} \right)^{(\gamma+1)/(\gamma-1)} \right]^{0.5} \quad \text{equation (3)}$$

$G_V$  = gas discharge rate [kg/s],  $M$  = molecular weight [g/mol],  $R$  = gas constant [Pa  $m^3$ /mol K],  $T$  = tank temperature [K],  $\gamma$  = heat capacity ratio

After the discharge rate is expressed the concentration at a distance  $x$ , can be calculated using equation 4.

$$C = \frac{G}{U \sigma_y \sigma_z \pi} \quad \text{equation (4)}$$

$\sigma_y$  and  $\sigma_z$  are spread parameters [m], as functions of the distance  $x$ ,  $C$  = concentration [ $kg/m^3$ ],  $G$  = discharge rate [kg/s],  $U$  = wind velocity [m/s]

The spread parameters  $\sigma_Y$  and  $\sigma_Z$  are expressed with complicated expressions in ref./3/. In order to derive an expression where  $x$  (C,...) the spread parameters can be approximated with equation 5 and 6, ref./4/.

$$\sigma_Y = ax^b \quad \text{and} \quad \sigma_Z = cx^d \quad \text{equation (5) and (6)}$$

The constants a, b, c and d are stability constants connected to the condition of the weather. In ref./1/ the weather was assumed to be normal and the stability constants will therefor be expressed for this situation.

If this approximation, using equation 5 and 6, is done it is easy to derive an expression for  $x$  (G, C, U,  $\pi$ , a, b, c and d):

$$x = \left( \frac{G}{CUac\pi} \right)^{1/(b+d)} \quad \text{equation (7)}$$

If the concentration C is expressed in ppm instead of  $\text{kg/m}^3$  equation 7 can be rewritten as equation 8.

$$x = \left( \frac{GRT * 10^6}{C_{ppm} M_p a Uac} \right)^{1/(b+d)} \quad \text{equation (8)}$$

### 2.1.2 The distributions of the parameters

The next step is to define the distribution of the different parameters. Some of them are set to be constants, for example  $C_D$  and the atmospheric pressure, while others are estimated as distributions. From ref./1/ the time to empty the tank when it is full (80 %) is about 28 minutes. If we assume that the tank always will carry at least 40 % of its volume, the shortest time to empty the tank will be about 14 minutes. The most likely time that it takes for the Fire Service to stop the discharge is assumed to be 20 minutes. This gives the distribution of the time,  $t$ , as triangular with the most probable value of 20, minimum value 14 and maximum value 28. The temperature in the tank is assumed to be the same as the temperature outside. If this assumption not had been made, the temperature distribution would have been of the same type as the pressure distribution. The other parameters are estimated and will be presented in table 1.

| Parameter                        | Liquid discharge  | Vapor discharge   |
|----------------------------------|---|---|
| t [min]                          | Triangular (14, 20, 28)   | Triangular (14, 20, 28)   |
| $C_D$                            | 0.6   | 0.8   |
| A [m <sup>2</sup> ]              | Triangular ( $7.85 \cdot 10^{-5}$ , $1.96 \cdot 10^{-3}$ , $1.96 \cdot 10^{-3}$ ) | Triangular ( $7.85 \cdot 10^{-5}$ , $1.96 \cdot 10^{-3}$ , $1.96 \cdot 10^{-3}$ ) |
| p [Pa]                           | Uniform (600 000, 778 000)  | Uniform (600 000, 778 000)  |
| $p_a$ [Pa]                       | 101325  | 101325  |
| $\rho$ [kg/m <sup>3</sup> ]      | 1400 kg/m <sup>3</sup>  | -   |
| M [g/mol]                        | 71  | 71  |
| R [Pa m <sup>3</sup> /mol K]     | 8.314   | 8.314   |
| T [K]                            | Triangular (263, 283, 303)  | Triangular (263, 283, 303)  |
| $\gamma$                         | -   | 1.32  |
| U [m/s]                          | Triangular (1, 4, 10)   | Triangular (1, 4, 10)   |
| a, b, c, d (stability constants) | 0.128, 0.905, 0.20, 0.76  | 0.128, 0.905, 0.20, 0.76  |

Table 1. The distributions of the used parameters

## 2.2 Results

In this report the recommended distance from the source to the LC50 concentration will be the distance at the 95 % percentile. This means that if 100 accidents occur, only 5 (5 %) of these will have a distance to the LC50 concentration which is greater than the recommended. This will give a conservative result, but it is better to be safe than sorry. The results from the simulations in @Risk are shown in table 2 and figure 1 to 4.

|                    | Liquid discharge, distance from source [m] | Vapor discharge, distance from source [m] |
|--------------------|--|---|
| 95 % percentile    | 1524                                       | 344                                       |
| Minimum            | 135  | 27  |
| Mean               | 869  | 195                                       |
| Standard deviation | 364  | 81  |
| Maximum            | 2856                                       | 643                                       |

Table 2. Results from the simulations in @Risk.

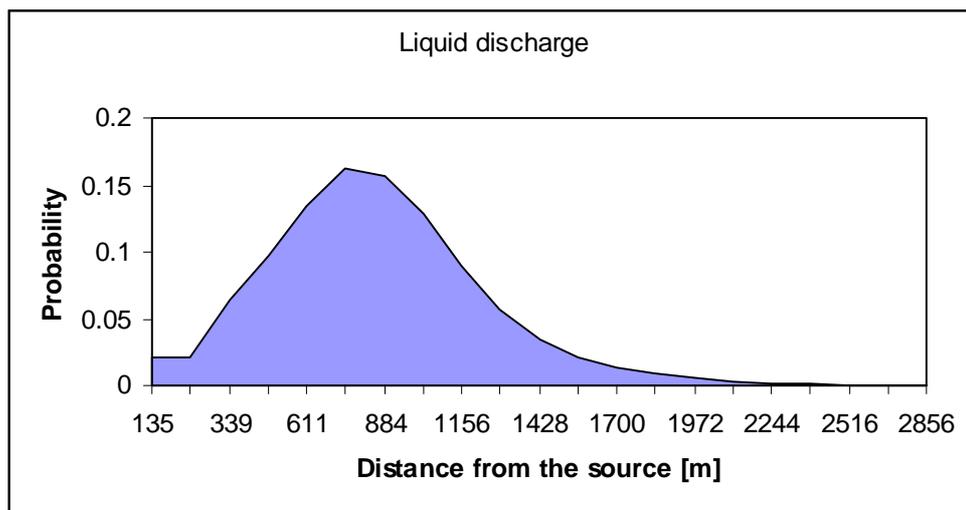


Figure 1. The probability as a function of the distance from the source for the liquid discharge

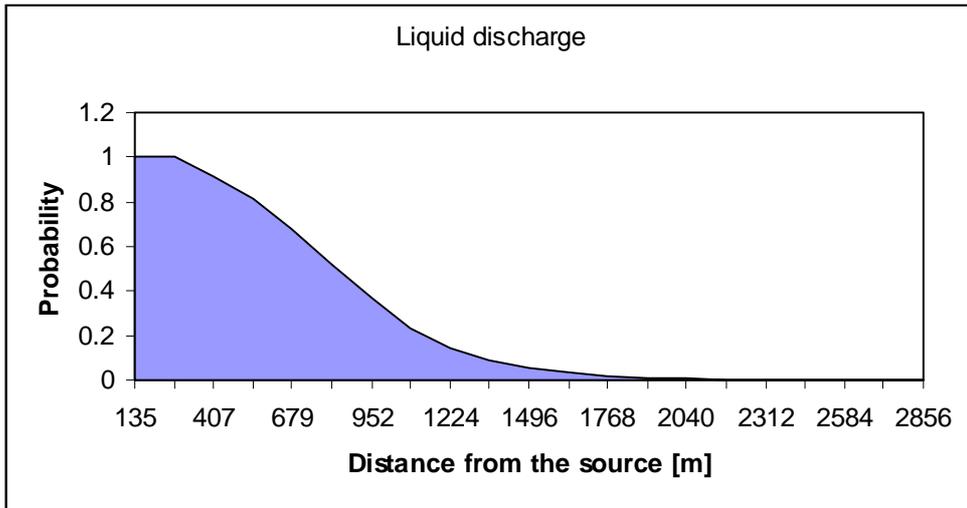


Figure 2. The probability as a CCDF-function of the distance from the source for the liquid discharge

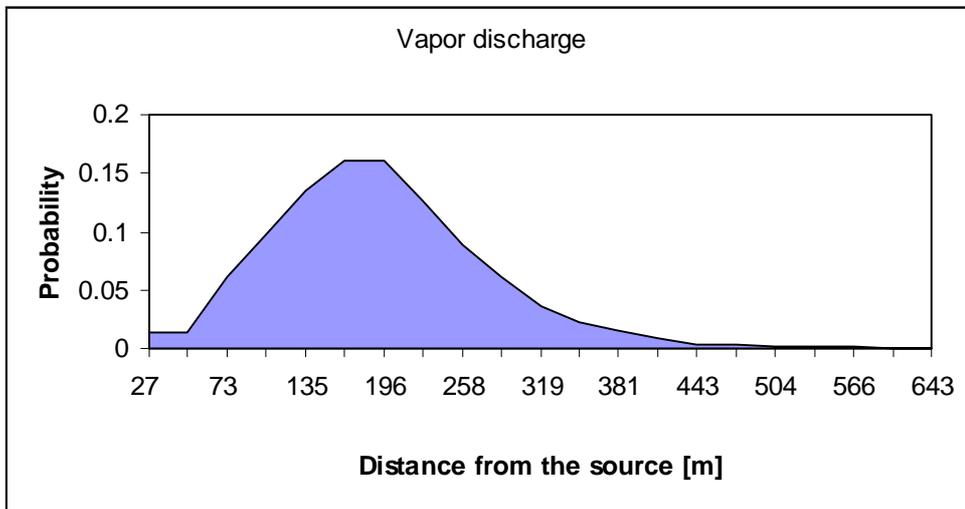


Figure 3. The probability as a function of the distance from the source for the vapor discharge

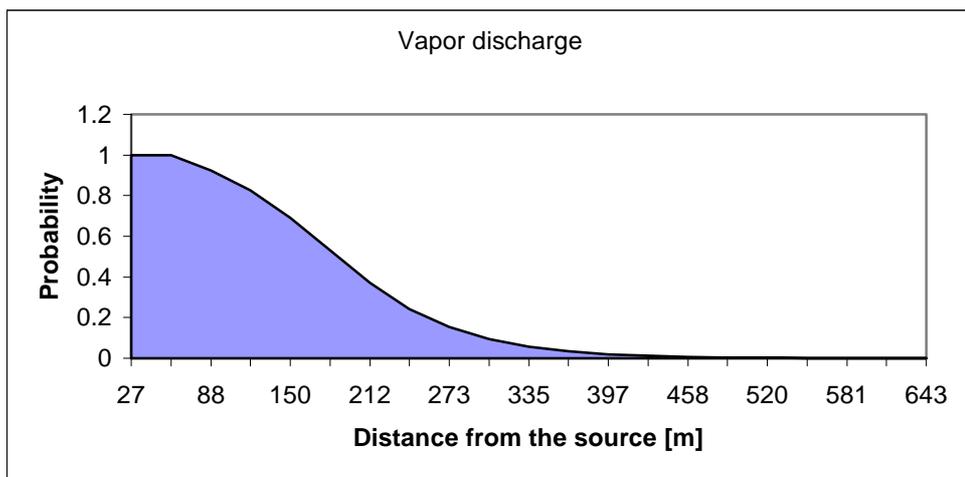


Figure 4. The probability as CCDF function of the distance from the source for the vapor discharge

### 2.3 Correlation

From the simulations in @Risk, it is also possible to evaluate how large influence the different parameters (that not is constant) have on the result. This is shown in figure 3 and 4. If the correlation coefficient is close to  $\pm 1$ , the correlation is large, i.e. the result is highly affected by this parameter.

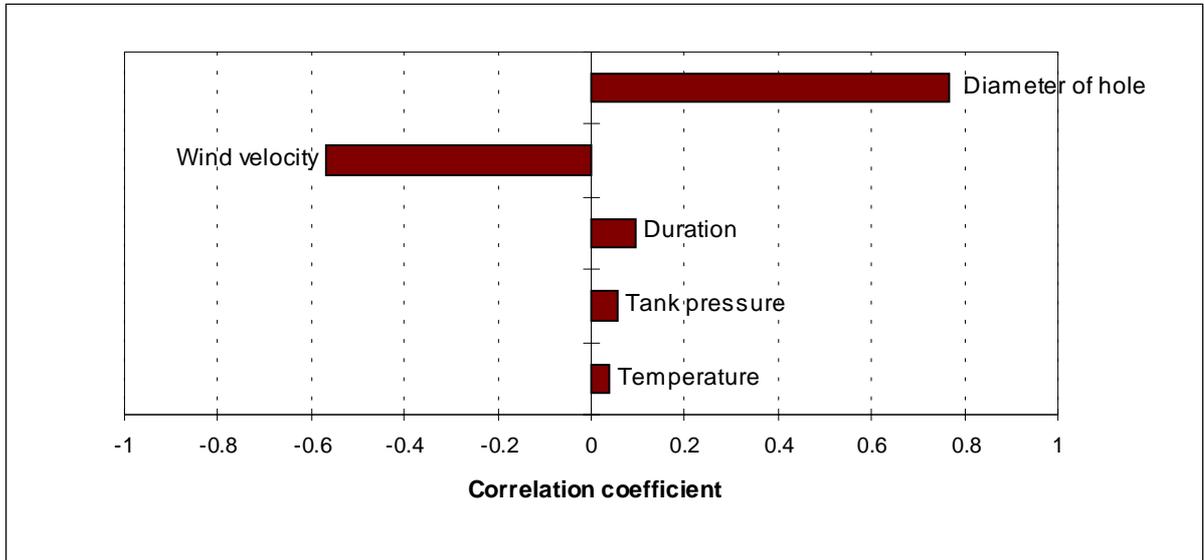


Figure 3. The correlation coefficient for the parameters when there is a liquid discharge

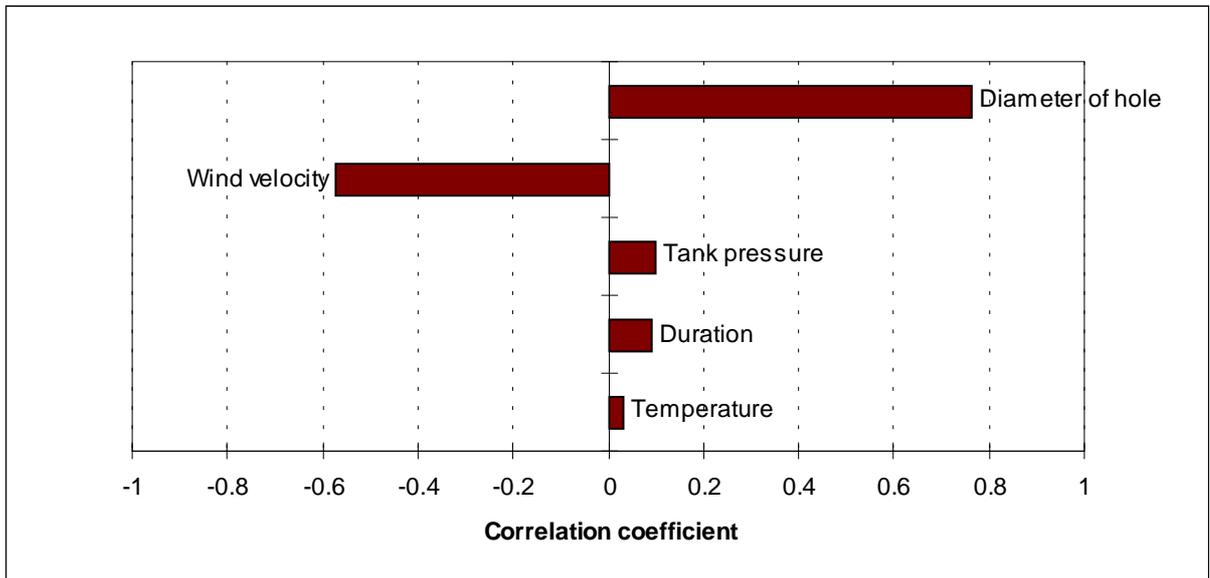


Figure 4. The correlation coefficient for the parameters when there is a vapor discharge

From figure 3 and 4, it is possible to see that the most important parameters are the “hole diameter” and the “wind velocity”. Therefore, in order to reduce the uncertainty in the result, these two parameters should be determined with high accuracy.

### 3. Risk evaluation

In this report both the individual risk and the societal risk has been evaluated. The individual risk can be presented in many ways and in applications like this report individual risk contours and F-N curves can be used. CPQRA ref./3/ gives the following description of individual risk contours:

*“The risk contours show the expected frequency of an event capable of causing the specified level of harm at a specified location, regardless of whether or not anyone is present at that location to suffer that harm”*

In this report, the individual risk is presented as risk contours, which also are described in words.

When the societal risk is to be calculated, it is necessary to know the number of people and different forms of activities around the facility. The societal risk in this report is presented as an F-N curve.

#### 3.1 Individual risk

In ref./1/ the probability for an accident and discharge of chlorine is calculated to  $7 \cdot 10^{-5}$ . If then the probability for vapor and liquid discharge (both 0.5, estimated from ref./3/), with a risk distance from the source of 344 m and 1524 respectively, this will give us the risk contour shown in figure 5. The risk distances represents the conservative values which are given in chapter 2.2 i.e. the distance at the 95 % percentile calculated in @Risk. The probability for vapor and liquid discharge is estimated from ref./3/.

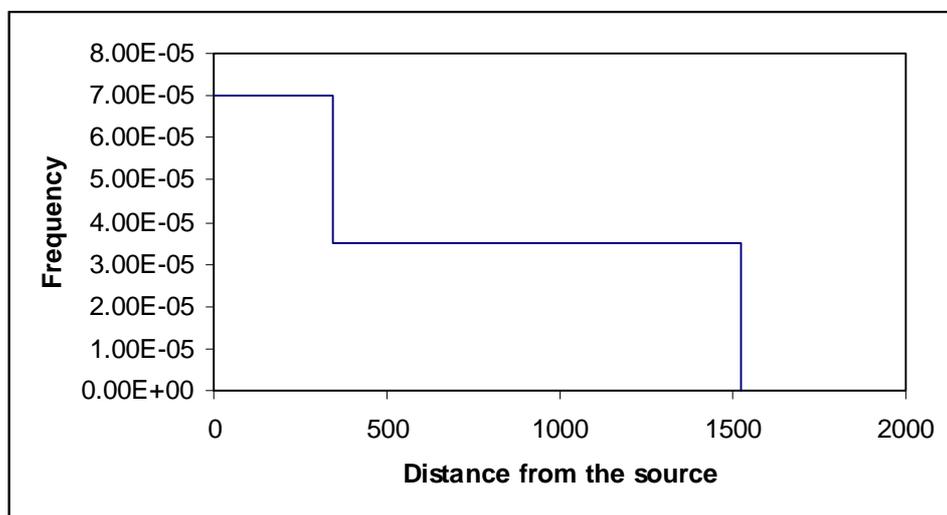


Figure 5. Individual risk at the accident with chlorine

If the result were presented as risk contours on a map, there would be two circles, one with a diameter of 344 m and with a probability of  $7 \cdot 10^{-5}$  and the other a diameter of 1524 m with a probability of  $3.5 \cdot 10^{-5}$ . This because the circle with the smaller diameter will be affected by both the events from the accident and the area between the two circles will only be affected by the liquid discharge event.

### 3.2 Societal risk

As described above the societal risk needs a definition of the population around the facility, including number of population and the probability that the people actually are there. In order to do this the area around the studied facility is divided into four areas, N, S, W and E. The names of the areas might look confusing but, the area called “N” (North) will be affected by a discharge if the wind blows from the north, area W will be affected by a wind blowing from the west etc. This is shown in figure 6.

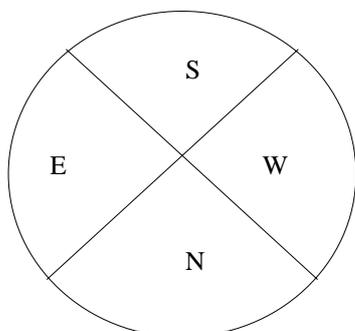


Figure 6. The area around the facility

When making an estimate of how many people that can be affected by a discharge the number of people is estimated for each area, for the two discharge cases. This is based on estimates of how many buildings that are used for industry and residents. The number of people per km<sup>2</sup> is estimated to 1000 and 6000 for industry and residents respectively. The probability of the wind direction is assumed to be equal for all four different directions. The affected area is calculated on the basis that the distance from the facility to the LC50 concentration is 344 m and 1524 for vapor and liquid discharge respectively. The number of deaths is then calculated as the number of affected people divided by 2, because of the distance from the facility is based on the LC50 concentration, where 50 % of the affected people dies. This is shown in table 3.

| Area           | Probability | Distribution                    | Affected area (km <sup>2</sup> )                               | Number of affected people | Number of deaths |
|----------------|-------------|---------------------------------|--|---------------------------|------------------|
| N <sub>v</sub> | 0.25        | 20 % residents<br>80 % industry | 0.37<br>(based on a radius of 344 m, the area is divided by 4) | 320                       | 160              |
| S <sub>v</sub> | 0.25        | 50 % residents<br>50 % industry |  | 185                       | 93               |
| W <sub>v</sub> | 0.25        | 80 % residents<br>20 % industry |  | 460                       | 230              |
| E <sub>v</sub> | 0.25        | 50 % residents<br>50 % industry |  | 320                       | 160              |
| N <sub>l</sub> | 0.25        | 20 % residents<br>80 % industry | 7.3<br>(based on a radius of 1524 m, the area is divided by 4) | 3650                      | 1825             |
| S <sub>l</sub> | 0.25        | 90 % residents<br>10 % industry |  | 10 040                    | 5020             |
| E <sub>l</sub> | 0.25        | 50 % residents<br>50 % industry |  | 320                       | 160              |
| W <sub>l</sub> | 0.25        | 80 % residents<br>20 % industry |  | 9130                      | 4565             |

Table 3. Number of affected people and number of deaths for different wind directions. Subscription v equals to the vapor discharge case and l equals the liquid discharge case.

If then the consequences for each wind direction and their probability are combined with the probabilities for liquid and vapor discharge, the risk can be calculated. This is done with the event tree in figure 6.

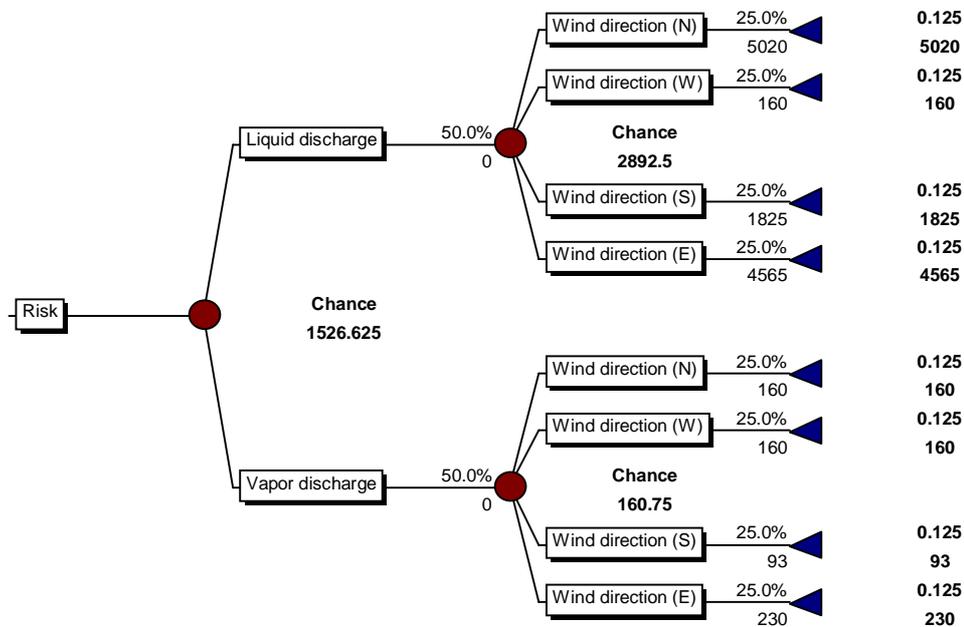


Figure 6. Event tree

The total risk is then calculated as the result from the event tree (1526.625) multiplied by the probability for the accident ( $7 \cdot 10^{-5}$ ). This give that one person will die during a period of ten years.

The societal risk can also be presented as an F-N curve, as shown in figure 7.

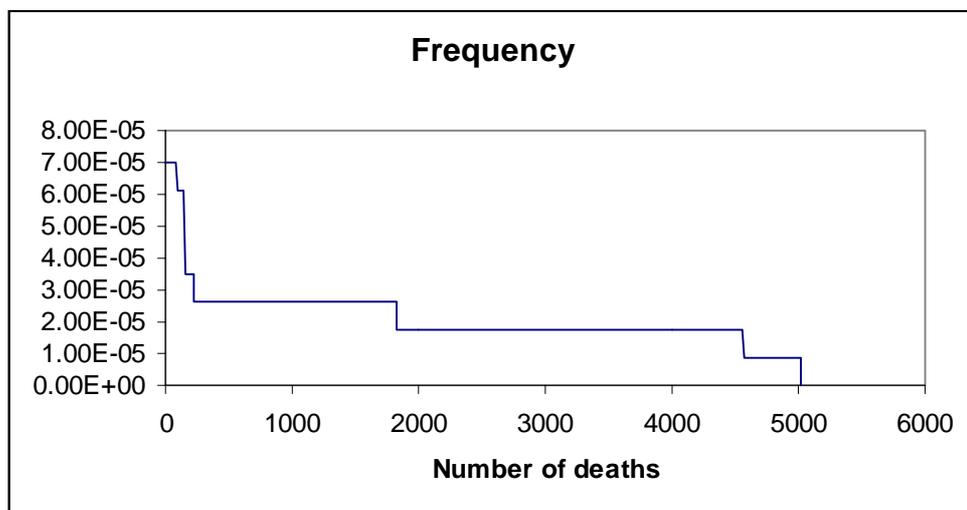


Figure 7. F-N curve, describing the societal risk.

#### **4. Conclusions**

In ref./1/ the safety distance for a discharge of liquid chlorine is calculated to 1000-1700 m. From the results in this report these figures can be said to be exaggerated. Although, a lower criteria for the concentration was used (100 ppm) in ref./1/ but almost the same risk distance is obtained in this report.

The individual risk is high compared to the suggested criteria in ref./5/ ( $10^{-5}$ ). Even the societal risk is high compared with criteria suggested in ref./5/, especially when the number of deaths increases. This can be a result from the number of approximations made in this report and in ref./1/. The probability for accidents including chlorine is exaggerated. This probability, calculated in ref./1/, includes all accidents with condensed gases and will therefor probably decrease the risk with a factor 1-100 when all transportation of condensed gas do not include chlorine. The used calculation model and the assumptions that all chlorine flashes will also make the results more conservative. Therefore the presented results in this report can be assumed to be safer than necessary.

The uncertainty analysis shows that, in order to reduce the uncertainty in the result, the hole diameter and wind velocity, has to be determined with high accuracy. If this not is done, the safety distance will vary in large range and it will be difficult to make any accurate decisions from the results. The main objective of this report has been to make this uncertainty analysis and no further conclusions will therefore be made about the presented results.

When only the two sub-scenarios in ref./1/ are analyzed the presented risk is not complete. In reality there are more events that has to be taken into account, but these are excluded from this report, where the purpose was to do an uncertainty analysis of the calculations in ref./1/.

## References

/1/ Hedskog, B. et. al., "**Risktänkande i Tretorns området**", Department of Fire Protection Engineering, Institute of Technology, Lund University, Lund, **1998**. (Swedish)

/2/ Palisade Corp. "**@Risk for windows version 3.5e**",USA, **1990-1997**.

/3/ Center for chemical process safety, "**Chemical Process Quantitative Risk Analysis**", New York, **1989**.

/4/ TNO. "**methods for the calculations of the physical effects of the escape of dangerous material (liquids and gases)**", Voorburg, **1979**.

/5/ Raddningsverket, "**Vardering av risk**", Karlstad, **1997**. (Swedish)