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A Deterministic and Probabilistic Analyses of the Carbon Tetrachloride Contaminant
Plume in Groundwater at the Former Union Carbide India Limited Factory in
Bhopal, Madhya Pradesh, India

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Abstract

A Deterministic and Probabilistic Analyses of the Carbon Tetrachloride Contaminant Plume in Groundwater at the Former Union Carbide India Limited Factory in Bhopal, Madhya Pradesh, India

By Vijay Selvan Ram

The Union Carbide India Limited (UCIL) factory in Bhopal, Madhya Pradesh is the site of one of the world's worst industrial disasters. In 1984, a gas release of Methyl Isocyanate (MIC) caused the deaths of thousands within weeks and thousands more since. After this incident, the factory operations ceased and the site was abandoned. However, remediation activities have yet to take place, which means that the pesticide products and their production intermediates serve as ongoing pollutants to the environment, in particular, the groundwater. In order to evaluate the effect of this contamination, the following study attempts to describe the contaminant plume of carbon tetrachloride (CCl_4) in the groundwater using analytical models provided by publicly the available software known as analytical contaminant transport analysis system (ACTS). CCl_4 is known to have adverse effects on human health when consumed through the drinking water and is classified as possibly carcinogenic by the Department of Health and Human Services (DHHS). The calibrated deterministic results show that concentrations of CCl_4 do not exceed the U.S. EPA maximum contaminant levels (MCLs) roughly 850m from the source in the northeast direction. Probabilistic simulations show that there is a 100% probability that CCl_4 concentrations exceed WHO specified MCL up to the year 2034 at sites 500m, 1000m and 2000m northeast of the UCIL site. Analytical models are an effective tool in decision making for environmental managers and policymakers. As many of the parameters used as inputs for the analytical model were based on sparse field data and literature values, it is recommended that future studies should aim to better characterize the hydrogeological system of which the land surrounding the UCIL site is a part. This information will help to generate more representative analytical models with which to analyze the contaminant plume.

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Background

The Bhopal Syndrome

The push to increase the productivity of agricultural lands through the application of pesticides begins in earnest after World War 2. David Weir, in his book, *The Bhopal Syndrome*, details the consequences of this effort. Increasing food production was possible by the application of increasing amounts of pesticides on crops. As a result, the pests being targeted began to develop resistance to these chemicals, which in turn led to an increasing amount of pesticides being sprayed on agricultural land, in a phenomenon termed the “pesticide treadmill” (Weir 1988). Pesticide manufacturers, experiencing saturated markets in the west, turned their attention to the export market with plans to develop manufacturing facilities closer to these markets in the developing world. In India, specifically, they found the absence of any stringent regulatory framework conducive to increasing what were becoming slim profit margins. These same regulatory policies would later be to blame by some for the poor conditions of pesticide plants around the country. The Union Carbide Corporation (UCC) was among the many multinational corporations producing pesticides, and the Union Carbide India Limited (UCIL) was the subsidiary branch operation in Bhopal, Madhya Pradesh (Weir 1988).

The Infamous MIC Gas Release

Bhopal, the site of UCIL, is the administrative capital of the central Indian state of Madhya Pradesh (Figure 1). On the night of December 2nd 1984, one of the world’s worst industrial disasters occurred at the UCIL site (Figure 2). Due to faulty safety systems and corrosion of the methyl-isocyanate (MIC) storage tank, water was inadvertently introduced into the 40 ton tank of MIC, causing an extreme exothermic reaction with such speed and momentum, the nearly 27 gases that formed eluded all safety apparatuses

and escaped into the environment (Labunska et al. 1999, Bucher 1987). Because MIC gas is more dense than air, and because of the relatively static wind conditions at the time, the gas cloud lingered in the ambient atmosphere where hundreds of thousands of residents residing in poorly insulated slum-dwellings and other apartment dwellings were exposed (Greenpeace 1999, Weir 1987)

Health Effects of MIC-Exposure

MIC, being an intermediary in the production process, was not widely studied in the field of toxicology before the gas explosion. However, this changed after the incident, when studies into the health effects of exposure to this gas became necessary (Bucher 1987). John Bucher notes that MIC has poor warning properties as it falls below the threshold of human detection, making it an especially potent toxin. In addition to the approximately 2,500 deaths, the exposure manifested itself in a number of adverse health outcomes for more than 100,000 people (Dhara et al. 1995). A number of studies have been done to date cataloging the acute- and long-term health effects. Epidemiological studies in the early aftermath of the incident describe the acute symptoms associated with exposure to MIC.

A survey conducted by Andersson et al. two weeks after the incident reported that the most common symptom among survivors was burning eyes. The authors go on to postulate that the irritating effect caused many residents to run outside of their homes in the direction of the gas cloud, thereby increasing their exposures. The survey participants were grouped into eight different housing zones exposed to the gas with two control groups. Diarrhea was reported with greater frequency in zones with greater mortality (Anderssen et al. 1988). Other initial symptoms reported include irritation of the eyes,

nose and throat, vomiting, urination and psychological manifestations such as depression, confusion and panic (Bucher 1987). In follow up studies, permanent changes to lung pathology were observed (Kamat et al., 1985).

In a review of the epidemiological studies linking health effects to MIC-exposure, written by Dhara et al. in 2002, longer-term health effects have been observed. Longer-term effects from MIC exposure have included chronic inflammation of the eye and inflammation of lung cells (Dhara and Gassert 2002). The review goes on to catalogue an increase in spontaneous abortions among households severely affected. In utero exposure to MIC gas has also led to a persistent hyper-responsive cellular and humoral immune state in affected individuals nearly twenty years after the incident (Mishra et al. 2009). A recent mortality figure associated with MIC exposure is estimated to be around 5,000 (Sarangi et al. 2010).

The threat to health from MIC-related exposure is ongoing, however, there are other environmental threats associated with the UCIL site that also demand attention. There is plenty of evidence to suggest that the UCIL plant is responsible for a number of toxic chemicals found in the groundwater supplying drinking water for residential neighborhoods in the vicinity of the plant (Labunska 1999).

Introduction

Union Carbide India Limited

The UCIL plant was in operation from 1977 to 1984. During that time they were charged with producing three different kinds of pesticides and their intermediates: Carbaryl, also known as Sevin, phosgene, monomethylamine (MMA), MIC, Aldicarb and γ -Hexachlorocyclohexane (γ -HCH), sold under the trade name, Sevidol. In order to

manufacture Sevidol, γ -HCH must be extracted from technical grade HCH, which includes an α -, β - and δ - isomer. After extraction, the remaining isomers are discarded as waste (Johnson et al. 2009). MIC, which was manufactured on site, in the presence of alpha-naphthol and carbon tetrachloride (CCl_4) produced Carbaryl. In addition to the aforementioned products, a number of other chemicals were used at the site for producing pesticides including chloroform as a solvent and heavy metals for sealants (Labunska et al. 1999).

Contaminated Groundwater in Bhopal

Dixit et al. conducted a study on the Shahpura Lake in Bhopal and found levels of copper, chromium, lead, cadmium and manganese higher than permissible levels. The authors postulate that these heavy metals arise from wastewater sources. Because this lake is used for fishing, there is the danger that these heavy metals will end up in the human body after bioaccumulating through the food chain (Dixit et al. 2008).

The extensive use of pesticides has also led to large-scale organochlorine contamination in drinking water sources. Dikshith et al, in a study examining residues of DDT and hexachlorocyclohexane (HCH) in major sources of drinking water in Bhopal, collected sixty water samples from different wells, handpumps and ponds and subjected them to GLC analysis. The well water showed levels of HCH between 1.576 – 7.747 parts per million (ppm) and levels of DDT between 3.153 – 9.356 ppm. Again, these compounds have the potential to bioaccumulate through the food chain, posing potential risks for those exposed (Dikshith et al., 1990).

In a different study, Dikshith et al. study levels of 1-Naphthol in soil and drinking water samples around Bhopal. Water sampled from hand-pumps showed a substantial

level of 1-naphthol with a range between 0.017 – 0.048 ppm with pond samples having a higher residual content. While the authors do note that the clinical and toxicological effects of 1-naphthol exposure are poorly understood, the presence of these chemicals, used for the production of pesticides, should be a major concern (Dikshit et al. 1990). This research highlights the concentrations of pollutants in drinking water and recreational water supplies in Bhopal; however, a number of studies document groundwater contamination as a consequence of the routine operations of the UCIL factory and the absence of management or remediation of the site following the MIC gas explosion.

Greenpeace

Labunska et al., associated with Greenpeace International, carried out an extensive survey of the soil and groundwater at the UCIL site in the summer of 1999. From a collection of soil-sludge taken in the former Sevin structure plant, elevated levels of mercury were found in a drain, which indicates contamination with a number of other heavy metals (chromium, copper, lead, nickel and zinc), all found at levels above background. From this sample they also isolated 73 organic compounds of which 49% were reliably identified. Polycyclic aromatic hydrocarbons (PAHs) among them are extremely toxic to humans. In addition to PAHs, hexachlorobutadiene and hexachloroethane were identified in this sample.

33 organic compounds, of which 64% were reliably identified, were found at the former UCIL formulation plant. Among the compounds identified were four isomers (alpha-, beta-, delta- and gamma-) of hexachlorocyclohexane (HCH), which were all involved either as production intermediaries that were recycled or discarded, or end-stage

products in the production process at UCIL. 400 meters north of the main UCIL site are the Solar Evaporation Ponds (SEPs), which collect waste after they have been neutralized and treated, and with the exception of mercury, the concentrations of other heavy metals were below background. An organic analysis found 15 compounds of which approximately 20% were identified; yet only a few organic compounds were identified reliably when compared with other sites (Labunska et al. 1999).

They collected groundwater samples from twelve drinking water wells both to the north and south of the UCIL site (Figure 3) and detected high levels of chloroform, carbon tetrachloride and chlorinated benzenes in wells close to the northern boundary of the plant (Labunska et al. 1999). A later study carried out in 2004 also found similarly high levels from a drinking water hand-pump located near the southern boundary of the plant (Labunska et al. 2004).

Pollution Monitoring Laboratory (PML)

In 2009, scientists from the Pollution and Monitoring Laboratory (PML), in association with the Centre for Science and Environment (CSE) collected soil and water samples from inside and outside the UCIL factory. These samples included water samples collected from handpumps, borewells and dugwells from residential areas around the UCIL plant, and from as far as 3.5 km away. Waste samples from waste storage sheds, soil samples from within the factory premises, the SEPs, and surface water samples show contamination of HCH isomers and heavy metals. They found results similar to Greenpeace, with groundwater samples being heavily contaminated with chlorinated benzene compounds and organochlorine pesticides (Johnson et al., 2009).

National Environmental Engineering Research Institute (NEERI)

NEERI, an institute devoted to the intersection of environmental concerns and human public health, performed three rounds of sampling and geophysical investigations on UCIL premises to determine the extent of contamination in both soil and groundwater. Soil sampling within UCIL premises, outside the UCIL premises, and groundwater sampling within and outside UCIL premises reveal a contamination profile that is less alarming than the two previously described studies. The geophysical investigations reveal the possibility of chemical contamination at three sites (Site I, Site III and Site V) (Figure 4). From the analysis of groundwater sampled from borewells within the UCIL premises and outside, pesticide contamination was found in 5 wells in the vicinity of UCIL premises along a Northeast axis (NEERI 2010).

Study Objectives

This study will attempt to characterize the contaminant plume for CCl_4 in groundwater and create future projections for the contaminant plume at sites along the axis of the direction of groundwater flow. More specifically, the aims for the study will be to 1) characterize the hydrogeology of the site as reported in the literature 2) estimate the source concentrations of CCl_4 3) run a deterministic model using single-point estimates to project the contaminant plume out in space and time, and 4) run a probabilistic model to project a range of likelihoods that the concentration of CCl_4 will exceed drinking water standards set by the World Health Organization (WHO) and the United States Environmental Protection Agency (US EPA).

As Labunska et al. report in their 1999 Greenpeace report, the groundwater under the site flows in the northeast direction. There is an abundance of human settlements along the northeast axis, raising the possibility of significant exposure to contaminated

groundwater for those populations that draw their drinking water from this source. The studies outlined above indicate a lengthy profile of contamination of both the soil and groundwater, which includes a number of pesticides and their production intermediates. However, for the purposes of this study, CCl_4 will help to elucidate some measure of exposure-risk for those residents who drink from this groundwater.

CCl_4 , a volatile organic compound (VOC) was chosen because of its reported distribution in the groundwater along the northeast axis. According to Labunska et al., CCl_4 is found in high concentrations in wells along the northern plant boundary, while those concentrations in wells along the southeast corner of the site are lower, though still significantly elevated (Labunska et al. 1999). In addition, the toxicological profile of carbon tetrachloride is well characterized, providing a good justification for assessing their risk.

In order to evaluate the behavior of CCl_4 and its' associated levels in the groundwater, the software Analytical Contaminant Transport System (ACTS) will be used to study the steady state and time dependent behavior of CCl_4 . The ACTS software utilizes environmental models commonly found in the literature for analytical purposes. It can be used as a screening-level tool for environmental managers and policy-makers to obtain some general knowledge of the system and its behavior. In order to utilize ACTS, hydrogeologic parameters and contaminant properties must be measured, in addition to characterizing the aquifer and contaminant plume. Because this study relies on values from the literature regarding Bhopal and the UCIL site, where uncertainty exists or information is unavailable, ACTS is capable of performing analysis using Monte Carlo

methods, producing a range of possible outputs (e.g. a range of contaminant levels at a specified distance after a specified period of time) (Anderson et al., 2010).

Chemical and Contaminant Properties of Carbon Tetrachloride

Chronic exposure to CCl_4 can have an adverse effect on liver functioning. Breakdown products have been shown to attack cell proteins, and in severe cases liver cells can be destroyed leading to a decrease in liver function. If exposure is short-term, these effects can be reversed. Kidneys are also sensitive to CCl_4 . It can cause a buildup of water and waste products in the body with potentially fatal consequences if the exposure is too high. There are also neurological symptoms associated with high exposure to CCl_4 . In the most severe cases, coma and permanent damage to nerve cells can result. Animal studies by the Department of Health and Human Services (DHHS) have shown CCl_4 to be possibly carcinogenic. IARC classifies CCl_4 in Group 2B (possibly carcinogenic to humans), while the EPA classifies CCl_4 as a probable human carcinogen (ATSDR 2005).

The World Health Organization (WHO) has set maximum contaminant level guidelines for drinking water for a range of chemical contaminants. The guideline for carbon tetrachloride is 0.004mg/L (WHO 2011). The EPA has set 0.005 mg/L for carbon tetrachloride as the maximum contaminant level (EPA 2011).

Methods

Modeling Approach and Assumptions

The aquifer under the UCIL pesticide manufacturing facility and the surrounding area was characterized within ACTS as a confined, two-dimensional, saturated, infinite model with constant dispersion coefficients. In order to define the modeling domain, the x-axis of the model grid is aligned with the reported direction of groundwater flow,

Southwest to Northeast, with a maximum length of 2 kilometers, and the y-axis centered on the UCIL facility, extended to include the whole facility with a width of roughly 500 meters. The following assumptions were made for modeling purposes:

1. The contaminant plume will be characterized as flowing in the reported direction of groundwater flow (Labunska 1999, NEERI 2010), with the location of the source remaining constant. Groundwater flow is assumed to be steady and uniform.
2. The surficial aquifer is characterized as infinite, meaning the boundaries of the aquifer are assumed to be far enough away that they do not affect the dispersion coefficient.
3. Because of the limited amount of data regarding soil and groundwater properties specific to the site, certain hydrogeologic parameters (porosity, bulk density of soil, etc) were estimated based on their typical values as reported in the literature.
4. It is assumed that the concentration of CCl_4 is constant and no source remediation has been performed. This is due to the high level concentrations of the contaminants found at the site approximately 15 years after the closing of the site (Labunska et al. 1999)

Model Input Parameters and Source Definition for Deterministic Simulations

Parameters pertaining to groundwater flow and contaminant characteristics are obtained from a variety of sources including relevant literature articles, existing site field data and measurements taken remotely through Google Earth (Table 1). All of the values for the deterministic analysis are shown in Table 2. The model was calibrated by manual adjustment of input parameters, which most closely approximated the measured concentrations found in field measurements generally located along the axis of groundwater flow (Labunska 1999, NEERI 2010).

In order to estimate the source concentration of CCl_4 , the model was calibrated by varying the concentration at the inflow boundary, assuming the source originated in 1984. By varying the concentration at the inflow boundary, and adjusting the field and chemical constants, it was determined that 4,000mg/L most closely approximated the concentration measured at the monitoring well used for calibration (Labunska et al. 1999). 4,000mg/L is approximately 5% of the solubility limit of CCl_4 .

Following calibration, a deterministic scenario was simulated using a constant source scenario under the assumption that there has been no source removal or remediation of the site.

Model Input Parameters for Probabilistic Simulations

In order to conduct probabilistic analyses of contaminant transport, two-stage Monte Carlo simulation was performed by generating probability density functions (PDFs) for three input parameters. In the first stage, PDFs were generated for each parameter that had a degree of uncertainty, in other words, the values were recorded in the literature or cited in field measurements as ranges. 10,000 realizations were simulated to characterize the variability in the parameters. In the second stage, another 10,000 realizations of the model were run within ACTS using the inputs of the PDFs for each parameter, thereby creating a range of probabilities of contaminant concentrations in the groundwater for specified times and distances.

The two parameters chosen for two-stage Monte Carlo simulations are the Darcy groundwater velocity and the retardation coefficient. The Darcy groundwater velocity underwent Monte Carlo simulations by varying proxy parameters that are required to calculate the Darcy groundwater velocity: hydraulic conductivity and porosity. Input

parameters and their distributions are presented in Table 3. Probabilistic simulations will be run for three points of interest, 500m, 1000m and 2000m northeast of the center of the UCIL site for three different time periods. These areas represent dense population centers.

Results

Calibration Results

In order to determine the parameters that best estimates measured concentrations of carbon tetrachloride, the model was calibrated by varying the input parameters that achieved results that most closely matched concentrations found in a well roughly 300 meters northeast of the center of the production facility. The concentration at the inflow boundary that most closely matched the concentration measured at IT9030 and IT9032 was 4,000mg/L (Table 4, Figure 3).

Deterministic Model Simulations

After having calibrated a set of parameters to appropriately model the system, simulations were conducted using single-value and distributed-value inputs to model the contaminant plume at a maximum distance of 2000 m with different time end-points. Given the initial source concentration, the deterministic model output shows a normalized concentration of 3.80×10^{-22} , which is 1.52×10^{-15} mg/L at a location 2000 meters from the source concentration in 2084. To put the results in context, the outcome of interest was the location of the plume, which approached the U.S. EPA MCL, which is represented in the figure as a normalized concentration of 1.25×10^{-6} (Figure 5a-c).

The model was run to simulate the plume at 10, 30 and 50 years since the closing of the UCIL site in 1984. 10 years after the end of operations at the site, the leading edge

of the level that represents the EPA level MCL is at a distance of approximately 850 meters from the source. Given a constant source scenario, after 10, 30 and 50 years, distances beyond roughly 850m are not projected to contain concentrations of CCl_4 above 0.005mg/L.

Probabilistic Model Simulations

The results for the probabilistic scenario include two histograms showing the probabilistic distributions for the two input parameters that underwent Monte Carlo simulations. Descriptive statistics of each of those input parameters are presented in Table 3 and Figures 6a – 6b.

Three different locations (500m, 1000m and 2000m) were chosen because of their central location in densely populated areas to the northeast of the site. The results of probabilistic simulations for each location show the likelihood of exceeding certain concentrations, particularly the WHO MCL of 0.004mg/L ($C/C_0 = 1 \times 10^{-6}$) at specified points in space and time. For all simulations (500m, 1000m and 2000m), there is a 100% probability that the concentration of CCl_4 exceeds the WHO MCL. For concentrations higher than this, the probabilities drop (Figures 6 – 9).

Discussion and Conclusion

Contaminant Plume

The EPA and WHO have both set drinking water standards for CCl_4 , 0.005mg/L and 0.004mg/L, respectively. The model simulations were run in order to determine at what locations and times this concentration is exceeded, and as a result, pose a health risk for the populations exposed to the groundwater. Deterministic simulations show that given a constant source, populations living up to roughly 850 meters from the source will

be exposed to concentrations of 0.005mg/L. Deterministic simulations show reduced concentrations for populations living further out than 850 meters.

In the probabilistic model simulations, for all distances and times simulated, there is a 100% probability that the concentration of CCl_4 will exceed the WHO MCL of 0.004mg/L ($C/C_0 = 1 \times 10^{-6}$). As the magnitude of the concentration increases, that probability decreases, but still remains a point of concern. For example, in 2014, at 500 meters away from the source, there is a roughly 70% probability that the concentration of CCl_4 will reach 10,000 times the WHO MCL. At 1000m, this probability reaches 60% and decreases only slightly at 2000m in 2014. Studies, which also use ACTS to characterize contaminant plumes, recommend that probabilities of exceeding below 13% are not actionable levels (Anderson et al. 2010). However, given that the probabilities demonstrated in the ACTS model almost guarantee that the concentration of CCl_4 will be far greater than the WHO and U.S. EPA MCL, it would be prudent for policy makers to began a remediation campaign for the groundwater.

Limitations and Recommendations

Various maps detail the locations of specific pesticide production processes on site at UCIL. The location for the source of CCl_4 was chosen based on Figure 2. However, the two locations chosen for calibration (IT9030 and IT9035), while located northeast of the chosen source, they were not along a linear axis. In order to determine the calibration concentration, an average of the CCl_4 concentrations measured in 1999 (Labunska et al. 1999) was chosen.

The ACTS software provides a convenient method for characterizing contaminant plumes in groundwater. The software relies on the user to collect contaminant and

hydrogeologic parameters for use as inputs into a user-generated model. ACTS is capable of running both deterministic and probabilistic scenarios. The deterministic model is used when single value inputs are used to produce a single value output, characterizing the concentration of contaminants at a point in space and time. The probabilistic model takes into account the uncertainty in parameters, and characterizes the contaminant plume as a range of probabilities that the concentration of the chosen contaminant exists at a certain location in space and time.

Because this study was performed remotely, all of the parameters were chosen from the literature. Many studies performed in Bhopal at the site of the UCIL factory report contaminant and hydrogeologic data; however, certain parameters (aquifer porosity and bulk density of soil) were chosen from a reference of typical values (Cherry and Freeze 1979, Wallace 1981). This introduces a level of uncertainty when running the model simulation in ACTS. This is dealt with to some degree in the probabilistic simulations.

There is also some disagreement regarding the direction of groundwater flow in the region of UCIL. Within the NEERI report from 2010, the direction of groundwater is reported to be in both the Northeast and Southeast direction. This, they claim, is due to the variable nature of groundwater flow depending on the conditions (NEERI 2010). The Greenpeace report from 1999, citing an earlier report by NEERI, state that the direction of groundwater flow is along a Northeast axis. Given that the contaminant concentrations used for calibration increased along the Northeast axis, it was assumed for the purposes of this study that the direction of groundwater flow was along the Northeast axis. More

detailed studies of the aquifer will be crucial to more accurately characterize the nature of the aquifer and contaminant plume.

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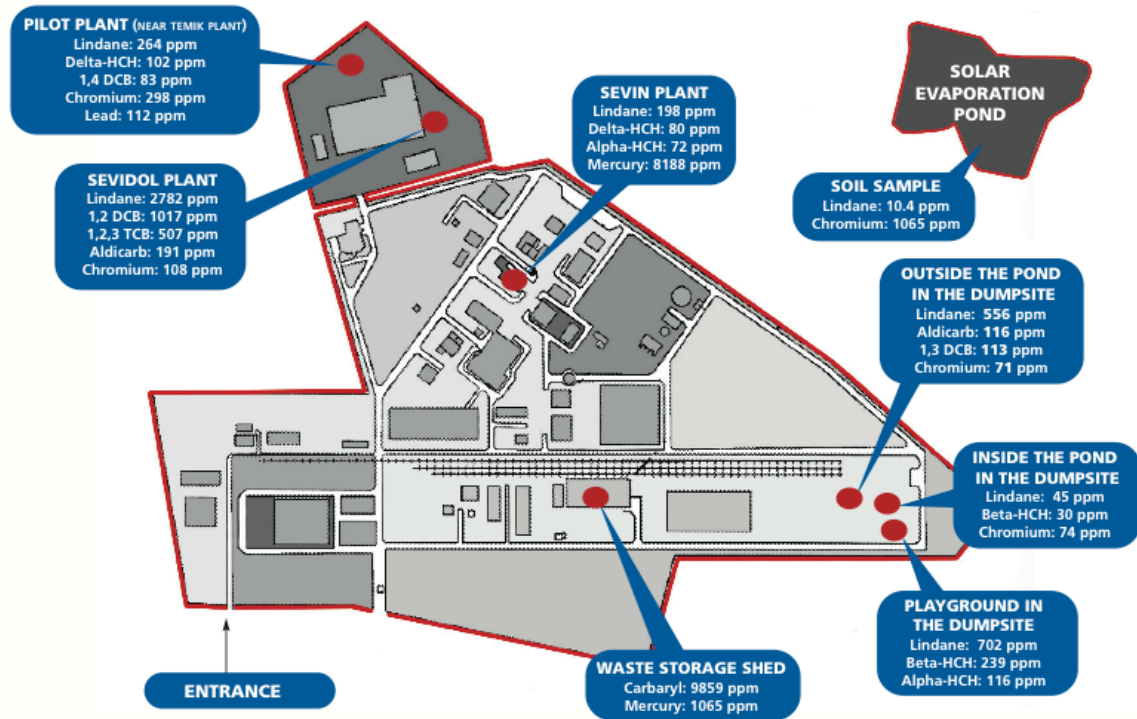
Figures

Figure 1: The Central Indian State of Madhya Pradesh



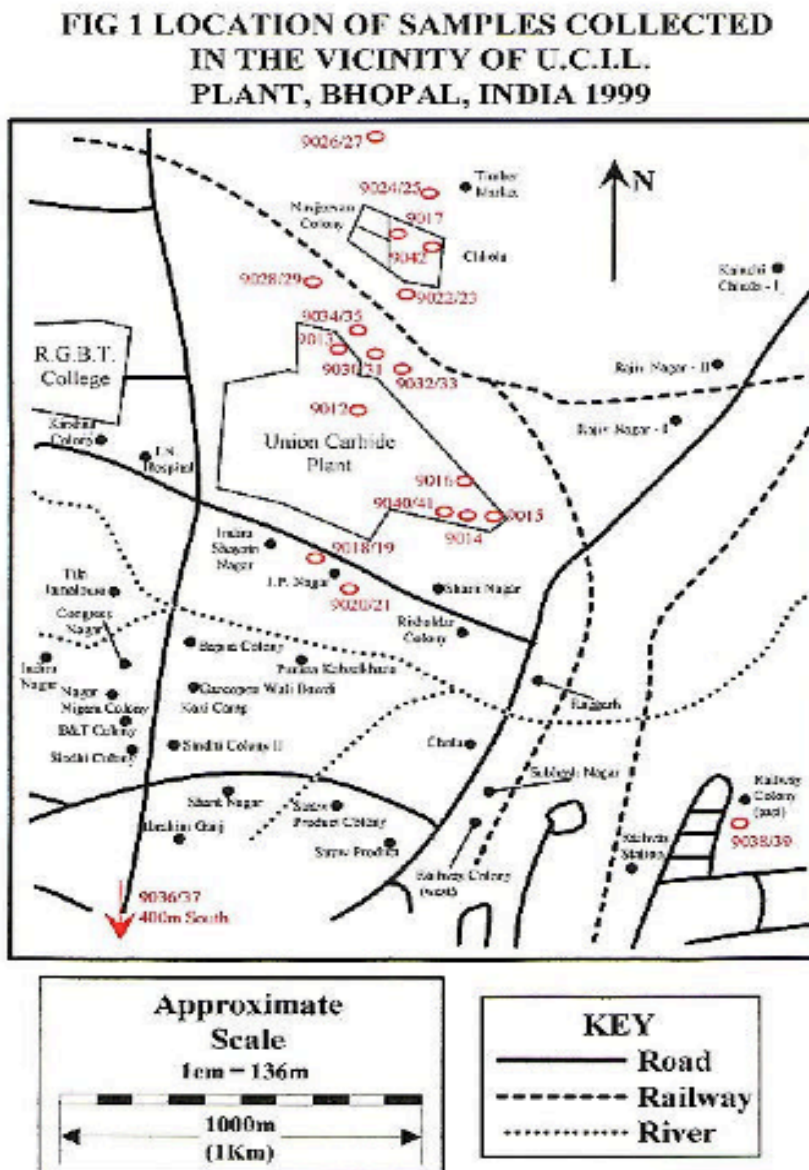
<http://raisin.nic.in/maps.htm#India%20MAP>

Figure 2: Center for Science and Environment Schematic of UCIL Factory



<http://cseindia.org/content/continuing-nightmare-bhopal-cse-laboratory-tests-soil-water-samples-union-carbide>

Figure 3: Greenpeace Sampling Locations at the UCIL Factory in Bhopal, India



<http://www.greenpeace.org/international/en/publications/reports/the-bhopal-legacy-toxic-cont/>

Figure 4: NEERI: Location of Suspected Dump Sites

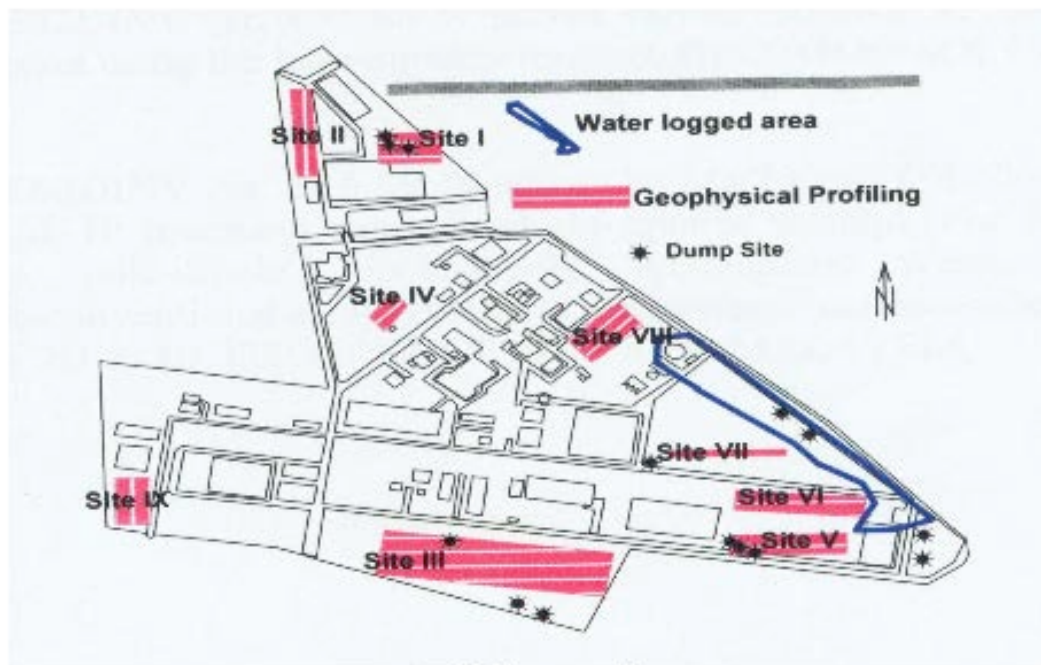


Figure 5: Locations of suspected dumps at UCIL premises

**Figure 5a: Deterministic Simulation Results for Calibration Target
Calibration of Carbon Tetrachloride (model simulation = 15 years)**

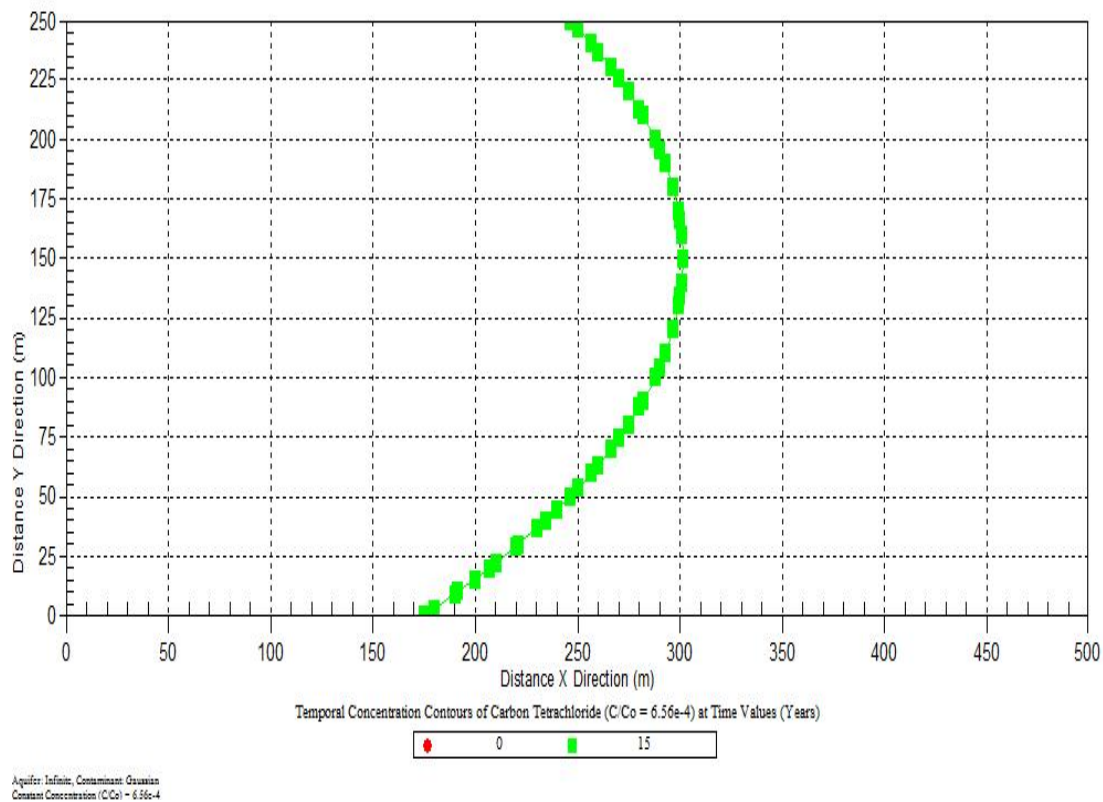


Figure 5b: Deterministic Simulation Results for 1994
Normalized Concentration of Carbon Tetrachloride (model simulation = 10 years)

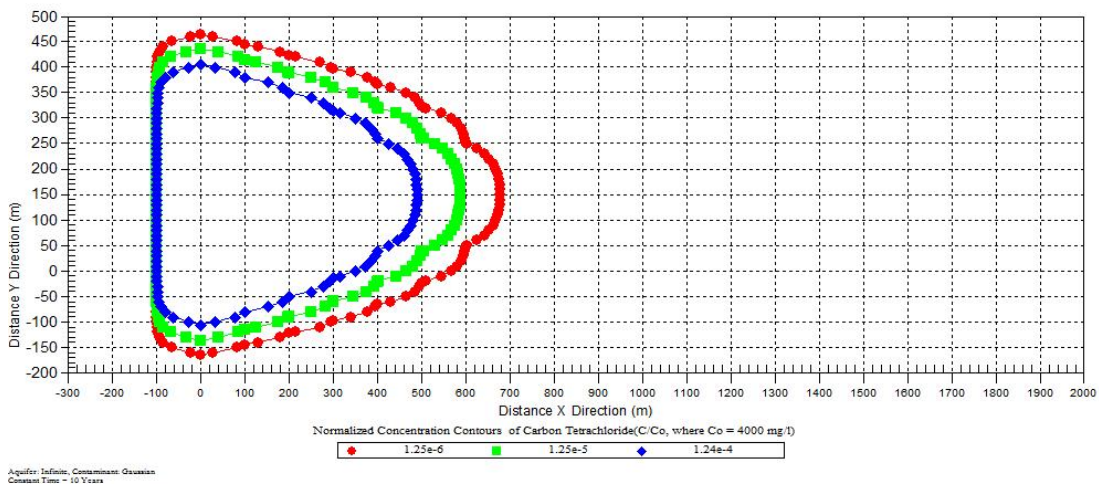


Figure 5c: Deterministic Simulation Results for 2014
Normalized Concentration of Carbon Tetrachloride (model simulation = 30 years)

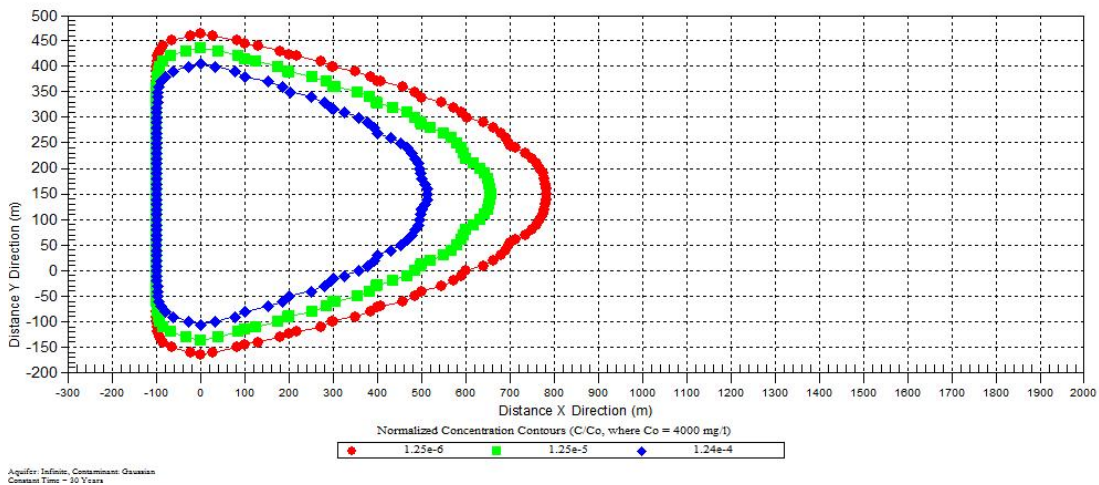


Figure 5c: Deterministic Simulation Results for 2034
Normalized Concentration Distribution of Carbon Tetrachloride (model simulation = 50 years)

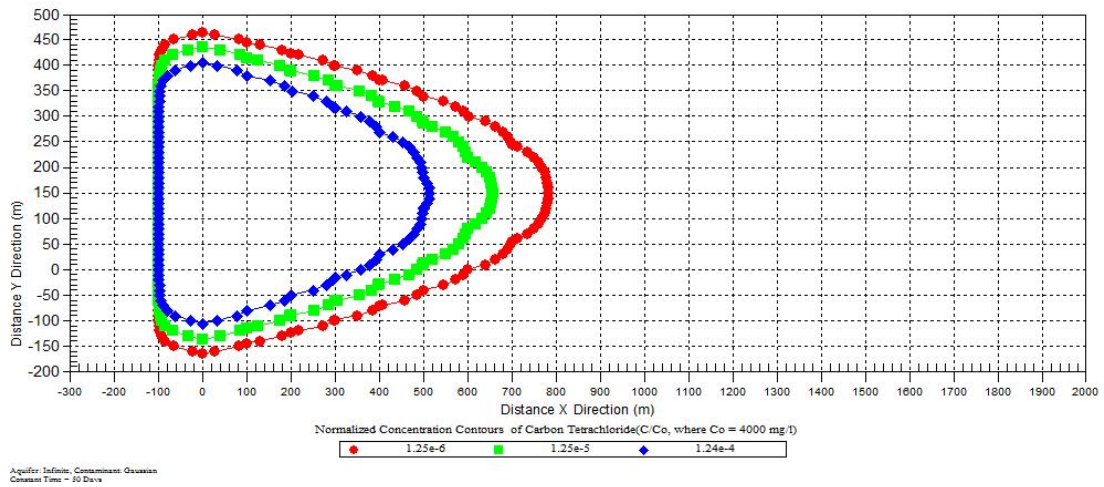


Figure 6a: Range of Values for Groundwater Velocity

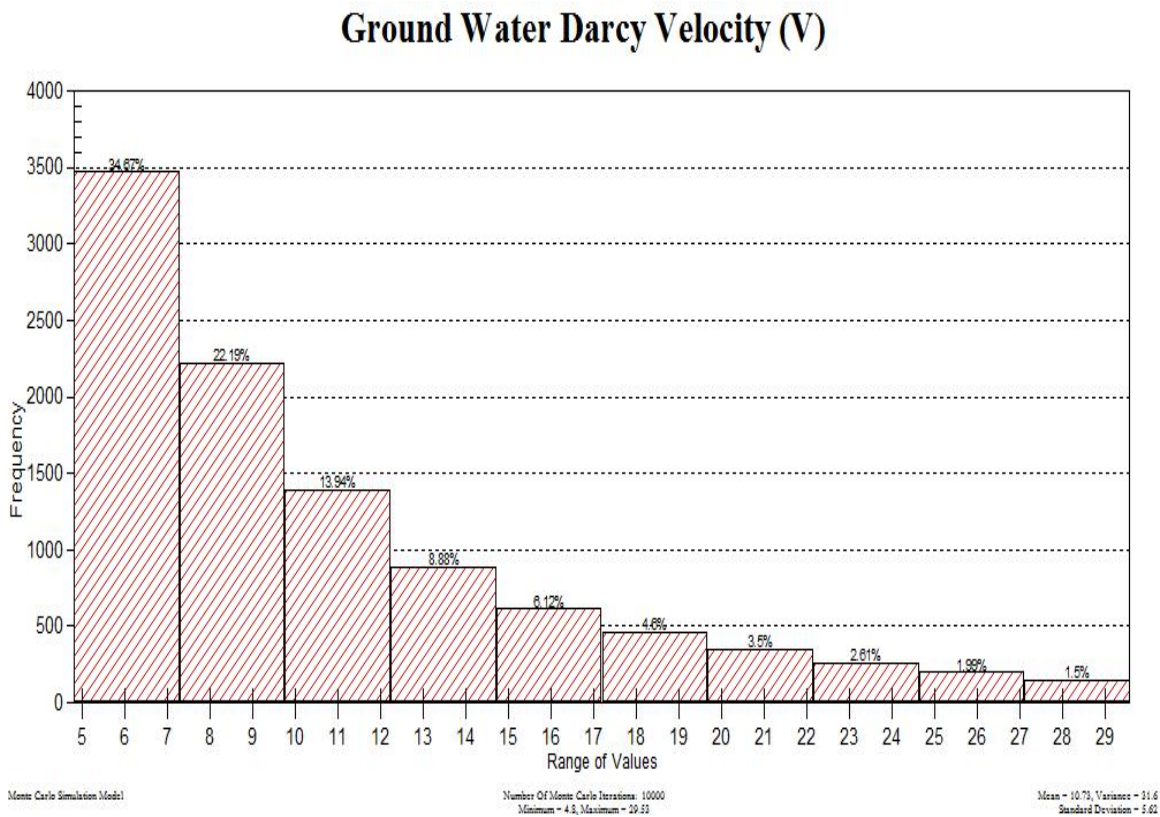


Figure 6b: Range of Values for Retardation Coefficient
Retardation Coefficient (R)

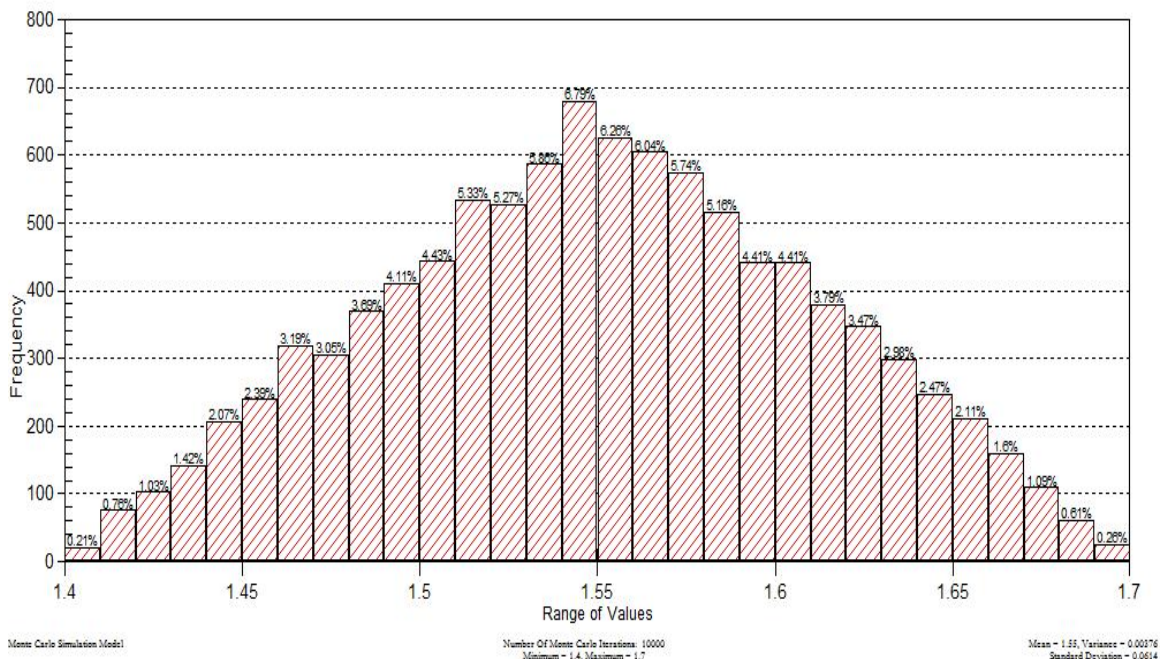


Figure 7a: Probability of Exceeding World Health Organization MCL for Carbon Tetrachloride in 1994 (500 meters from the Source).

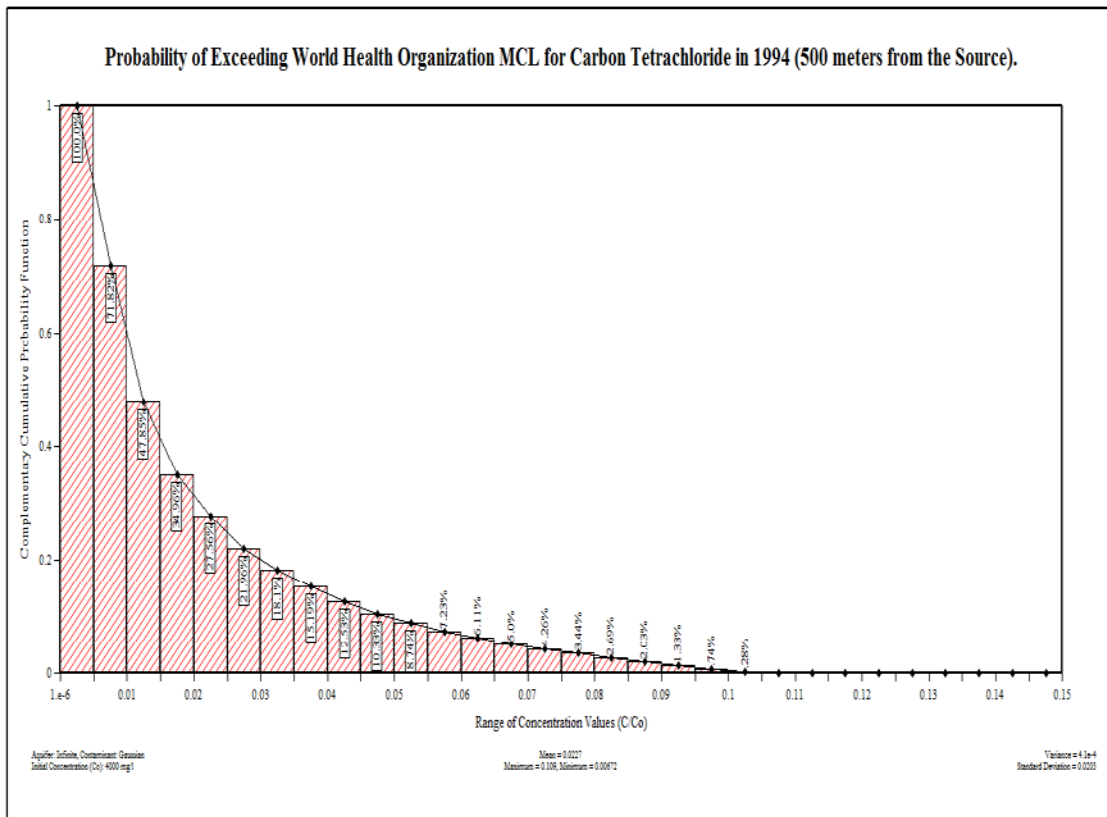


Figure 7b: Probability of Exceeding World Health Organization MCL for Carbon Tetrachloride in 2014 (500 meters from the Source)

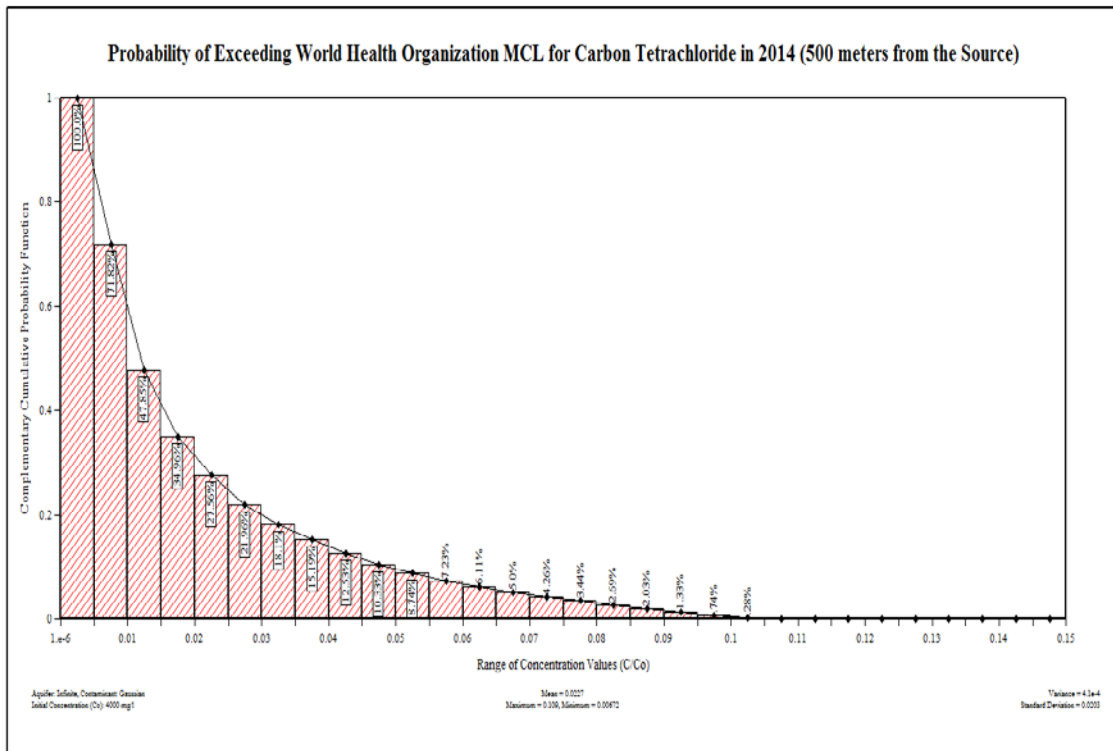


Figure 7c: Probability of Exceeding World Health Organization MCL for Carbon Tetrachloride in 2034 (500 meters from the Source)

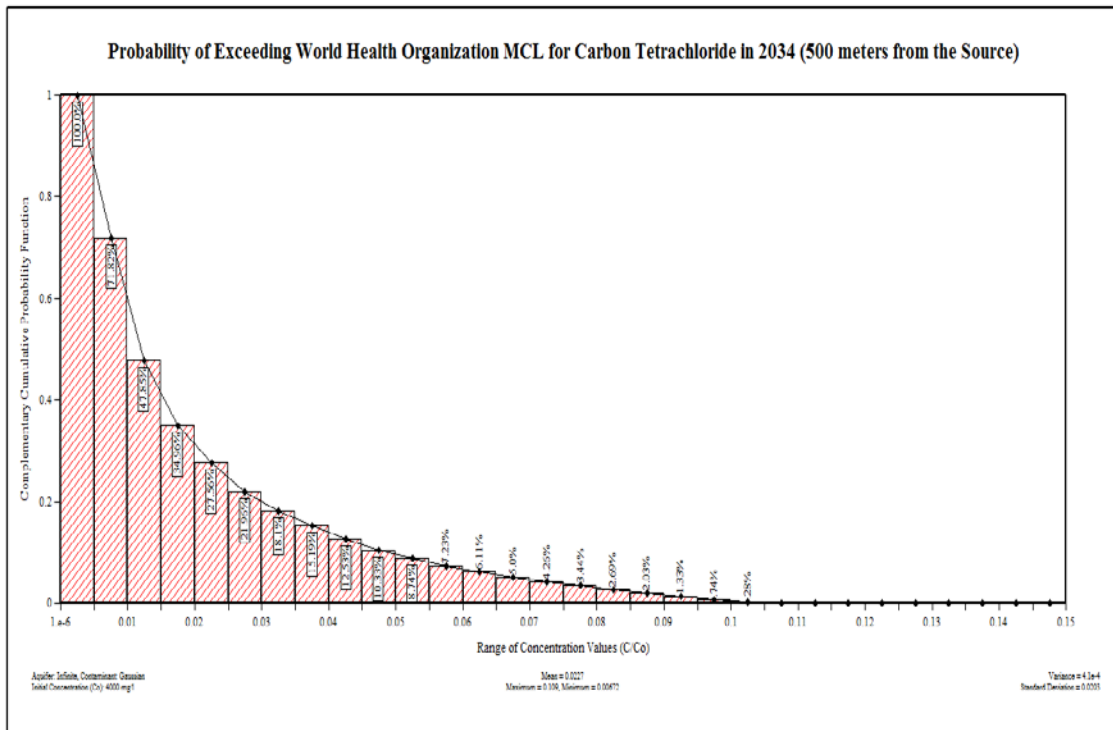


Figure 8a: Probability of Exceeding World Health Organization MCL for Carbon Tetrachloride in 1994 (1000 meters from the Source).

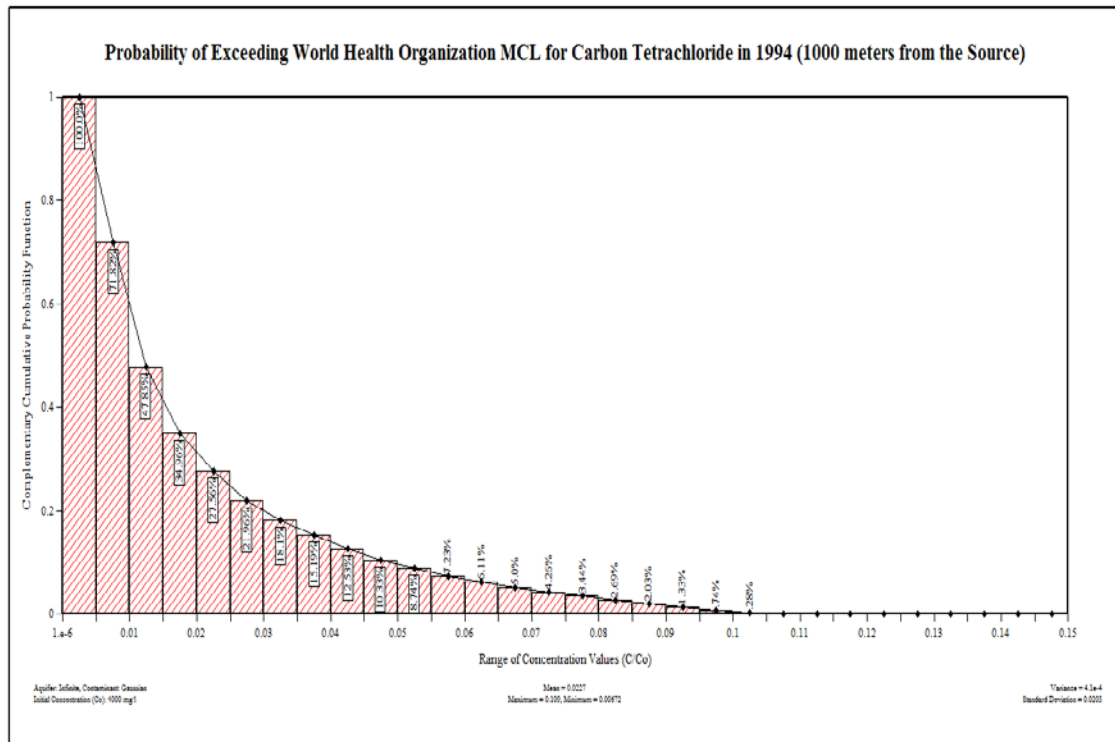


Figure 8b: Probability of Exceeding World Health Organization MCL for Carbon Tetrachloride in 2014 (1000 meters from the Source)

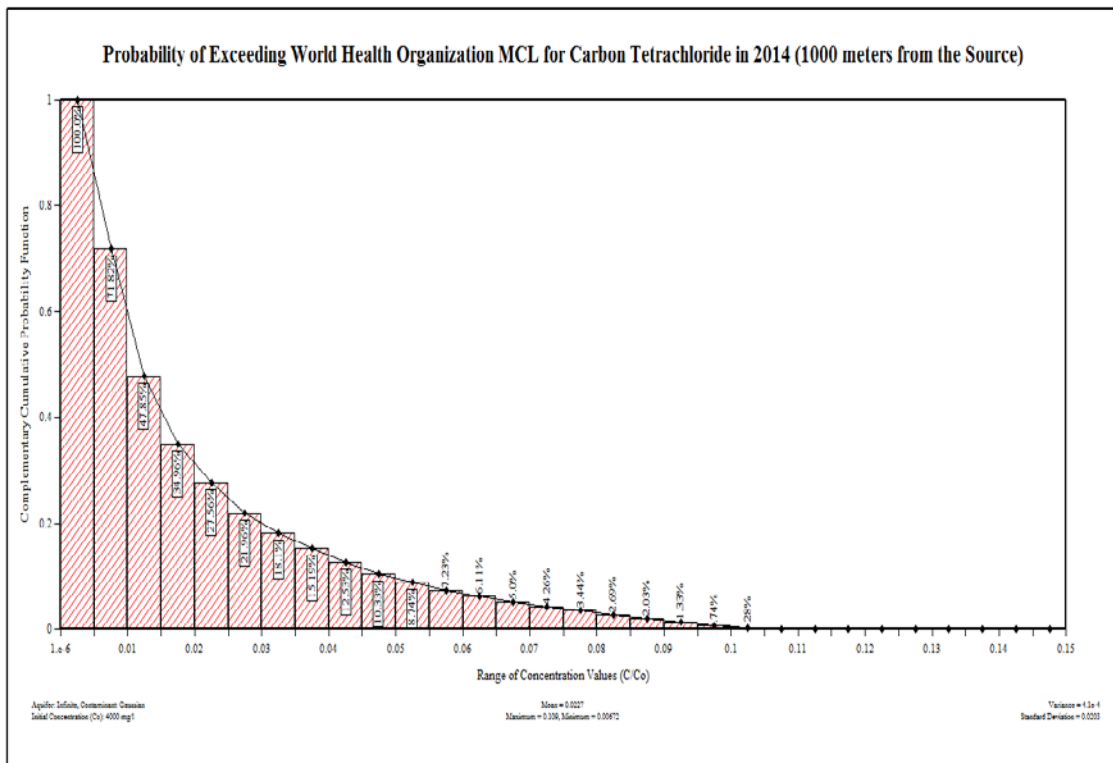


Figure 8c: Probability of Exceeding World Health Organization MCL for Carbon Tetrachloride in 2034 (1000 meters from the Source)

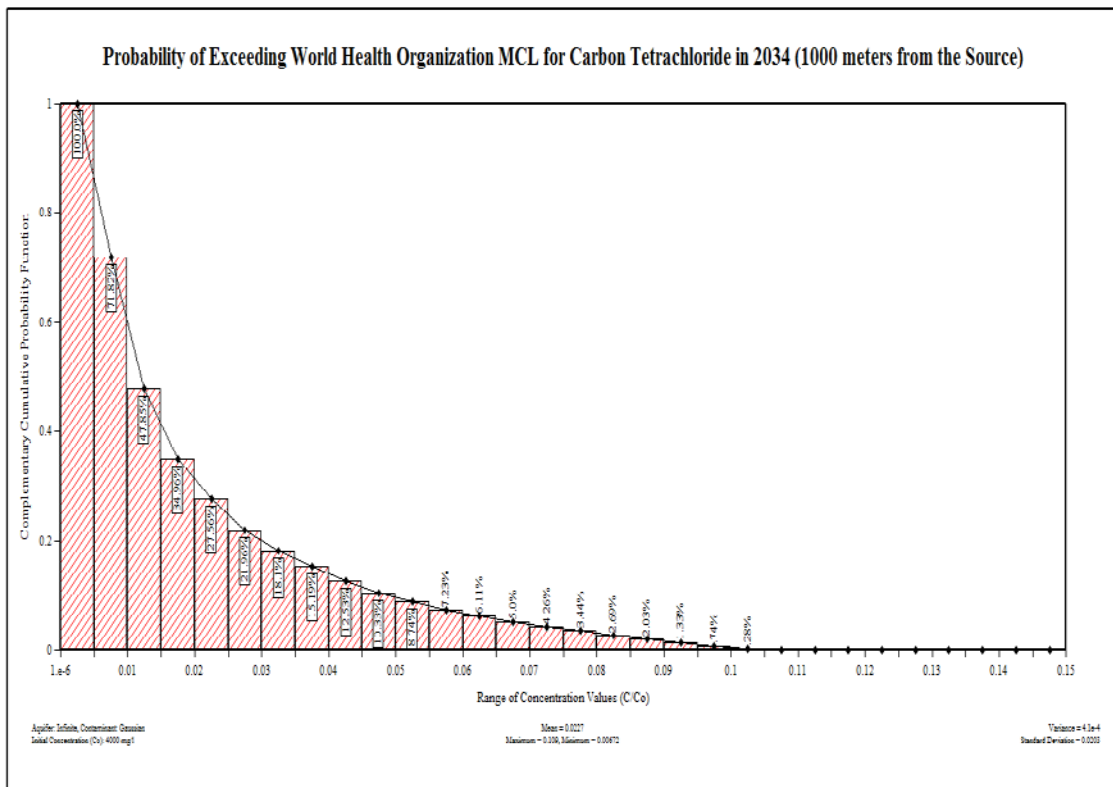


Figure 9a: Probability of Exceeding World Health Organization MCL for Carbon Tetrachloride in 1994 (2000 meters from the Source)

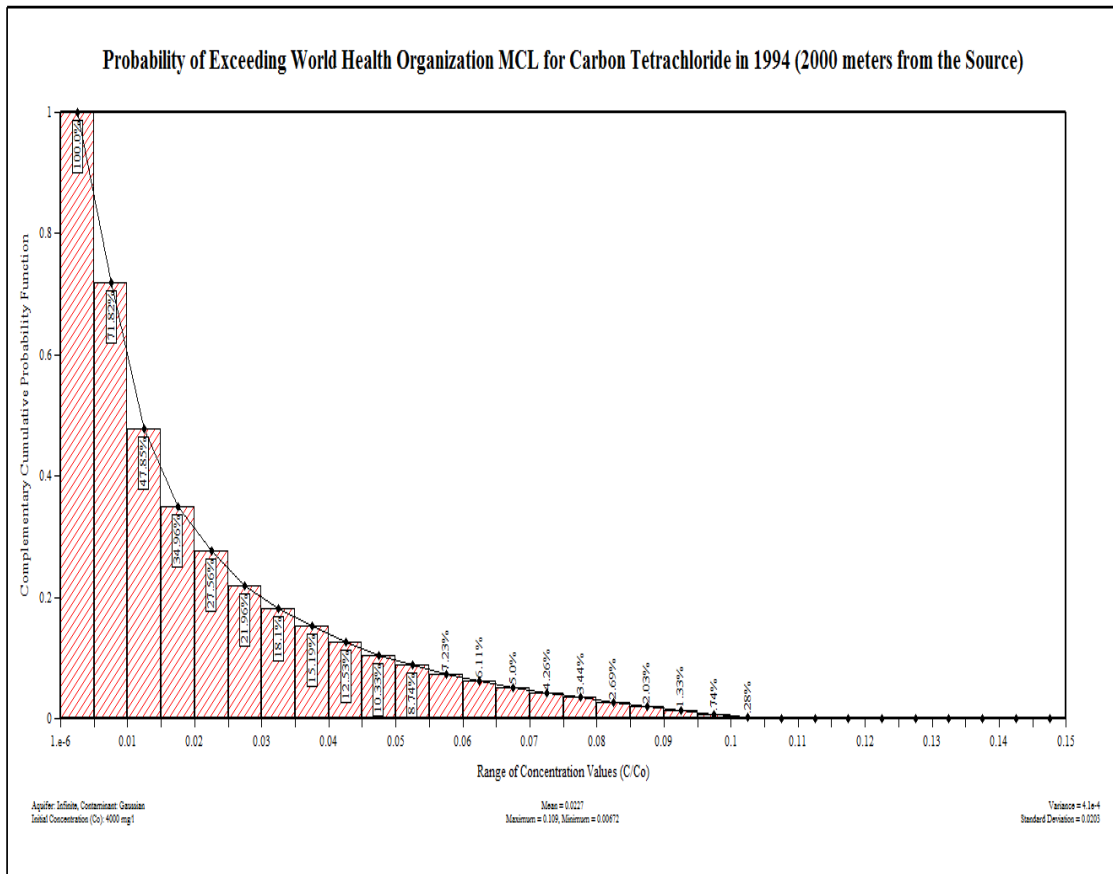


Figure 9b: Probability of Exceeding World Health Organization MCL for Carbon Tetrachloride in 2014 (2000 meters from the Source)

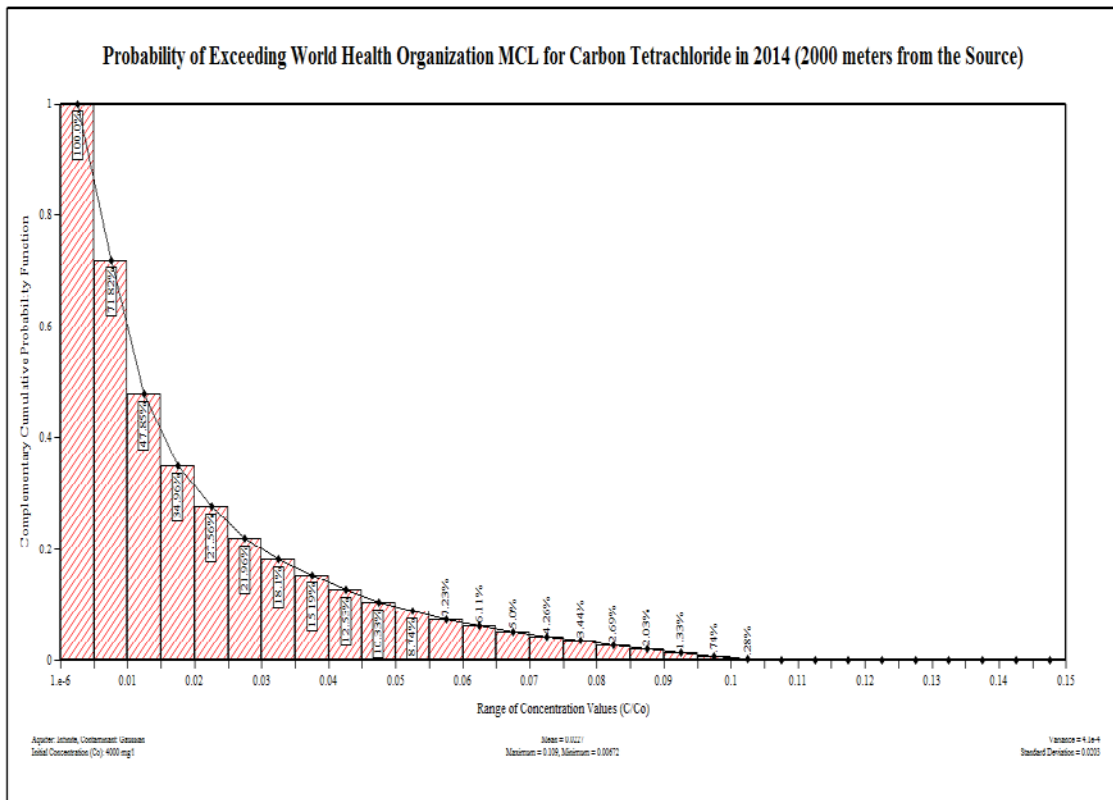
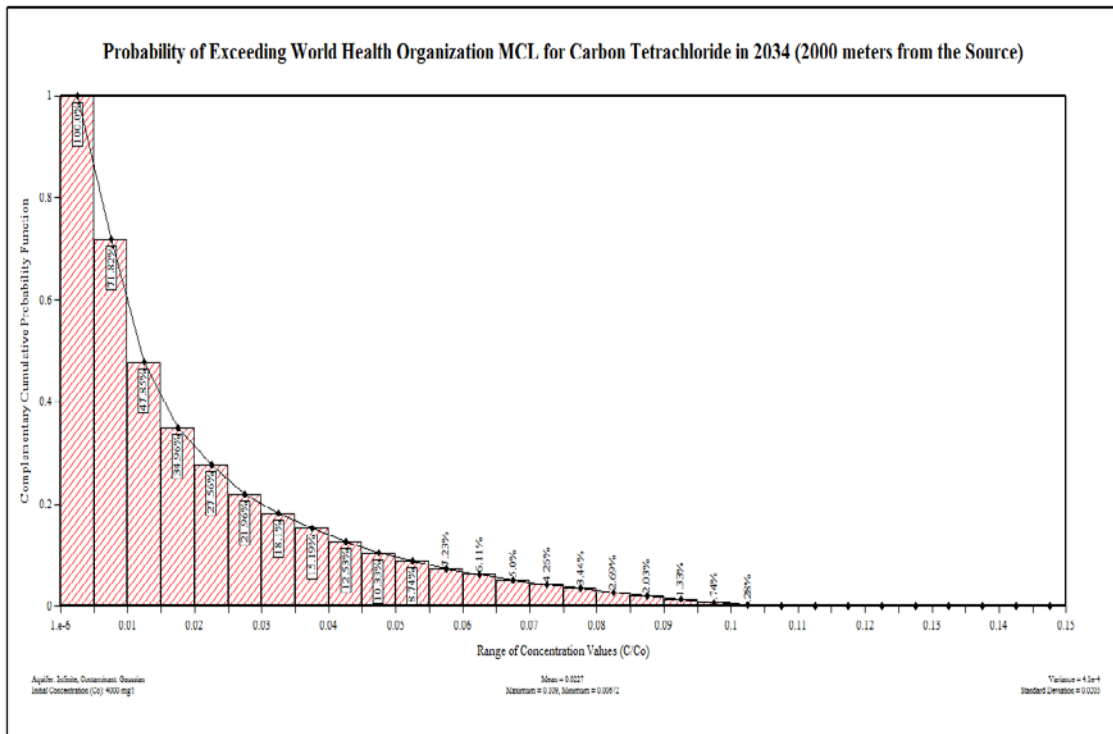


Figure 9c: Probability of Exceeding World Health Organization MCL for Carbon Tetrachloride in 2034 (2000 meters from the Source)



Tables

Table 1: Summary of Relevant Hydrogeologic and Contaminant Transport Parameters for the UCIL site in Bhopal, Madhya Pradesh

<u>Property</u>	<u>Value</u>	<u>Units</u>	<u>References</u>	<u>Notes</u>
Hydraulic Conductivity (K)	0.1 – 0.3	m/day	Powell et al. (1983)	Range of hydraulic conductivities for the Betwa Catchment, over which sits the UCIL factory
Porosity of soil (theta)	0.25 – 0.5		Cherry and Freeze (1979) values cited by the U.S. Department of Energy	Range of Porosity values for sand
Recharge to surficial aquifer (q)				$q = P - Q_s - ET$
Precipitation (P)	120.5	cm/year	Singh et al (2003)	Value for the state of Madhya Pradesh
Surface Runoff (Q_s)	54.23	cm/year	Singh et al (2003)	45% of the annual precipitation from Singh (2003)
Evapotranspiration (ET)	137.21 – 181.32	cm/year	Ramasastri	
	42.18	cm/year	Singh et al 2003)	35% of the annual precipitation as estimated from Singh et al (2003)
Bulk Density of Soil	1500	Kg/m ³	Wallace et al (1981)	Value for Silty Clay
	1.55	g/cm ³	Morris and Johnson (1967)	Value for Fine Sand
Longitudinal Dispersivity	200	M	10% of Aquifer Length (Fetter 1993)	

Ratio of Dispersivities	10 – 100		Fetter (1993)	
Solubility in Water				
Carbon Tetrachloride	800	mg/L	ATSDR Verschueren (1983)	
Retardation Coefficient				
Carbon Tetrachloride	1.4 – 1.7		ATSDR (Mackay et al. 1983)	

Table 2: Deterministic Input Parameters:

Parameter	Value	Data source / Calculation Method
Hydraulic Conductivity (K)	73 m/year	Arithmetic mean of the range of values listed in Powell et al (1983)
Hydraulic gradient (i)	0.068 m/m	Measured as a function of total head between wells IT9020 and IT9030 determined using Google Earth imaging
Porosity of soil (θ), unitless	0.375	Arithmetic mean of the range of values in the literature
Bulk density of soil (ρ_b)	1.55g/cm ³	Value for fine sand (Morris and Johnson 1967)
Specific discharge (V_d) m/year	4.96	$V_d = Ki$
Groundwater velocity (V)	7.45 m/year	$V = Ki/\theta$
Longitudinal dispersivity (α_L), m	200	10% of Study length (Fetter 1993)
Ratio of dispersivities (α_L/α_T), unitless	100	(Fetter 1993)
Longitudinal dispersion coefficient (D_x)	1490m ² /year	$D_x = \alpha_L V$
Lateral dispersion coefficient (D_y)	14.90m ² /year	$D_y = D_x(\alpha_L/\alpha_T)$
Recharge to surficial aquifer (q)	24.09 cm/year	Calculated using values for precipitation, surface runoff and evapotranspiration in Table 1.
Retardation coefficient for carbon tetrachloride (R), unitless	1.55	Arithmetic mean of range of values listed in ATSDR
Source concentration (C), in mg/L At time = 0 years (1984)	4,000 mg/uL	5% of solubility limit
Standard deviation of contaminant source width,	60m	Adjusted to achieve appropriate calibration target

assuming a Gaussian distribution		
Aquifer thickness	6.5m	ACTS computational grid geometry
X-coordinate length	2,000m	ACTS computational grid geometry
Y-coordinate length	500m	ACTS computational grid geometry
Discretization along y-direction	50m	ACTS computational grid geometry
Duration of simulation	100 years	
Temporal discretization	10	

Table 3: Values used to simulate the contaminant plume at the UCIL factory in Bhopal, India

Parameter	Mean Value	Range from which PDF was generated	PDF Distribution	Monte Carlo Statistics
Groundwater Darcy Velocity (V) (m/year)	7.45	4.8 - 29.6	Lognormal	<u>Minimum</u> : 4.8001 <u>Maximum</u> : 29.5333 <u>Standard Deviation</u> 5.6212
Retardation Coefficient (R), unitless	1.55	1.4 - 1.7	Triangle	<u>Minimum</u> : 1.4 <u>Maximum</u> : 1.6983 <u>Standard Deviation</u> : 0.06075

Table 4: Deterministic Result for Selected Calibration Targets

Model Calibration Target	Distance from Source (m)	1999 total carbon tetrachloride concentration ($\mu\text{g/L}$)	
		Measured	Simulated
IT9030 and IT9032 (Labunska et al. 1999)	300	3410 and 1730	2630 ($C/C_0 = 6.56 \times 10^{-4}$)