

USE OF A GENERAL FATE MODEL TO PREDICT
THE FATE OF TASTE AND ODOR COMPOUNDS IN
AN OKLAHOMA RESERVOIR

By

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2008

Submitted to the Faculty of the
Graduate College of the
Oklahoma State University
in partial fulfillment of
the requirements for
the Degree of
MASTER OF SCIENCE
December, 2011

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CHAPTER I

INTRODUCTION

1.1 Overview

Taste and odor problems in surface waters have drawn increasing attention worldwide from biologists, chemists and engineers for the past few decades (Yan et al., 2010). The majority of taste and odor events in drinking water are particularly associated with two compounds: namely geosmin and 2-methylisoborneol (MIB). Both geosmin and MIB are low molecular weight volatile tertiary alcohols. Geosmin and MIB are not harmful, but their presences in drinking water are aesthetically unpleasant. Presence of taste and odor in drinking water may result in decreased consumer trust and subsequently, decreased water consumption and could eventually cause the public to switch to alternate sources of drinking water such as bottled water and in-home treatment systems (Sorial and Srinivasan, 2011). These two compounds are secondary metabolites of actinomycetes (soil bacteria) and *Cyanobacteria* (blue green algae). However, these species produce geosmin periodically, not continually. Since taste and odor compounds are natural in origin it is very hard to control in source water. Moreover, the most problematic of these

these compounds are generally highly stable. The structure of these compounds makes them resistant to the conventional water treatment like coagulation, sedimentation and oxidation. However these taste and odor problems can be avoided or minimized by enhancing the water treatment process.

In addition to that, these compounds can make offensive odor and taste at extremely low threshold concentrations, at nanogram per liter levels to humans. It is very common for the average person to detect the presence of these compounds in the 10 to 30 ng/l (ppt) concentration range (Sorial and Srinivasan, 2011).

To better understand the behavior of these chemicals, both in the environment and in water plants, it is necessary to predict the chemical distribution and persistence of this chemical in multimedia environment. General fate models (GFM) are used to identify the fate and transport of chemicals in the environment. These models typically have the following purposes:

- A) To maximize our understanding of a monitored system.
- B) To obtain the best possible understanding of the likely behavior of a substance not yet being monitored.
- C) To enhance a monitoring program by providing guidance on the likely behavior of the substance of interest (Mackay, 2005).

There are many fundamentally different models used to understand and predict chemical fate for various purposes. They are conceptual models, statistical models and mass balance models. The mass balance models are also valuable educational and research tools for exploring and teaching new scientific concepts including the behavior of chemicals in physical and biological systems (Mackay, 2001). The United States National

Research Council defines a model as “A simplification of reality that is constructed to gain insights into select attributes of a particular physical, biological, economic or social system” (NRC, 2007). The model used in this paper to evaluate fate and transport of taste and odor compound in different media is called Level III from Center for Environmental Modeling and Chemistry (CEMC) (CEMC, 2011). This model is a steady state distribution model of a non-conserved chemical discharged at a constant rate into an open environment.

The Level III version 2.80 model predicts the chemical fate and transport of chemical by taking their chemical and environmental properties as input values. The Level III model also requires the user to specify the chemical’s mode-of-entry to the environment, i.e., to air, or water, or soil, or some combination of these media. The Level III model is founded upon the fundamental law that mass is neither created nor destroyed, and therefore, this model is classified as a mass balance models. A mass balance environmental model can:

- i) Reveal likely relative concentrations, i.e., it is useful for monitoring purposes by indicating likely relative concentrations between media such as air, water, and fish,
- ii) Show the relative importance of loss processes, i.e., the process rates that we need to know most accurately,
- iii) Link loadings to concentrations, i.e., identify key sources and ultimately their effects,
- iv) Enable time responses to be estimated, i.e., how long recovery will take, and
- v) Generally demonstrate an adequate scientific knowledge of the system (Webster et al., 2005).

In the study presented here, this model is used to predict the fate of geosmin and MIB in Lake Eucha, Oklahoma. It will also include a sensitivity analysis of input parameters to determine which are most important and which are less important.

1.2 Objectives

The specific objectives of this study are as follows:

- 1) To collect all pertinent inputs required by a general fate model (Level III) for geosmin and MIB,
- 2) To perform a sensitivity analysis on the general fate model to determine which inputs are most critical,
- 3) To use the general fate model to analyze the behavior of geosmin and MIB in Lake Eucha, Oklahoma.

CHAPTER II

REVIEW OF LITERATURE

2.1 Mass balance modeling concepts

Mass balance multi-compartment models pioneered by Mackay are the most commonly used models to quantify the fate, transport and transformation of organic chemicals in the environment (McKone and MacLeod, 2003). These models use mathematical expressions to combine chemical transport processes (e.g., diffusion in water and advection by wind) and chemical transformation processes (e.g., microbial degradation, hydrolysis) with thermodynamic principles to quantify chemical fate, transport and behavior. There are three important environmental processes to be considered in a mass balance model, including degradation processes, advection processes and intermedia exchange processes.

2.1 a) Transformation or degradation processes

A substance can be effectively removed from consideration by being transformed through a chemical reaction. This is often described as degradation and first-order reaction kinetics are frequently assumed in analogy with radioactive decay. These reactions

include photolysis, oxidation, hydrolysis, and biodegradation.

2.1 b) Advection processes

Advection processes such as wind transport and river currents can effectively remove a substance from the modeled system by transporting it to a different location.

2.1 c) Intermedia exchange processes

Exchange between environmental media can occur by a multitude of processes including diffusion, rain dissolution, wet and dry aerosol deposition, runoff, and sedimentation and resuspension. Depending on the specific model other processes may be included. The importance of each process is highly dependent upon the chemical being investigated.

2.2 Level III model

As noted, one key general fate model in use is called Level III (CEMC, 2011). In a Level III simulation, the chemical is assumed to be continuously discharged at a constant rate and achieves a steady state condition in which input and total output rates are equal. The loss processes are degrading reactions and advection. Level III model calculations require basic chemical property and reaction half-life information. Level III model also require the user to specify the chemical's mode-of-entry to the environment, i.e., to air, or water, or soil, or some combination of these media. Medium-specific emission rates, are now required because the results are strongly dependent on the receiving medium or media, i.e., the "mode-of-entry". The chemical distribution in the defined environmental compartments thus reflects the partitioning properties, inter-media transfer processes, degradation properties, advection rate information, and environmental properties. In the Level III model the equilibrium exist within the medium not between the medium. Without the equilibrium assumption the chemical's fugacities in each medium generally

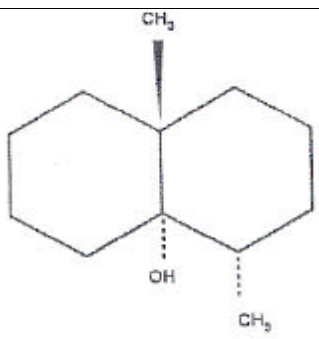
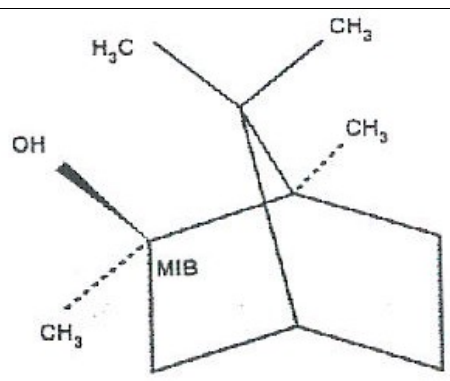
differ and, it is now necessary to describe active transport processes between environmental media. These can include processes such as diffusion, volatilization, deposition, resuspension, and runoff and require a variety of input data depending on the details of the environment modeled.

2.3 Background

Taste and odor problems are associated with aesthetic quality of water. The aesthetic quality of water comes under the USEPA's secondary standards for drinking water, which are not enforceable. However these taste and odor problems are often a source of consumer complaints when they are exceeded. For an average consumer, taste and odor is the only way of determining the safety of tap water (McGuire, 1995). As mentioned there are two organic compounds which are primarily responsible for producing taste and odor problems in finished drinking water. They are geosmin (trans-1, 10-dimethyl-trans-9 decalol, $C_{12}H_{22}O$) and MIB (2-methyl isoborneol, $C_{11}H_{20}O$) which have been identified to be the major taste and odor-causing compounds in drinking water obtained from surface water. Biodegradation and metabolism by actinomycetes (soil bacteria) and *Cyanobacteria* (blue green algae) are the main producers of geosmin and MIB in surface water. Certain environmental factors or conditions may influence the growth of blue-green algae and the production and release of geosmin: warm water temperatures, a stable water column (stratified conditions), a low ratio of total nitrogen to total phosphorus concentrations, high total phosphorus concentrations, predation by other organisms, and turbid conditions (Bowen, 2009). So the drinking water treatment plant which receives surface water as a raw water source will face taste and odor episodes significantly. In addition to the aesthetic and ecological problems, cyanobacterial blooms can have serious

consequences for drinking water supply by physically blocking the filtration processes in water treatment plants, and producing a range of metabolites such as harmful cyanotoxins in addition to taste and odor (T/O) compounds (Watson, 2004, van Apeldoorn et al., 2007, Watson et al., 2007, Pirbazari et al., 1993). Table 1 shows the physical and chemical characteristics of MIB and geosmin.

Table: 1 Physical and Chemical properties of MIB and geosmin (Pirbazari et al., 1992).

Parameter	Geosmin	MIB (2-methylisoborneol)
Molecular Formula	C ₁₂ H ₂₂ O	C ₁₁ H ₂₀ O
Molecular Weight [g/mole]	182	168
Boiling Point [°C]	165.1	196.7
Aqueous Solubility [mg/L]	150.2	194.5
K _{ow}	3.7	3.13
Henry's Law Constant (atm m ³ /mole)	6.66*10 ⁻⁵	5.76*10 ⁻⁵
Structure		

The treatment methods that have been successfully implemented by water treatment plants to remove geosmin and MIB are adsorption by granular/powdered activated carbon or advanced oxidation process by ozone, UV and H₂O₂. While these two earthy-muddy-smelling metabolites have been the focus of considerable research since early 1960s, geosmin and 2-MIB remain poorly understood throughout much of the water industry, and misconceptions which impede the prediction, treatment, and control of these volatile organic compounds (VOCs) persist (Juttner and Watson, 2007).

2.4 Sources of geosmin and MIB

Most taste and odor problems are produced by microbial metabolites in water environment which cause earthy, musty and muddy odors (Tucker, 2000). Geosmin and 2-methylisoborneol are the most common earthy musty metabolites found in cultures of *Cyanobacteria* and actinomycetes (Gerber and Lechevalier, 1965, Watson et al., 2008, Watson et al., 2003). The off-flavor geosmin and MIB may be released into the water in large amount, during the algae bloom development. The most common kinds of algae in lakes (e.g., blue-green algae diatoms, green algae, chrysophytes, and dinoflagellates) can produce a wide range of compounds that can be detected by humans as definable tastes and odors (e.g., moldy, musty, fishy, flowery, etc.) (Deas, 2009). *Cyanobacteria* (blue-green algae), photoautotrophs, were recognized as a more frequent source of geosmin and 2-methylisoborneol in water than actinomycetes (Krishnani et al., 2008). Geosmin and 2-MIB are tertiary alcohols, each of which exists as (+) and (-) enantiomers. Odor outbreaks are caused by biological production of the naturally occurring (-) enantiomers. The (-) enantiomers are ten times more potent than the (+) molecules (Juttner and Watson, 2007). Tables 2 present the various species producing MIB, geosmin and both, respectively.

Table: 2 Geosmin- and MIB-producing species (Krishnani et al., 2008)

Species	Origin	Habitat	References
<i>Phormidium</i>			
<i>Phormidium sp.</i> <i>Cal Aq.0100</i>	Aqueduct/USA	Periphyton	Taylor et al., 2006.
<i>Phormidium sp.</i> <i>HD798</i>	Algae/lake	Periphytic	Taylor et al., 2006.
<i>Phormidium sp.</i>	Lake/USA	Benthic	Izaguirre, 1992.
<i>Phormidium sp.</i>	River/Japan	Benthic	Matsumoto and Tsuchiya, 1988.
<i>Phormidium sp.</i>	Inland water/ Norway	Benthic	Berglind et al., 1983b.
<i>Other species</i>			
<i>Synechococcus sp</i> <i>CL792</i>	Lake/USA	Planktonic	Taylor et al., 2006.
<i>Nostoc sp.</i>	Water treatment plant /Taiwan		Hu and Chiang, 1996.
<i>T. granulatum</i>	Japan	Benthic	Tsuchiya and Matsumoto, 1988.
<i>Planktothrix</i> <i>agardhii</i>	Lake/Norway	Planktonic	Persson, 1988; Berglind et al., 1983a.
<i>O. brevis</i>			Berglind et al., 1983b.
<i>Actinomycetes</i>			
<i>Streptomyces</i>	Denmark	Streams/pond	Klausen et al., 2005.
<i>Streptomyces violaceusniger</i>	Water supply/ Jordan	Sediment	Saadoun et al., 1997.
<i>Streptomyces sp.</i>	USA		Gerber, 1977.

2.5 Production of geosmin and MIB

Geosmin and MIB are predominantly intracellular in healthy cells. It will be released into the water during algae blooms or when a water body is chemically treated using algaecides. The taste and odor outbreaks are more prominent under eutrophic conditions. Under this condition, the development of this bloom occur usually the combination of high nutrients content (especially nitrogen and phosphorous) and warm temperature (Srinivasan and Sorial, 2011). There is a direct correlation between the amount of phosphorus in a lake and the quantity of phytoplankton the lake can support. A concentration of 0.1 mgL⁻¹ of soluble inorganic nitrogen is considered the minimum concentration to maintain growth during the growing season. Geosmin showed a close relationship with temperature and MIB with nitrogen uptake (Watson et al., 2003). The highest concentration of geosmin and MIB were recorded during late summer and lower during winter. Other studies show that the blue green algae grow faster in the temperature between 25°C to 30°C which results in higher production of MIB. It also suggests that the production of musty odor chemicals by blue green algae was more prominent during late summer and early autumn (IWASE and Toshihiko, 2010). The previous studies show that the extracellular concentration and productivity of geosmin was maximum at 10°C temperature with a light intensity of 10 $\mu\text{mol m}^{-2}\text{s}^{-1}$. But under the low temperature and light intensity more intracellular geosmin was synthesized and accumulated in the cells (Zhang et al., 2009). Algal cells can produce geosmin at concentration of 10⁻⁵ ng/cell, so a relatively small algal bloom of 10,000 cells/ml would produce levels of 100 ng/l (Hall, 2006). Figure 1 shows the release of geosmin and MIB during biodegradation of algae cells (*Cyanobacteria*).

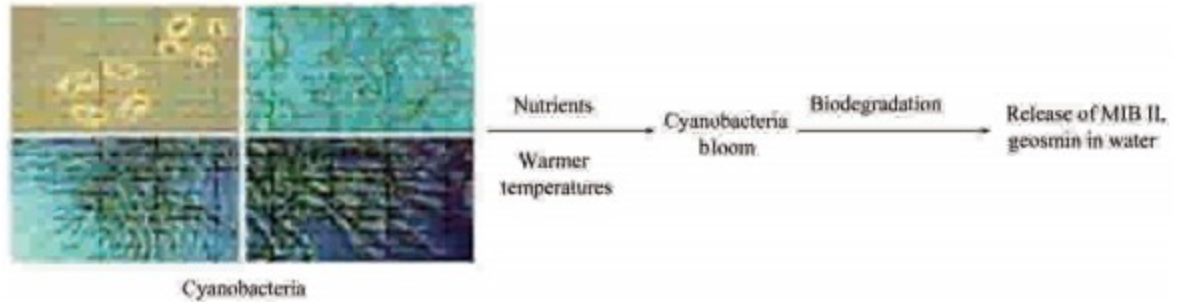


Figure: 1 Simplified pathway of geosmin/MIB formation (Srinivasan and Sorial, 2011).

2.6 Growth of algae blooms

Algae blooms can occur in source water (lakes and rivers), distribution systems and in water treatment processes. Previous studies have observed that the concentration of MIB increase during the decline of *Cyanobacteria* bloom (Tarrant et al., 2009). Abundant blue-green algae and the often associated taste and odor problems usually result from nutrient enrichment in lakes and reservoirs. Nitrogen and phosphorus wash off the land surface during storms and are delivered to lakes or reservoirs. Activities on the land, such as fertilizer application, livestock waste storage, and leaking sewage-disposal systems, often are sources of excess nitrogen and phosphorus that cause the gradual enrichment of lakes or reservoirs (Bowen, 2009). In another study it was found that positive correlation exist between the biomass of phytoplankton and the geosmin concentration in fish water, indicating that geosmin concentration increased with increase of phytoplankton biomass (Xu et al., 2010). Previous study identified the algal growth in uncovered sedimentation and coagulation basins which result in production of geosmin and MIB in water treatment processes (Bruce et al., 2002). Previous studies have investigated the geosmin and MIB at paper and pulp industry mills in the secondary effluent. They found that these compounds were lower or absent in upstream and downstream suggesting, that they were produced

within the bioreactor. They found correlation between the geosmin and MIB with different operating parameters. Since the geosmin and MIB are produced because of the metabolic activity of cells, they are introduced into the water in three ways. They are metabolic excretion of healthy cells, cell lysis and cell death. During the water treatment process addition of chemicals like chlorine may affect the microbial cells resulting in cell lysis which may introduce geosmin and MIB into the finished water (Ridal et al., 2001).

2.7 Treatment technology for geosmin and MIB

Conventional methods like coagulation, flocculation, sedimentation, filtration and disinfection have been used for taste and odor control. However the taste and odor compounds such as geosmin and MIB are extremely resistant to removal by the above conventional methods (Mamba et al., 2009). No removal was observed under a range of PH and coagulation conditions including various alum dosages (Bruce et al., 2002). Oxidation has been used as other common method for taste and odor control. The common oxidants such as Cl_2 , ClO_2 and KMnO_4 are not very effective for the removal of these compounds. But O_3 showed significant removal of geosmin and MIB (85% for 3.8 mg/L dosage rate at a contact time (CT) of 6.4 min) (Jung et al., 2004). The most prominent technology used by the most of water treatment plant are Granular/Powdered activated carbon (GAC/PAC) and Advanced oxidation processes. However its effectiveness of PAC in removal of geosmin and MIB is less when compare to other contaminants.

2.8 Granular/Powdered activated carbon (GAC/PAC)

Granular activated carbon(GAC) or powdered activated carbon(PAC) are the most common strategies widely used in the drinking water treatment plant to encounter the

taste and odor events during late summer to early fall (Srinivasan and Sorial, 2011). In GAC the activated carbon is used as a granular media above the sand/gravel media filter for the removal of Geosmin and MIB from the water passing through it. Although the removal efficiency of GAC is achieved below odor threshold concentration. The complex procedure and high cost makes this method hard to implement in the drinking water treatment plant. The removal efficiency of GAC depends on many factors like surface area of activated carbon, concentration of dissolved organic carbon(DOC), contact time and filter age.

The surface area of activated carbon is directly proportional to the removal efficiency of geosmin and MIB. The large surface area can adsorb large amount of geosmin and MIB, however there is a competition between geosmin/MIB and other organic compounds to reserve a seat in the activated carbon. So whenever the concentration of DOC in the water is high it directly affects the removal efficiency of GAC towards the target compounds (Geosmin/MIB). The other factor which affects the GAC performance is contact time. The contact time is the period over which water flows through the GAC filter. The removal efficiency increases as the contact time is increased. The GAC performance is also depend on filter age, it is found that the removal efficiency of geosmin and MIB decreased below odor threshold level after 12 months. Because of various reason like uneven distribution of sand and gravel media, mixing of these two media over the time period and high concentration of DOC (Ridal et al., 2001). However the complete removal of geosmin and MIB occur only GAC is accompanied by biofilter or is followed by ozonation. In the case of PAC, the higher dosage is needed when the concentration of

geosmin and MIB are high. So there is a possibility of occurring large amount of sludge which leads to higher operating cost (Srinivasan and Sorial, 2011).

2.9 Advanced oxidation processes (AOP)

The other effective method is using AOPs such as ozone, UV and H_2O_2 for the removal of geosmin and MIB. The previous studies observed that the geosmin oxidization during ozonation was at higher degree compared to MIB. The ozonation removes 80 to 90% MIB on all surface water under baseline conditions. The parameters like pH, H_2O_2 , temperature and ozone dose may affect the removal percentage of geosmin and MIB. The maximum removal percentage of MIB (>95%) was obtained during the addition of H_2O_2 . The percentage MIB removal is independent of initial MIB concentration (50 ng/L versus 100 ng/L) across all the nanopure water and natural water conditions evaluated. Lowering pH reduces MIB oxidation by 20% to 50%. Second order rate constants for ozone and HO are slightly higher for geosmin than MIB, leading to higher geosmin removal during ozonation. (Westerhoff et al., 2011). Another study determined the degradation of geosmin and MIB of about 90 and 65% with the UV dose of 1200 mJ/cm² and 6 mg/L H_2O_2 . Under identical conditions, but in the absence of H_2O_2 , only about 20% was degraded with UV photolysis. This study suggest that geosmin and 2-MIB concentrations are mainly reduced by reaction with hydroxyl radical (formed by photolysis of H_2O_2) though a small amount may also degraded by direct photolysis (Jo et al., 2011). In another pilot study showed that two different kinds of GAC (carbon or wood) were used both have the capability of removing MIB more than 90% for at least 9 and 6 months. It also suggests that presence of chlorine reduce the removal percentage of

MIB. The large column experiment determined that 80% of MIB were removed through adsorption and 20% of them through biodegradation.

2.10 Identification and quantification of geosmin and MIB

Geosmin and MIB can cause earthy and musty smell in the finished drinking even at low odor threshold concentration, in the range of nanograms level. So the process of identifying and quantifying are very essential for the removal of these compounds. These compounds can be detected through sensory evaluation like flavor profile analysis however it is very hard to identify and quantify analytically. These compounds can make offensive odor and taste at low threshold concentration, at nanogram levels. The odor threshold concentration (OTC) for geosmin and MIB are 30 and 10 ng/l (Persson, 1980).

Table 3 shows the odor threshold concentration of geosmin and MIB.

Table: 3 Odor Threshold concentrations (Persson, 1980).

VOCs	Odor	General OTC (ng/l)
Geosmin	Earthy	30
2-MIB	Musty	10

It is very essential to use the method which can measure Geosmin and MIB at ng/l level. Conventional methods like liquid-liquid extraction requires large water sample volumes and intensive sample procedures to measure sample at nanogram level (Rashash et al., 1996). On the other hand methods like closed loop analysis and purge & trap have complex equipment and procedures.

2.11 Analysis of geosmin and MIB in water samples

Odor threshold for these compounds is very low, and people can detect them in low nanograms-per-liter (ng/L) concentrations in drinking water, typically 30 and 10 ng/L for

geosmin and MIB, respectively (Persson, 1980) and (Korth et al., 1992). Thus, many water utility companies and beverage manufacturers must detect geosmin, 2-MIB at concentrations of 1–3 ng/l. Solid-phase microextraction (SPME) is a relatively new and simple method for the analysis of volatile and semi volatile compounds occurring in a wide variety of food, water, and environmental matrices (Belardi and Pawliszyn, 1989, Eisert and Levsen, 1996, Pawliszyn, 1997). SPME relies on the partitioning of organic compounds from a matrix directly into a solid phase. SPME integrates sampling, extraction, concentration and sample introduction in a simple process, and most importantly, it uses no solvent during extraction. The extensive applications of SPME were almost based exclusively on separation and analysis by gas chromatography (Sung et al., 2005). The compound should have some properties for the successive extraction through SPME. First the compound should be sufficiently volatile and we know that Geosmin and MIB are volatile organic compounds. Moreover the compound should possess dissolve phase and thermally stable. This SPME method has many advantages compare to conventional method. The conventional method like liquid-liquid extraction require large sample volumes (100-1000ml) and intensive sample concentration procedures for the detection and quantification of this compounds at nanogram level, but SPME method require smaller volume of samples (Rashash et al., 1996). Moreover SPME uses no solvent in the extraction process. The SPME method is solvent less and uses smaller volume of samples which makes the extraction process extremely faster and time saving. Conventional analytic method like closed loop stripping and purge & trap has relatively complex equipment when compare to SPME which is really small in size and portable.

2.12 Algaecides

Algaecide is a substance that used to kills or inhibits the growth of algae. Algaecides are used in reservoirs to control algal or cyanobacterial growth and to prevent the associated water quality problems. There are different types of algaecides are available in the market. Copper sulphate has been used widely as an algaecide to control algal blooms in water supply storages and lakes for nearly 100 years (McKnight et al., 1983). It is generally regarded as effective, economical and safe to use for operators, although copper can have adverse environmental impacts on the aquatic ecosystem. The effectiveness of copper algaecide treatment is determined by three major factors

- Chemical factors - the chemistry receiving water determines the speciation and thereby the toxicity of copper
- Biological factors - the sensitivity of the target organism to copper
- Physical factors - the distribution of copper in the reservoir after application may affect contact with the target organism (Burch, 1990).

An extensive survey of water utilities in the U.S. and Canada in the 1980's indicated that copper sulphate is by far the most widely used algaecide, although other alternatives are used under some circumstances (AWWA, 1987). Table 4 shows the common algaecides and their chemical formulation.

Table: 4 Common algaecides, their formulations and key references (Burch et al., 91).

Compounds	Formulations
Copper sulfate	$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
Copper II alkanolamine complex	$\text{Cu Alkanolamine} \cdot 3\text{H}_2\text{O}^{++}$
Copper - ethylenediamine complex	$[\text{Cu}(\text{H}_2\text{NCH}_2\text{CH}_2\text{NH}_2)_2(\text{H}_2\text{O})_2]^{++}$ SO_4
Copper - triethanolamine complex	$\text{Cu N}(\text{CH}_2\text{CH}_2\text{OH})_3 \cdot \text{H}_2\text{O}$
Copper citrate	$\text{Cu}_3[(\text{COOCH}_2)_2\text{C}(\text{OH})\text{COO}]_2$
Potassium permanganate	KMnO_4
Chlorine	Cl_2
Lime	$\text{Ca}(\text{OH})_2$
Barley straw	

2.13 Copper sulfate

Copper sulfate has been regarded as the algaecide of choice because it is economical, effective, relatively safe and easy to apply, has no significant human health implications, and has been considered not to cause extensive environmental damage (McKnight, 1983). copper and other heavy metals differ from some other toxic contaminants in that they are not biodegradable, and once they have entered the environment their potential toxicity is controlled largely by their speciation or physiochemical form (Florence, 1982). Toxicity of copper is determined by cupric ion (Cu^{2+}) activity and not by the total copper

concentration. So the physiochemical form of copper in water determines the toxicity of copper. The four important processes which controls the physiochemical forms are

- Precipitation (tenorite, malachite and azurite)
- Adsorption (with suspended particles)
- Formation of complex with organic or inorganic ligands. (copper hydroxide, copper carbonate)
- Biological concentration

The effective dosage rate to kills the *Cyanobacteria* is in the range of 0.125 - 0.5 mg Cu L-1. The effective dose for a particular species in particular water was affected by factors such as the abundance and physiological state of the algae, pH, temperature, alkalinity, and dissolved organic matter concentration of the water (Holden, 1970).

2.14 Chelated copper

The performance of copper sulfate was reduced in hard alkaline water (Palmer, 1962). The loss of cupric ions in the form of precipitations like tenorite, malachite and azurite may serve as a reason for poor performance. In order to overcome this issue chelated copper was introduced instead of copper sulfate. Examples of copper chelated algaecides include copper ethanolamine, copper ethylene-diamine and copper citrate. Copper citrate has been used as an algaecide in the U.S. It is claimed that the use of citric acid as a chelating agent enhances the solubility of copper allowing it to remain in solution longer under alkaline conditions (Raman, 1988), Which result in the maintenance of toxic cupric ionic activities and the inhibition of algal growth for longer periods after dosing (McKnight et al., 1983). It is acknowledged that, despite their relatively widespread use

in the U.S., the efficacy of chelated copper algaecide in relation to water chemistry is poorly understood (AWWA, 1987).

2.15 pH and alkalinity

The most rapid changes in copper chemistry occur in the pH range 6.5 - 8.0. The presence of cupric ion is high as pH decrease. In alkaline water, where the pH greater than seven favors the precipitation of copper, whereas acidic water favors copper solubility. So the copper dose needed to treat water varies based on alkalinity. Even though the production of ionic copper is high as pH decreases, the level of toxicity is significantly high as pH increases for the same given amount of ionic copper. The efficacy of copper sulphate treatment is largely dependent on water chemistry like alkalinity, pH, hardness and dissolved organic content.

High pH - high dosage of algaecide concentration is needed.

Low pH - Low dosage of algaecide concentration is needed (Andrew et al., 1977).

2.16 Mechanism of copper algaecides

Copper is an essential micronutrient for growth of algae and *Cyanobacteria*, and is required for various metabolic and enzyme processes (Cid, 1995). However the higher concentration of copper may serve as toxic to cells (Florence, 1982). The mechanism of copper toxicity is likely to be concentration dependent. Evidence of cell lysis was also found in one study where membrane damage was seen within 24 hours in cultured cells of the cyanobacterium *Microcystis aeruginosa* following treatment with copper (0.64 mg Cu L⁻¹ as CuSO₄) (Kenefick, et al., 1993). At lower concentrations metals need to be transported into the cell to exert physiological and toxic effects. Copper ions are believed to be transported into cells by a process of facilitated diffusion across the membrane

(Florence, 1986). Figure 2 explains the transport of copper complexes into the cell membrane by diffusion.

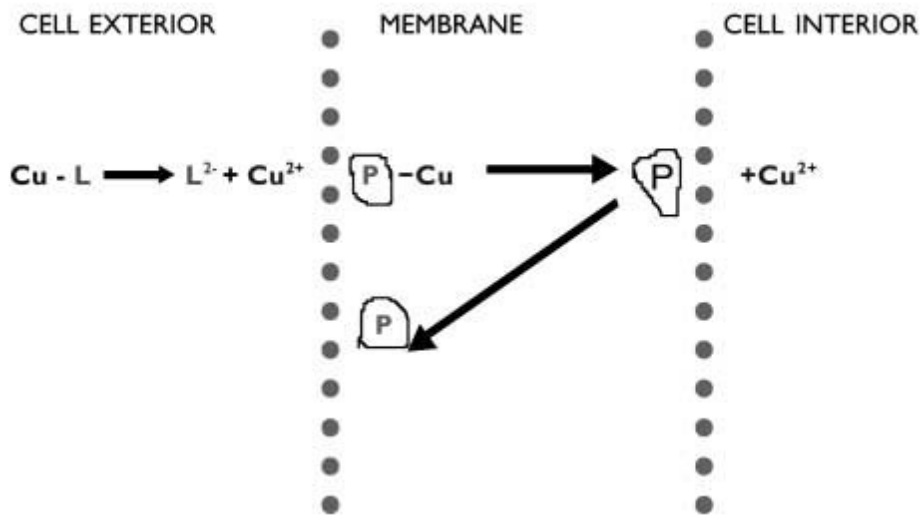


Figure: 2 Diagrammatic representation of the transport of copper complexes through a membrane and into the cell by facilitated diffusion. Diagram after Florence (Florence, 1986).

Copper availability for transport is therefore dependent upon strength of binding and rates of dissociation from the solution ligands at the membrane surface. This has implications for the use and toxicity of copper chelates as algacides.

CHAPTER III

METHODOLOGY

3.1 Overview

It is essential to understand the fate and transport of any chemical in environmental pathways like air, water, soil and sediment. This will give an overall idea where the chemical is finally deposited and in which way it can be controlled, preventing possible concerns for human and animal health issues. This study is concerned with the taste and odor problems in drinking water. The major chemical responsible for the taste and odor problem reported in most of the literature is geosmin, so it is the primary focus here.

3.2 Descriptions of Level III model

The software model developed by Canadian Environmental Modeling Network (CEMN) is used to analyze the fate and transport of this chemical. A key contribution of models is their ability to bring together knowledge about chemical properties, environmental properties, and processes. The software model used in this paper is CEMN's Level III model (version 2.80). These models are most useful for chemicals that are multimedia in nature, i.e., realistically present in all environmental media.

A Level III simulation describes a situation which is one step more complex and realistic than previous version. In this model, a chemical is assumed to be continuously discharged at a constant rate and achieves a steady state condition in which input and output rates are equal. The loss processes are degrading reactions and advection. In the Level III model, equilibrium between media is not assumed and, in general, each medium is at a different fugacity. A mass balance applies not only to the system as a whole, but to each compartment. Rates of intermedia transport are calculated using D values (fugacity rate constants) which are transport parameters contain information on mass transfer coefficients, areas, deposition and resuspension rates, diffusion rates, and soil runoff rates. It is also necessary to define the inputs to each medium separately. The distribution of the chemical between media depends on how the chemical enters the system, e.g. to air, to water, or to both. This mode of entry also affects persistence or residence time.

Mass balances are calculated for the four bulk media of air (gas + aerosol), water (solution + suspended particles + biota), soil (solids + pore air + pore water), and sediment (solids + pore water). Equilibrium exists within, but not between media. For example, sediment solids and pore water are at equilibrium, but sediment is not necessarily at equilibrium with the overlying water.

Physical-chemical properties are used to quantify a chemical's behaviour in an evaluative environment. Three types of chemicals are treated in this model: chemicals that partition into all media (Type 1- excluding ionizing chemicals), non-volatile chemicals (Type 2), and chemicals with zero, or near-zero, solubility (Type 3). The chemical geosmin and MIB are analyzed in this study and they come under Type 1.

3.3 Screenshots of Level III model

The Level III simulation model contains of two major parts called model input tab and model output tab. The model input parameter consists of four divisions, namely simulation ID, chemical properties, environmental properties and emissions and inflows.

Figure 3, 4 and 5 shows the screenshots of the input parameters of the model.

Chemical Properties

Chemical Name: geosmin [New Chemical]

Chemical Type: 1

Molar Mass (g/mol): 182

Data Temperature (°C): 20

Partitioning Data for Type 1

Water Solubility (g/m³): 150.2

Vapour Pressure (Pa): 0.076

Log Kow: 3.7

Melting Point (°C): 47.08

Reaction Half-lives (h)

Air (gaseous)	17	<input type="checkbox"/> Negligible
Water (no sus. part.)	55	<input type="checkbox"/> Negligible
Soil	170	<input type="checkbox"/> Negligible
Sediment	170	<input type="checkbox"/> Negligible
Suspended Particles	1.00E+11	<input checked="" type="checkbox"/> Negligible
Fish	1.00E+11	<input checked="" type="checkbox"/> Negligible
Aerosol	1.00E+11	<input checked="" type="checkbox"/> Negligible

Database Operations

[Save] [Delete]

[OK] [Cancel] [Help]

Figure: 3 Chemical properties of geosmin for Level III model

Environmental Properties

Environment Name:

Dimensions	Densities	Org. Carb. & Advection	Transport Velocities
Volume Fractions			
Air: Aerosol <input type="text" value="2E-11"/>			
Water: Susp. Particles <input type="text" value="0.000005"/> Fish <input type="text" value="0.000001"/>			
Soil: Air <input type="text" value="0.2"/> Water <input type="text" value="0.3"/> Solids <input type="text" value="0.5"/>			
Sediment: Water <input type="text" value="0.8"/> Solids <input type="text" value="0.2"/>			

Dimensions	Densities	Org. Carb. & Advection	Transport Velocities
Air	Area (m ²) <input type="text" value="2.98E+11"/>	Depth (m) <input type="text" value="2000"/>	
Water	<input type="text" value="11574009"/>	<input type="text" value="8.47"/>	
Soil	= Air - Water	<input type="text" value="0.1"/>	
Sediment	= Water	<input type="text" value="0.01"/>	

Database Operations

Figure: 4 Environmental properties of geosmin in Lake Eucha for Level III model

Emissions and Inflows

Emission Rate (kg/h)

Into Air

Into Water

Into Soil

Into Sediment

Advective Inflow Concentrations

Concentration in Air (ng/m³)

Concentration in Water (ng/L)

Figure: 5 Selected emissions of geosmin for Level III model

3.4 Input parameters of the Level III model

The simulation ID is a unique name or number of the specific simulation given by the user, mostly the name of the chemical in this case, geosmin. The next input division is chemical properties, where it is subdivided into three categories namely basic properties, partitioning data for type and reaction half-lives. The final input parameters in the Level III model are emissions and inflows. Here the mode of entry of the chemical should be specified for each medium. The mode of entry can be air, water, soil and sediments. Geosmin is a naturally occurring component, released through metabolism and degradation of algae blooms. So here, the major input is through the water environmental pathways.

The other major input properties in the Level III simulation are environmental properties, which require various input parameters to create a realistic simulated environment. The data required for environmental properties are structured into four categories, including dimension, density, organic carbon mass, and advection and transport velocity. Some of the data required for the environmental properties are extracted from the literature and other published sources. But many data are not available readily in any literature paper or other sources. In such cases default values suggested by the model are adopted. Tables 5, 6, 7, 8, 9 and 10 shows the input parameters of geosmin for the simulation.

In the Table 5, the chemical properties of geosmin are shown. The few data are extracted from the literature, Pirbazari, 1992. Then some data are taken from the EPIWEB 4.1. Estimation Program Interface Suite (EPI) was available from the EPA website. The software was run on computer with Windows operating system. The chemical name should be selected from the database provided in the EPI Suite 4.1. Then the physical-

chemical property are simulated for the given input, here is geosmin/MIB. The simulation results of geosmin/MIB are given in the appendices. The values for reaction half-lives of geosmin in the four compartments are extracted from the EPI Suite 4.1. These reaction half-lives are default values of EPI Suite not for geosmin or MIB.

Table: 5 Chemical properties of geosmin used for model input

Parameters	Chemical properties	Geosmin	Reference
Chemical type	Type	1	-
	Molar mass (g/mol)	182	Pirbazari et al., 1992
	Data temperature (°C)	20	-
Partitioning data for type	Water solubility (g/m ³)	150.2	Pirbazari et al., 1992
	Vapor Pressure (Pa)	0.076	EPIWEB 4.1
	Log kow	3.7	Pirbazari et al., 1992
	Melting point (°C)	47.08	EPIWEB 4.1
Reaction half-lives	Air (h)	17	EPIWEB 4.1
	Water (h)	55	EPIWEB 4.1
	Soil (h)	170	EPIWEB 4.1
	Sediment (h)	170	EPIWEB 4.1
	Suspended particles (h)	1×10 ¹¹	Level III
	Fish (h)	1×10 ¹¹	Level III
	Aerosol (h)	1×10 ¹¹	Level III

Table 6 shows the dimension of the Lake Eucha. The area and depth of water compartment are extracted from the report, prepared by the Water Quality Division of the

Oklahoma Conservation Commission (OCC) for the Lake Eucha, 1997. The default values are used for the other three compartments.

Table: 6 Dimensional environmental properties for model input

Compartment	Area (m ²)	Depth (m)	Reference
Air	2.98E+11	2000	Level III
Water	1.15E+07	8.47	Wagner, 1997.
Soil	2.97E+11	0.1	Level III
Sediment	1.15E+07	0.01	Level III

The Table 7 shows the values of volume fraction in the subcompartment. The most of the air compartment is aerosol. Then the water compartment is divided into two including, suspended particles and fish. The volume fraction of suspended particles is higher compare to fish volume. The soil compartment is classified into three sub compartment, which includes air, water and soil. Finally the sediment compartment is divided into two, which includes water and solids.

Table: 7 Volume fractional environmental properties for model input

Subcompartment		Volume fraction (Default)
Air	Aerosol	2.00E-11
Water	Susp. particles	5.00E-06
	Fish	1.00E-06
Soil	Air	0.200
	Water	0.300
	Soil	0.500
Sediment	Water	0.800
	Solids	0.200

Table: 8 Organic carbon mass environmental properties for model input

Sub compartment	Mass Fraction (g/g) (Default)
Soil	0.0200
Sediment	0.0400
Susp.Particles	0.200
Fish Lipid	0.0480

Table: 9 Advection residence times environmental properties for model input

Compartment	Residence times (h)	Reference
Air	40	Level III
Water	3317	Wagner, 1997
Sediment	50000	Level III

Table 8 and 9 shows the values of organic carbon mass and advection times. The most of the data used in these two columns are default values provided in the Level III model. But the advection residence times of water is calculated for Lake Eucha. The value of advection residence times of water is the volume of water divided by the flow of water. The default transport velocity values are used in the simulation and it is shown in the Table 10.

Table: 10 Transport velocities environmental properties for model input

Transport Velocity	m/h (Default)
Soil air boundary layer mass transfer coefficient	5
Sediment-water mass transfer coefficient	0.0001
Sediment deposition velocity	1E-07
Sediment resuspension velocity	2E-07
Soil water runoff rate	5E-05
Soil solids runoff rate	1E-08
Air side air-water mass transfer coefficient	5
Water side air-water mass transfer coefficient	0.05
Rain rate	0.001
Aerosol deposition velocity	10
Soil air phase diffusion mass transfer coefficient	0.02
Soil water phase diffusion mass transfer coefficient	1E-05

Like geosmin, values for MIB were observed in the literature. The fate and transport of MIB can also be simulated using Level III model in Lake Eucha, Oklahoma. The environmental properties were same as geosmin.

In the Table 11, the chemical properties of MIB are shown. The few data are extracted from the literature, Pirbazari, 1992. Then some data are taken from the EPIWEB 4.1. Estimation Program Interface Suite (EPI) was available from the EPA website. The software was run on computer with Windows operating system. The chemical name

should be selected from the database provided in the EPI Suite 4.1. Then the physical-chemical property are simulated for the given input, here is MIB. The values for reaction half-lives of MIB in the four compartments are extracted from the EPI Suite 4.1. These reaction half-lives are default values of EPI Suite not for MIB. The fate of geosmin and MIB are analyzed in the Lake Eucha, Oklahoma. So the environmental properties are same as given in the Tables 6, 7, 8, 9 and 10 for the MIB Level III simulation.

Table: 11 Chemical properties of MIB used for model input

Parameters	Chemical properties	MIB	Reference
Chemical type	Type	1	-
	Molar mass (g/mol)	168	Pirbazari et al., 1992
	Data temperature (°C)	20	-
Partitioning data for type	Water solubility (g/m ³)	194.5	Pirbazari et al., 1992
	Vapor Pressure (Pa)	4.27	EPIWEB 4.1
	Log kow	3.13	Pirbazari et al., 1992
	Melting point (°C)	31	EPIWEB 4.1
Reaction half-lives	Air (h)	17	EPIWEB 4.1
	Water (h)	55	EPIWEB 4.1
	Soil (h)	170	EPIWEB 4.1
	Sediment (h)	170	EPIWEB 4.1
	Suspended particles (h)	1×10 ¹¹	Level III
	Fish (h)	1×10 ¹¹	Level III
	Aerosol (h)	1×10 ¹¹	Level III

3.5 Determination of input rate of geosmin and MIB

Algal cells can produce geosmin and MIB at concentration of 10^{-5} ng/cell, so a relatively small algal bloom of 5000-10,000 cells/ml would produce levels of 100 ng/l (Hall, 2006). Based on the report given above the geosmin and MIB are calculated for the Lake Eucha, Oklahoma. The volume of water observed in the Lake Eucha is 98×10^6 cubic meter (Wagner, 1997). The production of geosmin and MIB can be calculated by multiplying the mass of geosmin/MIB produced per cell of algae by number of algae cells per volume of water with volume of water. The mathematical expression is represented as follows:

Geosmin production calculation

Mass of geosmin produced per cell of algae	=	10^{-5} _____
Number of algae cells per volume of water	=	$5000 - 10000$ _____
Volume of water	=	$98 * 10^6$ m ³

$$\frac{\text{_____}}{\text{_____}} \times \frac{\text{_____}}{\text{_____}} \times \frac{\text{_____}}{\text{_____}}$$

It should be noted that this represents a maximum emission rate, and this will yield maximum aqueous concentrations. Here we assumed the geosmin input is continuously discharged, which is not realistic in a real setting. The release of geosmin from algae is not continuous but that is a necessary assumption for the Level III model. In addition, in our calculation for geosmin production, the release of geosmin per cell is an approximate value not a specific value for Lake Eucha.

CHAPTER IV

RESULTS AND DISCUSSIONS

4.1 Overview

The Level III model was simulated with the data provided in the chapter III which included chemical properties, environmental properties and emissions. The model was simulated for both the chemical geosmin and MIB. The results were presented in overall output diagram and charts. The overall output diagram shows the chemical input and output, chemical concentration in multimedia compartments, and chemical loss through degradation, advection and intermedia exchange. The charts show the amount of geosmin presented in each compartment in kilograms and relative amount percentage in pie chart. Before running the simulation it is very important to determine the critical input parameters which decide the concentration of geosmin and MIB in the water compartment. To determine the most critical input parameters, sensitivity analyses were performed for both the chemical geosmin and MIB.

4.2 Sensitivity analyses for geosmin

The model lends itself to an efficient sensitivity analysis of the input parameters. These parameters, which include chemical and environmental properties, can be tested individually. This sensitivity analysis helps to determine the sensitive parameters which

decide the fate and transport of the chemical. The sensitivity analysis is done to identify the change in geosmin concentration in water compartment, where the highest geosmin concentration is observed. Table 12 shows the results of sensitivity analysis of the chemical properties of geosmin. The property with uncertainty and default values are taken for sensitivity analyses. The sensitivity analyses for chemical properties are performed by doubling the values of each property individually. Then the output geosmin concentration in water compartment is observed for any variation and the percentage differences are recorded.

Table: 12 Sensitivity analyses of chemical properties (geosmin)

Parameters	Chemical properties	Geosmin value	Geosmin value $\times 2$	Change in Geosmin Water conc?	Percentage diff in water conc
Partitioning data for type	Log Kow	3.7	7.4	Yes	+ 13.77
Reaction half-lives	Air (h)	17	34	No	-
	Water (h)	55	110	Yes	+ 93.54
	Soil (h)	170	340	No	-
	Sediment (h)	170	340	No	-

The sensitivity analysis in the Table 12 shows that two parameters make the change in geosmin concentration in water, when it is doubled. As expected the half life of geosmin in water makes a large percentage difference in the geosmin concentration in water when it is doubled. The half life of geosmin in water shows a linear relationship with the geosmin concentration in water. Further research is needed to identify the half life of

geosmin in water to obtain better results with the Level III model. Table 13 shows the sensitivity analysis of environmental properties of Lake Eucha.

Table: 13 Sensitivity analyses of environmental properties (geosmin)

Environmental Properties	Parameters	Geosmin value (default)	Geosmin value ($\times 1000$)	Change in Geosmin water conc?	Percentage Difference
Dimension	Area(m ²) (Air: Bulk)	2.98E+11	2.98E+14	No	Nil
	Depth(m) (Air: Bulk)	2000	2000000	No	Nil
	Vol fraction (Water: Sus particles)	5E-06	5E-03	Yes	+ 431
	Vol fraction (Water:Fish)	1E-06	1E-06	Yes	+22
	Vol fraction (Air:aerosol)	2E-11	2E-08	No	Nil
Advection flow	Residence time(h): Air	40	40000	No	Nil
	Residence time(h): sediment	50000	5E+7	No	Nil

Table: 13, continued					
Transport velocity	soil air boundary layer MTC	5	5000	No	Nil
	sediment-water MTC	0.0001	0.1	No	Nil
	sediment deposition velocity	1E-07	1E-04	Yes	-80
	sediment resuspension velocity	2E-07	2E-04	No	Nil
	soil water runoff rate	5E-05	5E-02	No	Nil
	soil solids runoff rate	1E-08	1E-05	No	Nil
	air side air-water MTC	5	5000	No	Nil
	water side air-water MTC	0.05	50	No	Nil
	rain rate	0.001	1	No	Nil
	aerosol deposition velocity	10	10000	No	Nil
	soil air phase diffusion MTC	0.02	20	No	Nil
	soil water phase diffusion MTC	1E-05	1E-02	No	Nil

The sensitivity analysis is done for the environmental properties of Lake Eucha. The input parameters of the environmental properties are increased by one thousand fold. The change in predicted geosmin concentration in water compartment is observed. Only three

parameters were identified as sensitive parameters for determining the geosmin concentration in water. They are volume fraction (water: suspended particles), volume fraction (water: fish) and sediment deposition velocity. The geosmin concentration increased by 431% when the volume of suspended particles in water is increased by one thousand fold. But the geosmin concentration decreased by 80% when sediment deposition velocity is increased by one thousand fold. When both these input parameters were increased by one thousand fold simultaneously, the net output geosmin concentration increased by 11%. When both input parameters are increased simultaneously the input suspended particles move from the water compartment to the sediment compartment and ultimately the geosmin concentration in the sediment increased significantly compared to the water compartment. These three parameters play a critical role in determining the concentration of geosmin in water compartment. As such, greater care is needed in ensuring that their input values are as accurate as possible.

4.3 Sensitivity analyses for MIB

The sensitivity analyses were also performed for chemical and environmental properties by following the same procedure for the geosmin and results were recorded in the Table 14 and 15.

Table: 14 Sensitivity analyses of chemical properties (MIB)

Parameters	Chemical properties	MIB value	MIB value $\times 2$	Change in MIB water conc?	Percentage diff in water conc
Partitioning data for type	Log Kow	3.13	6.26	Yes	+ 13
Reaction half-lives	Air (h)	17	34	No	-
	Water (h)	55	110	Yes	+ 85
	Soil (h)	170	340	No	-
	Sediment (h)	170	340	No	-

The sensitivity analysis in the Table 14 shows that the same two parameters show significant change in MIB concentration in water when doubled. The half life of MIB in water and the Kow make large percentage difference in MIB concentration in water when doubled. The half life of MIB in water also shows a linear relationship with geosmin concentration in water. Table 15 shows the sensitivity analysis of environmental properties of Lake Eucha. Again, the same critical parameters are identified.

Table: 15 Sensitive Analysis of Environmental properties (MIB)

Environmental Properties	Parameters	MIB Value (default)	MIB value ($\times 1000$)	Change in MIB water conc?	Percentage Difference
Dimension	Area(m ²) (Air: Bulk)	2.98E+11	2.98E+14	No	Nil
	Depth(m) (Air: Bulk)	2000	2000000	No	Nil
	Vol fraction (Water: Sus particles)	5E-06	5E-03	Yes	+ 126
	Vol fraction (Water:Fish)	1E-06	1E-06	Yes	+6.35
	Vol fraction (Air:aerosol)	2E-11	2E-08	No	Nil
Advection flow	Residence time(h): Air	40	40000	No	Nil
	Residence time(h): sediment	50000	5E+7	No	Nil

Transport velocity	soil air boundary layer MTC	5	5000	No	Nil
	sediment-water MTC	0.0001	0.1	No	Nil
	sediment deposition velocity	1E-07	1E-04	Yes	-48
	sediment resuspension velocity	2E-07	2E-04	No	Nil
	soil water runoff rate	5E-05	5E-02	No	Nil
	soil solids runoff rate	1E-08	1E-05	No	Nil
	air side air-water MTC	5	5000	No	Nil
	water side air-water MTC	0.05	50	No	Nil
	rain rate	0.001	1	No	Nil
	aerosol deposition velocity	10	10000	No	Nil
	soil air phase diffusion MTC	0.02	20	No	Nil
	soil water phase diffusion MTC	1E-05	1E-02	No	Nil

The sensitivity analysis is done for the environmental properties of Lake Eucha. The input parameters of the environmental properties are increased by one thousand fold. The change in predicted MIB concentration in water compartment is observed. Only three parameters were identified as sensitive parameters for determining the MIB concentration

in water. They are volume fraction (water: suspended particles, water: fish) and sediment deposition velocity. The MIB concentration increased by 126% when the volume of suspended particles in water is increased by one thousand fold. But the MIB concentration decreased by 48% when sediment deposition velocity is increased by one thousand fold. When both these input parameters were increased by one thousand fold simultaneously, the net output geosmin concentration increased by 18%. When both input parameters are increased simultaneously the input suspended particles move from the water compartment to the sediment compartment and ultimately the geosmin concentration in the sediment increased significantly compared to the water compartment. These three parameters play a critical role in determining the concentration of MIB in water compartment. As such, greater care is needed in ensuring that their input values are as accurate as possible.

4.4 Simulation output for geosmin

In order to run the simulation some of the unknown values need to be assumed or default values are used. The following paragraphs give the results of fate of geosmin and MIB with the input data provided in the Chapter III.

Figure 6, shown below, is the overall output diagram from the Level III version 2.80.1 for the geosmin in Lake Eucha. The data for chemical and environmental properties are collected from the various literature papers and default data are used for those not available in the literature papers. The diagram shows the mode of emission is through the water. The highest amount of geosmin is found in water, which contains almost 98.3 % of the remaining chemical. Moreover, the concentration of geosmin is highest in the water compartment, about 1610 ng/l, which is on the same order of magnitude as that observed

in Lake Eucha during periods of high geosmin concentration. The maximum geosmin concentration in water may create taste and odor problem in drinking water, as it is well above the odor threshold.

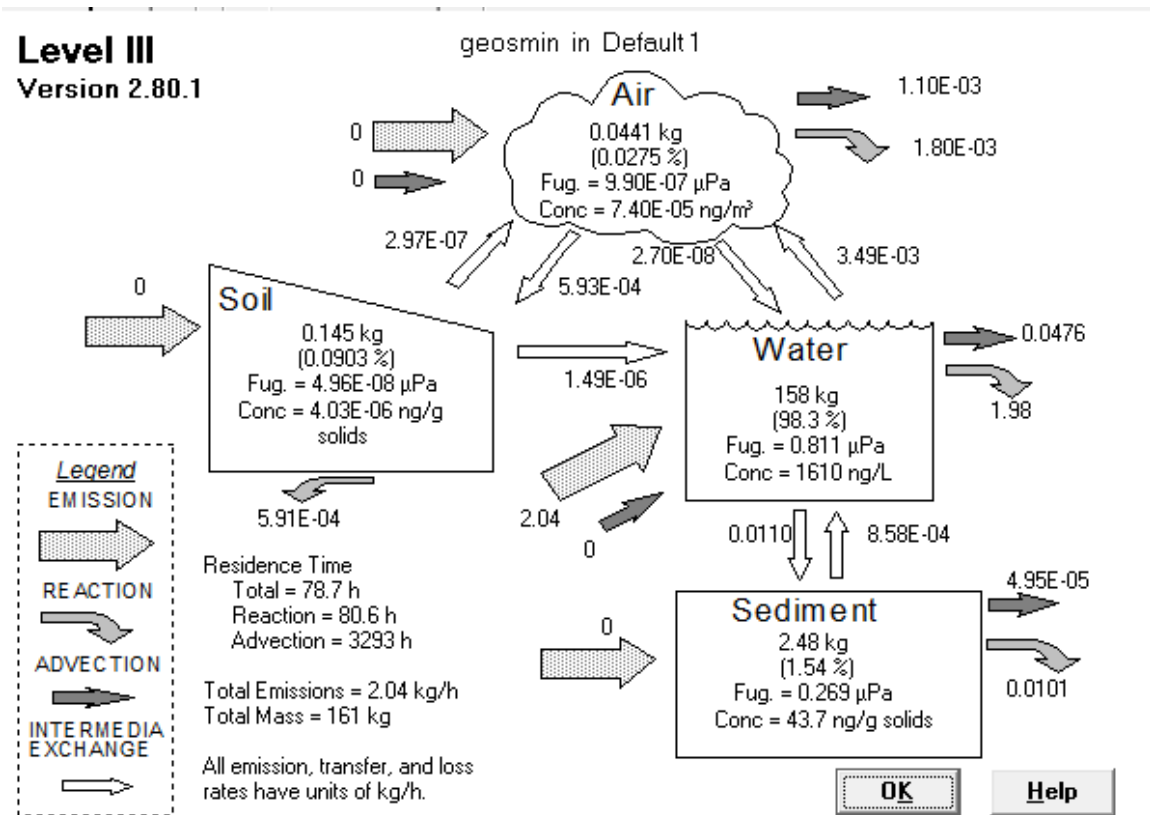


Figure: 6 Output diagram (Geosmin in Lake Eucha)

The loss of chemical from any compartment can happen in three ways, including chemical reaction (degradation), chemical transport (water and air current) and intermedia exchange. Almost 97 % of the geosmin input is chemically transformed (reacted) in the water compartment. The reaction time is 80.6 hrs, which is the time that would be taken to remove the chemical by degradation alone.

Then 2.33 % of the geosmin input is carried out of the system by advection. The advection time is 3293 hrs, which is the time that would be taken to remove the chemical by transporting to neighboring region (assuming no degradation).

Figure 7 below shows the bar graph that clearly indicates the maximum amount of geosmin is found in water compartment when compare to the other three compartments.

Figure 8 shows the relative amount of geosmin in each of the four compartments. The majority portion of geosmin is occupied in the water compartment.

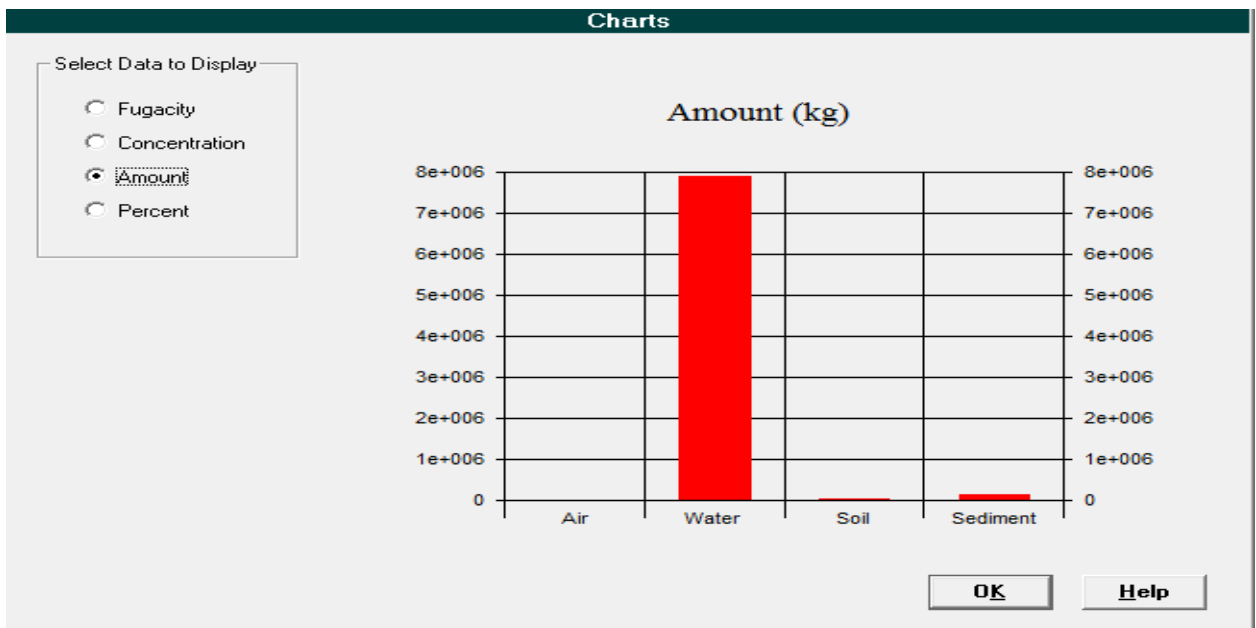


Figure: 7 Amount of geosmin in each compartment

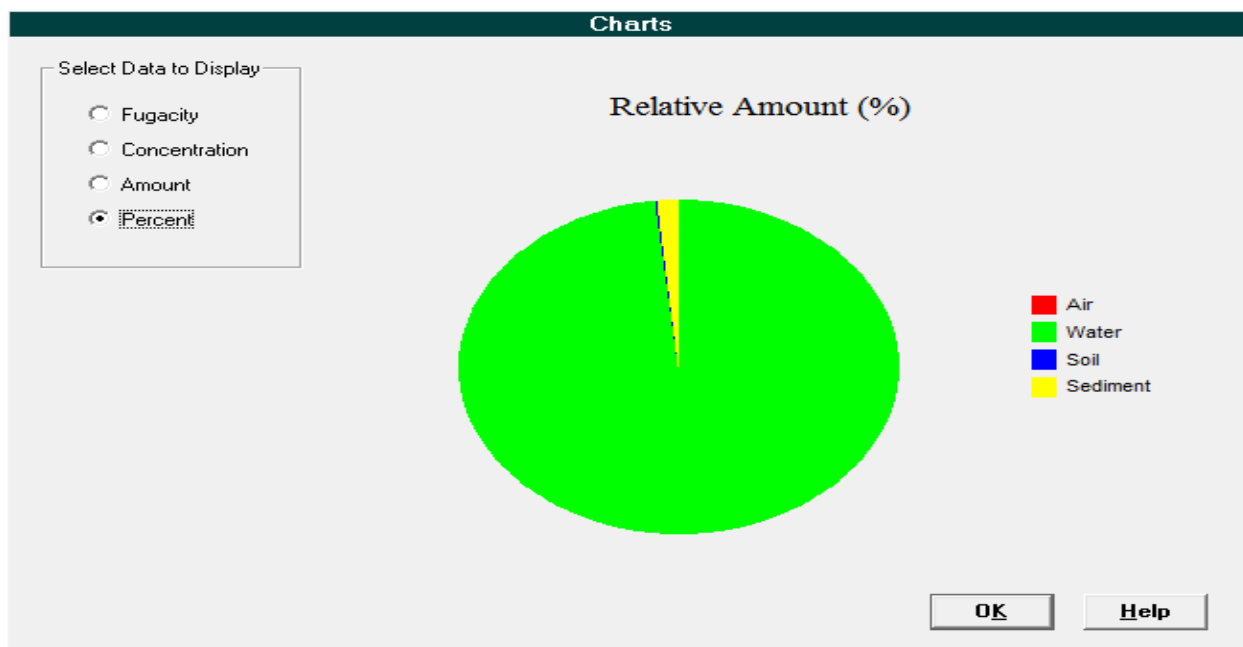


Figure: 8 Relative amounts (%) of geosmin in pie chart

4.5 Simulation output for MIB

Figure 9 shown below is the overall output diagram from the Level III version 2.80.1 for the MIB in Lake Eucha. The data for chemical and environmental properties are collected from the various literature papers and default data are used for those not available in the literature papers. The diagram shows the mode of emission is through the water. The highest amount of MIB is found in water, which contains almost 98.2% of the residual. Moreover, the concentration of MIB is highest in the water compartment, about 1521 ng/l. The maximum MIB concentration in water may create taste and odor problem in drinking water, as it is well above the odor threshold.

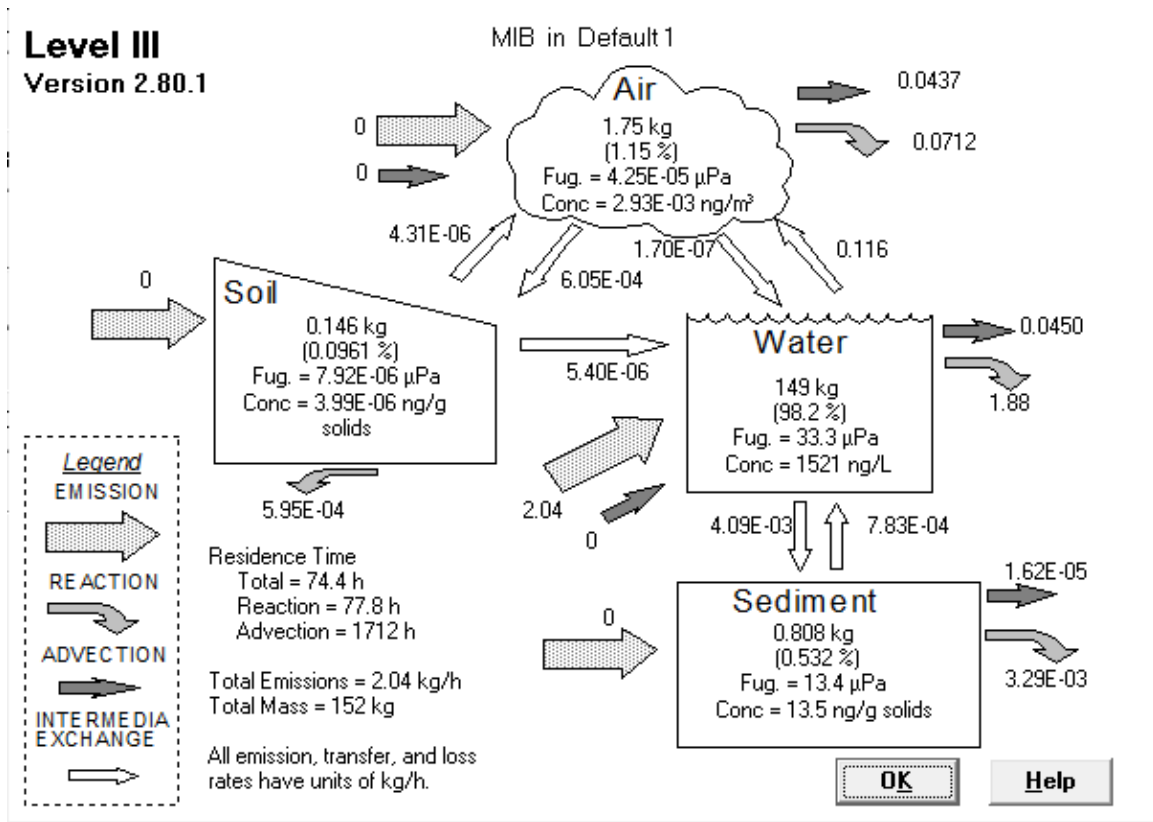


Figure: 9 Output diagram (MIB in Lake Eucha)

The loss of chemical from any compartment can happen in three ways, including chemical reaction (degradation), chemical transport (water and air current) and intermedia exchange. Almost 92% of the MIB input is chemically transformed (reacted) in the water compartment. The reaction time is 77.8 hrs, which is the time that would be taken to remove the chemical by degradation alone. Then 2.2% of the MIB input is carried out of the system by advection. The advection time is 1712 hrs, which is the time that would be taken to remove the chemical by transporting to neighboring region.

Figure 10 below shows the bar graph that clearly indicates the maximum amount of MIB is found in water compartment when compare to the other three compartments. Figure 11 shows the relative amount of MIB in each of the four compartments. The majority portion of MIB is occupied in the water compartment.

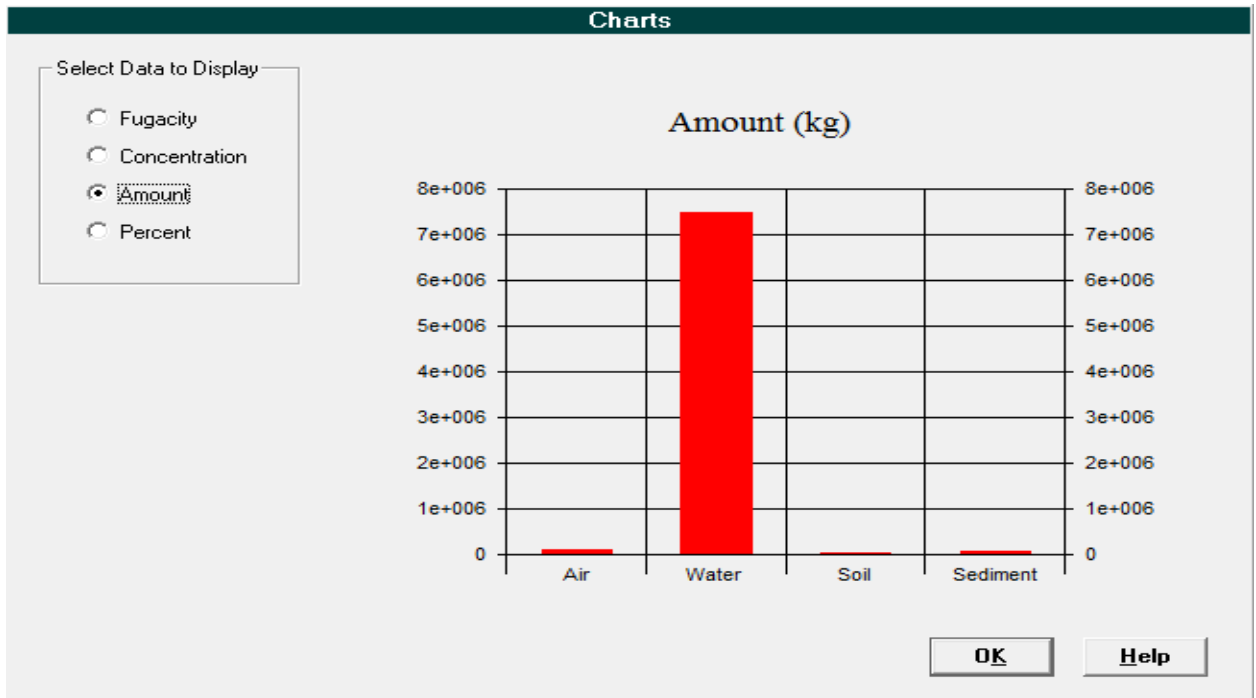


Figure: 10 Amount of MIB in each compartment

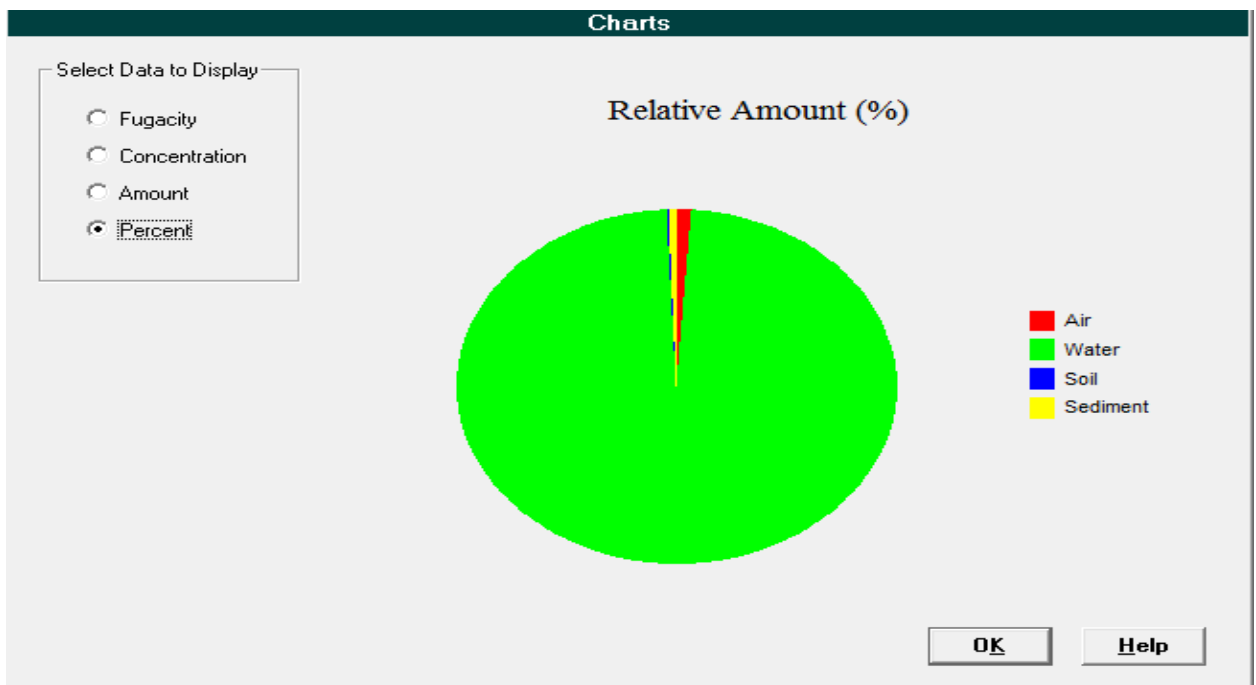


Figure: 11 Relative amounts (%) of MIB in pie chart

CHAPTER V

CONCLUSIONS

The Level III model was used to predict the fate and transport of the chemicals geosmin and MIB in Lake Eucha, Oklahoma. The input parameters were taken from relevant literature for the chemical and environmental properties where available. The mode of entry of geosmin was assumed to be only in the water. The Level III software produced simulations with the given input parameters for the geosmin and MIB and the results were generated in the form of diagram, charts and tables. A sensitivity analyses for the model was also performed. The research yielded the following conclusions.

Sensitivity analyses: The sensitivity analysis was performed to determine the key parameters that decide the fate and transport of geosmin and MIB in this simulated environment. From the results, the critical parameters were identified to be log K_{ow} , the half life in water, the volume fraction (suspended particles: water), volume fraction (fish: water) and sediment deposition velocity. The remaining input parameters were found to have relatively little or no impact for the chemicals and scenario tested here. It is very important to fix these parameters in future research, which could help the model to predict the fate and transport of chemical with more accuracy.

Fate of geosmin: From the given input emission, 98% of the residual geosmin was predicted to remain in the water compartment. Hence the maximum geosmin concentration was observed in the water compartment and it was 1610 ng/l. Almost 97 % of the geosmin input is chemically transformed (reacted) in the water compartment. The reaction time is 80.6 hrs, which is the time taken to remove the chemical by degradation alone. Then approximately 2% of the geosmin input is carried out of the system by advection. The advection time is 3293 hrs, which is the time taken to remove the chemical by transporting to neighboring regions.

Fate of MIB: From the given input emission, 98.3% of the residual MIB was predicted to remain in the water compartment. Hence the maximum MIB concentration was observed in the water compartment and it was 1521 ng/l. Almost 92% of the MIB input is chemically transformed (reacted) in the water compartment. The reaction time is 77.8 hrs, which is the time taken to remove the chemical by degradation alone. Then approximately 2% of the MIB input is carried out of the system by advection. The advection time is 1712 hrs, which is the time taken to remove the chemical by transporting to neighboring regions.

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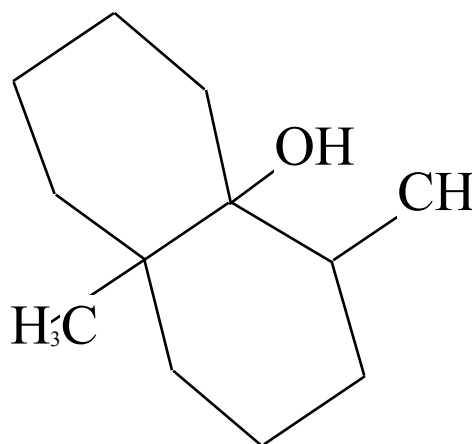
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APPENDIX

Lake Eucha Morphological characteristics

Parameters	Values	Reference
Surface area	2860 Acres	Wagner, 1997.
Mean depth	27.8 Feet	Wagner, 1997.
Volume	79600 Acre / feet	Wagner, 1997.
Flow	8.221 Cubic meter / sec	OWRB, 2002.

EPI Suite Results For CAS 019700-21-1



SMILES : CC1CCCC2(C)CCCCC12O

CHEM : Geosmin

MOL FOR: C12 H22 O1

MOL WT : 182.31

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.68 estimate) = 3.57

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

Boiling Pt (deg C): 248.80 (Adapted Stein & Brown method)

Melting Pt (deg C): 47.08 (Mean or Weighted MP)

VP(mm Hg,25 deg C): 0.00057 (Modified Grain method)

VP (Pa, 25 deg C) : 0.076 (Modified Grain method)

BP (exp database): 270 deg C

Subcooled liquid VP: 0.000907 mm Hg (25 deg C, Mod-Grain method)

: 0.121 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):

Water Solubility at 25 deg C (mg/L): 156.7

log Kow used: 3.57 (estimated)

no-melting pt equation used

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 294.88 mg/L

ECOSAR Class Program (ECOSAR v1.00):

Class(es) found:

Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:

Bond Method : 1.18E-005 atm-m³/mole (1.20E+000 Pa-m³/mole)

Group Method: 3.15E-006 atm-m³/mole (3.19E-001 Pa-m³/mole)

For Henry LC Comparison Purposes:

User-Entered Henry LC: not entered

Henry's LC [via VP/WSol estimate using User-Entered or Estimated values]:

HLC: 8.726E-007 atm-m³/mole (8.841E-002 Pa-m³/mole)

VP: 0.00057 mm Hg (source: MPBPVP)

WS: 157 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:

Log Kow used: 3.57 (KowWin est)

Log Kaw used: -3.317 (HenryWin est)

Log Koa (KOAWIN v1.10 estimate): 6.887

Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model) : 0.2929

Biowin2 (Non-Linear Model) : 0.0462

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.3721 (weeks-months)

Biowin4 (Primary Survey Model) : 3.2778 (days-weeks)

MITI Biodegradation Probability:

Biowin5 (MITI Linear Model) : 0.4564

Biowin6 (MITI Non-Linear Model): 0.4075

Anaerobic Biodegradation Probability:

Biowin7 (Anaerobic Linear Model): -0.7922

Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):

Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 0.121 Pa (0.000907 mm Hg)

Log Koa (Koawin est): 6.887

Kp (particle/gas partition coef. (m³/ug)):

Mackay model : 2.48E-005

Octanol/air (Koa) model: 1.89E-006

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model : 0.000895

Mackay model : 0.00198

Octanol/air (Koa) model: 0.000151

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 22.3859 E-12 cm³/molecule-sec

Half-Life = 0.478 Days (12-hr day; 1.5E6 OH/cm³)

Half-Life = 5.734 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):

0.00144 (Junge-Pankow, Mackay avg)

0.000151 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

Koc : 284.4 L/kg (MCI method)

Log Koc: 2.454 (MCI method)

Koc : 307.8 L/kg (Kow method)

Log Koc: 2.488 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:

Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):

Log BCF from regression-based method = 2.019 (BCF = 104.5 L/kg wet-wt)

Log Biotransformation Half-life (HL) = 0.3185 days (HL = 2.082 days)

Log BCF Arnot-Gobas method (upper trophic) = 2.430 (BCF = 268.9)

Log BAF Arnot-Gobas method (upper trophic) = 2.430 (BAF = 269.1)

log Kow used: 3.57 (estimated)

Volatilization from Water:

Henry LC: 3.15E-006 atm-m³/mole (estimated by Group SAR Method)

Half-Life from Model River: 252.3 hours (10.51 days)

Half-Life from Model Lake : 2866 hours (119.4 days)

Removal In Wastewater Treatment:

Total removal: 14.87 percent

Total biodegradation: 0.20 percent

Total sludge adsorption: 14.52 percent

Total to Air: 0.15 percent

(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

Mass Amount Half-Life Emissions

(percent) (hr) (kg/hr)

Air 0.484 11.5 1000

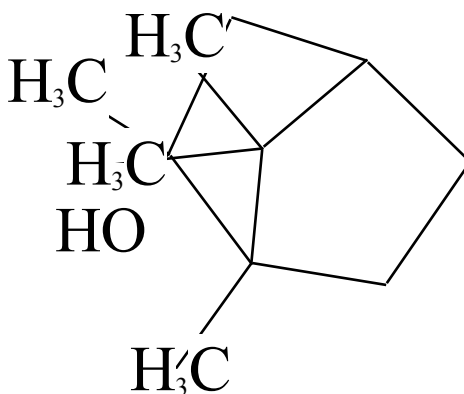
Water 20.2 900 1000

Soil 78.9 1.8e+003 1000

Sediment 0.326 8.1e+003 0

Persistence Time: 996 hr

EPI Suite Results For CAS 002371-42-8



SMILES : C(CC1(C2(O)C)C)C(C2)C1(C)C

CHEM : exo-1,2,7,7-Tetramethylbicyclo[2.2.1]heptan-2-ol

MOL FOR: C11 H20 O1

MOL WT : 168.28

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.68 estimate) = 3.31

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

Boiling Pt (deg C): 210.08 (Adapted Stein & Brown method)

Melting Pt (deg C): 31.00 (Mean or Weighted MP)

VP(mm Hg,25 deg C): 0.032 (Modified Grain method)

VP (Pa, 25 deg C) : 4.27 (Modified Grain method)

Subcooled liquid VP: 0.0362 mm Hg (25 deg C, Mod-Grain method)

: 4.83 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):

Water Solubility at 25 deg C (mg/L): 305.1

log Kow used: 3.31 (estimated)

no-melting pt equation used

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 345.4 mg/L

ECOSAR Class Program (ECOSAR v1.00):

Class(es) found:

Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:

Bond Method : 8.90E-006 atm-m³/mole (9.02E-001 Pa-m³/mole)

Group Method: 2.68E-006 atm-m³/mole (2.72E-001 Pa-m³/mole)

For Henry LC Comparison Purposes:

User-Entered Henry LC: not entered

Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:

HLC: 2.322E-005 atm-m³/mole (2.353E+000 Pa-m³/mole)

VP: 0.032 mm Hg (source: MPBPVP)

WS: 305 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:

Log Kow used: 3.31 (KowWin est)

Log Kaw used: -3.439 (HenryWin est)

Log Koa (KOAWIN v1.10 estimate): 6.749

Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model) : 0.1156

Biowin2 (Non-Linear Model) : 0.0105

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.1909 (months)

Biowin4 (Primary Survey Model) : 3.1446 (weeks)

MITI Biodegradation Probability:

Biowin5 (MITI Linear Model) : 0.4876

Biowin6 (MITI Non-Linear Model): 0.3828

Anaerobic Biodegradation Probability:

Biowin7 (Anaerobic Linear Model): -0.8055

Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):

Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 4.83 Pa (0.0362 mm Hg)

Log Koa (Koawin est): 6.749

Kp (particle/gas partition coef. (m³/ug)):

Mackay model : 6.22E-007

Octanol/air (Koa) model: 1.38E-006

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model : 2.24E-005

Mackay model : 4.97E-005

Octanol/air (Koa) model: 0.00011

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 7.2400 E-12 cm³/molecule-sec

Half-Life = 1.477 Days (12-hr day; 1.5E6 OH/cm³)

Half-Life = 17.728 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):

3.61E-005 (Junge-Pankow, Mackay avg)

0.00011 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

Koc : 112.5 L/kg (MCI method)

Log Koc: 2.051 (MCI method)

Koc : 221.1 L/kg (Kow method)

Log Koc: 2.345 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:

Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):

Log BCF from regression-based method = 1.848 (BCF = 70.41 L/kg wet-wt)

Log Biotransformation Half-life (HL) = 0.0813 days (HL = 1.206 days)

Log BCF Arnot-Gobas method (upper trophic) = 2.177 (BCF = 150.2)

Log BAF Arnot-Gobas method (upper trophic) = 2.177 (BAF = 150.2)

log Kow used: 3.31 (estimated)

Volatilization from Water:

Henry LC: 2.68E-006 atm-m³/mole (estimated by Group SAR Method)

Half-Life from Model River: 284.7 hours (11.86 days)

Half-Life from Model Lake : 3215 hours (134 days)

Removal In Wastewater Treatment:

Total removal: 9.51 percent

Total biodegradation: 0.15 percent

Total sludge adsorption: 9.22 percent

Total to Air: 0.14 percent

(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

Mass Amount Half-Life Emissions

(percent) (hr) (kg/hr)

Air 0.897 35.4 1000

Water 21.7 1.44e+003 1000

Soil 77.3 2.88e+003 1000

Sediment 0.166 1.3e+004 0

Persistence Time: 1.29e+003 hr

VITA

MOHANKUMAR MUTHUSWAMY

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RESERVOIR

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A general fate (Level III) model was used to predict the fate and transport of geosmin and MIB in Lake Eucha, Oklahoma. The Level III model produced simulations with given input parameters for chemical geosmin and MIB. A sensitivity analyses for the model was also performed. The sensitivity analysis was performed to determine the key parameters that control the fate and transport of geosmin and MIB in a multiphase environment. From the results, the critical parameters were identified to be log Kow, the half life in water, the volume fraction (suspended particles: water), volume fraction (fish: water) and sediment deposition velocity. Almost 97 % of the geosmin input was chemically transformed (reacted) in water compartment. From the given input emission, 98 % of the residual geosmin was predicted to remain in the water compartment. Then approximately 2 % of the geosmin input was carried out of the system by advection. In the case of MIB, almost 92 % of the MIB input was chemically transformed (reacted) in water compartment. From the given input emission, 98.3 % of the residual MIB was predicted to remain in the water compartment. Approximately 2 % of the MIB input was carried out of the system by advection.

ADVISER'S APPROVAL: Dr. Gregory Wilber
