Modeling and Evaluation of Pollutant Emissions from Industrial Biofilters by Dispersion Models

by

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AUTHOR'S DECLARATION

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

I understand that my thesis may be made electronically available to the public.
Abstract

With gradually increasing strict environmental regulations that control emissions of volatile organic compounds (VOCs), reduced sulphur compounds and nuisance odors from industries, there is a growing need for air pollution control systems. Biofiltration systems have been widely used in the treatment of odorous and toxic volatile organic compounds. As compared to traditional physical and chemical systems, biofiltration is cost-effective, environmentally friendly, and highly efficient for many biodegradable pollutants. The biofilter concept is about using microorganisms to metabolize the variety of contaminants such as volatile organic compounds, reduced sulphur compounds and hydrocarbons. Although the biofilters are designed to eliminate pollutants with greater than 90% efficiency, accidental releases do occur due to biofilter failures; hence, this poses serious threats to health, especially to those who live in the vicinity of biofilter locations.

This research investigates the dispersion of air pollutants that are accidentally released from industrial biofilters. Two commercial biofilters that were installed in different industrial sites, located in (Hickson) and (Toronto), Ontario, Canada, were used as test cases. A mathematical (Gaussian) dispersion model, a screening model (SCREEN3), and a non-steady state Lagrangian California Puff Model (CALPUFF), were used at different biofilter removal efficiencies to predict pollutant concentrations, dispersion and health effects, and to examine the impacts of topographical and meteorological conditions on concentration of pollutant emissions at receptor locations.

The study shows that geographical variations (i.e., flat versus elevated surfaces) of the location of a biofilter have an effect on the wind, and hence on pollutant dispersion. The results confirmed that the
wind direction has a direct impact on the pollutant plume path, whereas the wind speed and atmospheric stability class influence the pollutant concentration. The results elucidated that the high concentration of pollutants due to low removal efficiency of a biofilter can cause serious health problems. The results of this work can be used as a basis to evaluate biofilter performance under various atmospheric and geographical conditions and to improve biofilter design.
Acknowledgements

First and foremost, all praise and thanks are due to Almighty Allah for providing me with the strength and patience to accomplish this work.

I would like to express my profoundest gratitude to Dr. Ali Elkamel for accepting me as his master’s student and for providing me such a great opportunity to achieve my master’s degree under his supervision. I would also like to extend my sincere appreciation to Dr. Zarook Shareefdeen (American University of Sharjah) for introducing me to this interesting topic and for the time and effort he spent guiding me in my research. Although I only spent a short time working under the supervision of both Dr. Elkamel and Dr. Shareefdeen, I have gained invaluable lessons, and an enormous amount of knowledge. The experience has not only encouraged me to pursue my goal but has also increased my self-confidence as a researcher.

My deep gratitude goes to my thesis committee members, Dr. Mazda Biglari and Dr. Aiping Yu for accepting to serve on my thesis committee.

To my beloved parents, Ali and Norah, thanks for never tiring of praying and believing in me. My thanks also to my sisters, Najlaa, Naseem, Rajaa, Asmaa, and Sarah and to my beloved brother, Abdullah, for their engorgement and support during my journey. Last but not least, my sincere appreciation and gratitude to my husband Ali, for his unlimited love, support and sacrifices. Without him, I would not have been able to complete this work.
Dedication

To my beloved daughter Lamar
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Chapter 1
Introduction

The air pollution that accompanies different industrial activities has affected environment quality and thus human health. It can cause a variety of environmental problems such as climate change, ozone depletion, and damage to crops and the forest. Additionally, the emissions of volatile organic compounds (VOCs) and inorganic odors, such as dimethyl sulfide, amines, hydrogen sulfide, ammonia, and dimethyl disulfide, which are considered major air pollutants, cause many sub-chronic health effects including eye and nose irritation, headache, and drowsiness (Shareefdeen et al. 2002). High concentrations of these odors with long-term exposure can cause serious diseases, such as cancer and liver damage (Probert et al. 2009). In most countries, including Canada, environmental protection agencies regulate the emissions of VOCs, and conduct strenuous efforts to prevent their release into the atmosphere and the surrounding areas. Hence, air pollution control systems have been employed to regulate a wide set of volatile organic compounds (VOCs) produced by numerous industrial facilities (Steyn et al. 2010).

In recent years, biological control systems, including biofilters, biotrickling filters, and bioscrubbers have become more desirable than the air pollution control methods due to their effective removal of VOCs and biodegradability pollutants, operational simplicity, and economical costs (Shareefdeen et al. 2005). Biofiltration is promising technology and immobilized bacteria in this system degrade VOC pollutants into carbon dioxide (CO₂) and water (H₂O) (Shareefdeen et al. 2001, Islam 2006). Although biofilters are designed to eliminate
pollutants with greater than 90% efficiency, an accidental release could occur due to a failure in performance, placing the people who live in the vicinity of biofilter locations at risk (Shareefdeen et al. 2002). This failure could occur due to a shortage in one of biofilter parameters such as temperature, moisture content, pH, flow rate, contaminant loading rate and structure failures. In such circumstances, estimating the concentration of pollutants is necessary to manage the situation and to maintain good air quality (Shareefdeen et al. 2005).

Maintaining proper air quality usually involves using a complex set of management methods to address different interconnected air quality issues (de Nevers et al. 1995). However, the complexity of these methods can consume a significant time and cost. As a result, air dispersion models have been used as alternative tools to evaluate different emission control scenarios. They can be applied in such cases to estimate the total pollutant concentrations for specific locations and times. Additionally, they can be used to understand the interactions of an emission source and geophysical and meteorological conditions. Moreover, we can take advantage of these models to determine the environmental exposure to the pollutants and assess the health effects associated with it (GAQDBC 2008).

There are a number of air dispersion models that are continually developed to predict the dispersion of industrial air releases and the subsequent contaminant concentrations in adjacent areas, including AERMOD, Industrial Source Complex 3 (ISC3), and Lagrangian puff models (CALPUFF). However, it is important to choose the model that satisfies the requirements of the study of interest because no particular model can address all cases and the range of implementation (AQMG 2013, Ainslie et al. 2009).
The present project is intended to use three air quality dispersion models (Gaussian, SCEEN3, and CALPUFF) to predict the concentrations of accidental releases from industrial biofiltration systems.

1.2 Objectives:

By using air dispersion models, the following objectives can be achieved.

- To estimate the concentration of pollutants that is released accidentally from biofilters and assess their health impacts.
- To identify the effect of meteorological conditions on pollutant dispersion.
- To determine the influence of stack height and building downwash on the concentration of pollutants.
- To investigate the relationship between the failure of biofilter performance and pollutant concentration.
- To compare the different dispersion models as tools for estimating concentration and dispersion.

1.3 Thesis Outline

This thesis is organized into five chapters with appendices and references. As the first chapter provided an introduction and the objectives of this research work, the second chapter provided a general overview of VOCs and odor regulations in Canada; biofiltration systems used to control VOCs and odor emissions and a potential failure in their performance; and air dispersion models
that can be used to predicate the concentration of pollutants. In Chapter 3, the methodology and materials that were used in this research are described. In chapter 4, the results obtained from conducting the air dispersion models and their analyses are provided. Finally, Chapter 5 provides a summary and recommendations for future work.
Chapter 2

Background Information and Literature Review

2.1 Recent Changes in VOC and Odor Regulations in Canada:

2.1.1 Volatile organic compounds

Volatile Organic Compounds (VOCs) are carbon-based substances that are volatile at ambient temperature and contribute to atmospheric photochemical reactions, which are considered a major contributor to smog (Probert et al. 2009, Steyn 2010). According to the United States Environmental Protection Agency (U.S. EPA), VOCs are defined as “organic compounds having vapor pressure exceeding 0.1 millimeters of mercury (mm Hg) at standard conditions (20°C and 760mm Hg).” These compounds have a significant adverse impact on human health, depending on the concentration of VOCs in the air, the type of compound, and the period of exposure to it. VOCs are generally regulated due to their effects on human health, which include (i) irritation and toxic effects; (ii) formation of ground level ozone that is responsible for damaging human health and environmental systems; (iii) decay in the ozone layer of the atmosphere caused by the existence of some elements of VOCs in the stratosphere of the earth’s which can cause skin cancer and other health problems such as eye infections due to increased exposure to ultraviolet radiation, and (iv) enhancing global warming. Some examples of VOCs include toluene, styrene, ethanol and methane (Shareefdeen et al. 2005, ECA Report no 19).
2.1.2 Odor

Odors occur as a result of one or more volatile or inorganic chemical compounds in the air. In general, at very low concentrations of odors are recognized via sense of smell (Shareefdeen et al. 2005, Chen et al. 2009). Air pollution accusations or complaints are mainly due to odors. Odorous substances behave differently and thus some of them put human health to higher risks. The concentrations needed for humans to observe an odor often differs by compound, and by the human smelling that odor. The concentration at which an average person can observe an odor from a special substance is called the “odor threshold”, and each substance has its own exclusive threshold (Bokowa et al. 2010). Hence, it is hard to set an “odor scale” that could allow for reliable and quantitative measurements of applicable to all chemical elements. Odorous compounds are usually emitted from different industrial sources such as sewage treatment works, solid waste composting works, bio-industries, etc. The examples of odorous molecules are organic sulfides, mercaptans, ammonia, inorganic and organic amines, organic acids, aldehydes and ketones (WHO report no 85, Revah et al. 2005).

2.1.3 Approaches used to regulate VOCs and odor

There are various approaches that have been used to the improve of VOC and odor legislations, including but not limited to:

1. **Forbidding of nuisance laws**: This law is established on either “quality of life” or “nuisance” narrative principles. The exact guidelines vary by administration, but necessarily require that odors from a facility do not cause a nuisance or create pollution.
2. Ambient concentration standards for particular chemicals: Numerous administrations in North America, though generally not in other regions in the world, have measurable ambient concentration guidelines for particular chemicals that are odorous. The managerial condition of these guidelines differs by administration with instructions for applicable standards.

3. Ambient concentration guidelines for odor: Odor can be calculated using an odor panel that contains of a number of specially qualified workers, and an olfactometer. The general idea is to dilute a specimen with odor free air until it can be discovered via only 50% of the odor panel. Dilution to threshold (D/T), and odor units (OU) are well-known units for odor concentration. Ambient odor concentration guidelines are used to manage odor in numerous administrations in North America, Europe, Asia, and Australasia. However, in several administrations these instructions are used for design functions only and are not to be applicable.

4. Minimum partition distances: Many administrations regulate odors along with nuisances using fixed or variable minimum segregation distances or buffer zones.

5. Technology of guidelines: Many administrations have prerequisites to fulfill the state-of-the-science control technology or familiar techniques that identify the essential levels of odor treatment controls or any structural and managerial practices that are used for existing facilities. These prerequisites are typically qualitative ((Bokowa et al. 2010, Lee et al 2003, USGS report 2006).

2.1.4 Odor restrictions in Canada:
Canada is one of many countries that have placed air quality "limit values". These may be presented as general standards or necessary air quality guidelines (WHO AQG). Facilities are
allowed to pollute in accordance with these standards, which meet quantitative limits. The main target of air quality standards is to provide a foundation to protect the public health from the negative effects of air pollution. This basis will help to eliminate or reduce to a minimum rate those air contaminants that are considered to be hazardous or possibly hazardous to human health and the environment. The provinces of Ontario, Alberta, and Manitoba are the only Canadian administrations for which information was provided. These standards have been put into place for a vast variety of chemical substances and are based on certain factors that include odor, health effects, ozone formation capacity and negative impacts on vegetation (Table 2-1). The Ontario Ministry of the Environment (MOE) has developed ambient air quality standards (AAQC) for more than 300 substances, containing 231 VOC types. The Government of Québec Ministry of the Environment has also developed air quality norms and conditional management guidelines for over 700 air contaminants. However, the majority of the ambient guidelines for these VOC substances were established based on the Texas Effects Screening Level (ESL). The ESLs were developed on the foundation of health effect thresholds, odor nuisance potential, vegetative effects and corrosion (ECA Report no 19, Ayers et al 2002).
Table 2-1: Ambient air quality standards for volatile organic compounds in Alberta (Ayers et al 2002).

<table>
<thead>
<tr>
<th>Substance</th>
<th>Guideline 1-hour average conc. (µg/m³)</th>
<th>Guideline 1-hour average conc. (ppb)*</th>
<th>Substance</th>
<th>Guideline 1-hour average conc. (µg/m³)</th>
<th>Guideline 1-hour average conc. (ppb)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetaldehyde</td>
<td>90</td>
<td>50</td>
<td>Formaldehyde</td>
<td>65</td>
<td>53</td>
</tr>
<tr>
<td>Acetic Acid</td>
<td>250</td>
<td>102</td>
<td>Methanol</td>
<td>2600</td>
<td>2000</td>
</tr>
<tr>
<td>Acetone</td>
<td>5900</td>
<td>2400</td>
<td>Methylene bisphenyl diisocyanate</td>
<td>0.51</td>
<td>0.05</td>
</tr>
<tr>
<td>Benzene</td>
<td>30</td>
<td>9</td>
<td>Monoethylamine</td>
<td>1.19</td>
<td>0.6</td>
</tr>
<tr>
<td>Dimethyl ether</td>
<td>19100</td>
<td>10100</td>
<td>Phenol</td>
<td>100</td>
<td>26</td>
</tr>
<tr>
<td>Ethyl chloroformate</td>
<td>0.57</td>
<td>0.13</td>
<td>Phosgene</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>Ethylene</td>
<td>120 (6-hour average) 50 (30-day)</td>
<td>104 (6-hour average) 43 (30-day)</td>
<td>Styrene</td>
<td>215</td>
<td>52</td>
</tr>
<tr>
<td>Ethylene oxide</td>
<td>15 (30-minute average) 8 (30-minute average)</td>
<td></td>
<td>Vinyl chloride</td>
<td>130</td>
<td>51</td>
</tr>
</tbody>
</table>

* Standard conditions of 25°C and 101.325 kPa are used as the basis for conversion from µg/m³ to ppbv (parts per billion by volume) or from mg/m³ to ppmv (parts per million by volume).

2.1.5 Recent modifications of exposure standards

The MOE has been revising, reassessing and updating existing air quality norms to insure that they are up to date for human health and ecosystem protection. The substances for which these guideline values are presently being revised are given in Table 2-2.
Table 2-2: Compounds currently under evaluation for ambient air quality norms located in Ontario (Ayers et al. 2002)

<table>
<thead>
<tr>
<th>Contaminant</th>
<th>Existing</th>
<th>Amendment</th>
<th>Contaminant</th>
<th>Existing</th>
<th>Amendment</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Contaminants to be changed</strong></td>
<td></td>
<td></td>
<td><strong>Contaminants to be added</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ethyl benzene</td>
<td>4,000 (S)</td>
<td>3,000*</td>
<td>Acrylonitrile</td>
<td>300 (G)</td>
<td>180*</td>
</tr>
<tr>
<td>Methanol</td>
<td>84,000 (S)</td>
<td>12,000*</td>
<td>Chloroform</td>
<td>1,500 (G)</td>
<td>300*</td>
</tr>
<tr>
<td>Methyl ethyl ketone</td>
<td>31,000 (S)</td>
<td>30,000*</td>
<td>Ethyl ether</td>
<td>30,000 (G)</td>
<td>7,000*</td>
</tr>
<tr>
<td>Trichloroethylene</td>
<td>85,000 (S)</td>
<td>3,500*</td>
<td>n-Heptane</td>
<td>-</td>
<td>33,000*</td>
</tr>
<tr>
<td><strong>Standards (no change)</strong></td>
<td></td>
<td></td>
<td><strong>Isopropyl benzene</strong></td>
<td>100 (G)</td>
<td>100</td>
</tr>
<tr>
<td>Ammonia</td>
<td>3600 (S)</td>
<td>3600*</td>
<td>Methyl isobutyl ketone</td>
<td>1200 (G)</td>
<td>1200</td>
</tr>
<tr>
<td>Chlorine</td>
<td>300 (S)</td>
<td>300*</td>
<td>Mineral spirits</td>
<td>30,000 (G)</td>
<td>7800*</td>
</tr>
<tr>
<td>Hydrogen Chloride</td>
<td>100 (S)</td>
<td>100*</td>
<td>Propylene oxide</td>
<td>13,500 (G)</td>
<td>450*</td>
</tr>
<tr>
<td>Toluene</td>
<td>2000 (S)</td>
<td>2000*</td>
<td>Vinylidene chloride</td>
<td>70 (G)</td>
<td>30</td>
</tr>
<tr>
<td>Xylenes</td>
<td>2300 (S)</td>
<td>2300*</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(S) – Current standard, (G) – current guideline

*Interim standard, subject to re-evaluation through Risk Management Framework

Air quality norms are legal standards, while conditional management norms are approved guidelines. These norms have been established based on the outcomes of a review of regulations used by environmental organizations around the world, as well as collected toxicological data.
The sources of information used by the Ministry include the United Nations Environment Program, U.S. EPA, U.S. Public Health Service, and California Environmental Protection Agency. Twenty-four hour management norms for most substances are identical to ambient air quality norms developed for the same substances by the government of Ontario (Ayers et al 2002).

### 2.2 Control Strategies for Air Pollution

A control strategy is a group of various pollution prevention measures and treatment technologies that are established and applied to decrease the air pollution, and hence, reduce the overall risk to human health or the environment. These strategies may differ by source type, such as fixed or mobile, as well as by the contaminant that is targeted. The air control strategy is developed and mentored by environmental organizations to assurance that its performance not only meets, but also will continue to meet, the policy requirements. Additionally, the control strategy advancements define the finest set of methods to deliver the emission reductions that are essential to reach the air quality goals. These methods may include waste dumping, prevention of emissions, and recycling activities. However, to date, many of the air quality enhancements have been attained through technological expansions. Air pollution control technologies have obtained impressive results to lessen the releases from industrial and mobile source regions by approximately 90 to 99% (Lee et al 2003, Bokowa et al. 2010).
2.2.1 Considerations to design a successful control strategy

Designing a successful air control strategy depends on three fundamental factors, which are:

- Environmental aspects such as apparatus sites, surrounding air quality conditions, sufficient supplies (i.e., water for scrubbers), valid needs, noise levels, and the contribution of the control system as a pollutant;

- Engineering aspects such as pollutant characteristics (harshness, toxicity, etc.), gas flow characteristics, and operational characteristics of the control system; and

- Economic aspects such as capital and operational costs, equipment preservation, and the life span of the equipment. Pollution prevention should include removing as much of the pollution releases as achievable at the source, and replacing raw (and less toxic) materials, as well as considering alternative-manufacturing processes (Li et al 2008, U.S. EPA report 2010).

2.2.2 Primary types of emission control methods:

There are two main types of treatments to control odor: physical/chemical and biological. Choosing a suitable control technique for VOCs and odors is based on the physical, thermodynamic and reaction properties of the compound of interest. Furthermore, it is recommended to consider the flow rate and contaminant concentration when selecting the control method (as shown in Figure 2-1), as well as temperature, stream structure, solubility, the oxygen
content of waste gas, the operating schedule, utility and maintenance requests, which are important aspects to define the selection (Revah et al. 2005).

![Figure 2-1](image)

**Figure 2-1 Usage of different technologies to control air pollution based on airflow rates and concentrations of pollutants, (Shareefdeen et al. 2005).**

### 2.2.2.1 Physical and chemical methods:

The primary concept of physical/chemical technologies is to remove malodorous emissions through physical means such as the adsorption and absorption processes, or through chemical reactions as chemical scrubbing and oxidation. Mostly, these processes are applied for pollutants that have a high flow and concentration (Shareefdeen et al. 2005). The physical/chemical control methods that are most effective at controlling VOCs and odor emissions are: (i) thermal oxidation, which can occur by burning VOC emissions at high
temperatures (650–800 °C) or at a sufficient enough temperature to cause complete oxidation; (ii) carbon adsorption, in which pollutants are adsorbed onto the surface of activated carbon (iii) scrubbing, which refers to the process where gaseous VOCs are absorbed into a scrubbing solution such as water or solvents. Although these methods have been applied to remove different air pollutants for decades, they are considered expensive and some of them generate undesirable byproducts such as greenhouse gases (carbon dioxide or nitrous gases emissions) (Shareefdeen et al. 2005; Siefers 2010; Noyola et al. 2006).

2.2.2.2 Biological methods

The principle of biological technologies is to remove emissions using microorganisms such as bacteria, fungi, and yeasts, which can degrade these pollutants into harmless products. However, the selection of the microbial population is decided by the types of contaminant to be treated (Revah et al. 2005). These methods can effectively remove the highly soluble and low molecular weight VOCs such as methanol, ethanol, and acetates. However, low molecular compounds with complex bond structures are not easily biodegradable because they require more energy to be destroyed, which is not permanently available to the microbes. These treatments are more preferable than physicochemical methods due to their lower capital and operating costs, simplicity of operation (i.e. ambient temperature and pressure), low energy requirement, high removal efficiency, and low quantity of secondary pollution. There are three main types of this technology, which include biofilters, biotrickling filters, and bioscrubbers, and they have been used to remove pollutants in a variety of applications (Shareefdeen et al. 2005, Islam et al 2006), as shown in Table 2-3.
Table 2-3 Applications of biological air treatment (Revah et al. 2005)

<table>
<thead>
<tr>
<th>General</th>
<th>Specific</th>
<th>Specific (cont.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Industrial activities including production, transport and storage</td>
<td>Asphalt, Chemical, Food, feed and beverage, Foundries, Fragrance, Leather</td>
<td>Petroleum and petrochemicals, Pharmaceutical, Pulp and paper, Textile, Viscose processing</td>
</tr>
<tr>
<td>Naturally generated odors</td>
<td>Compost, Farms, Food and feed, Landfill gases</td>
<td>Sewage, Slaughter and rendering plants, Tobacco, Wastewater treatment</td>
</tr>
<tr>
<td>Other trades</td>
<td>Paint shops, Print shops</td>
<td>Soil remediation</td>
</tr>
</tbody>
</table>

2.3 Biofilter System:

Biofilter is widely used in air pollution control. This technology shares the same basic mechanism as the other biological air treatments (bioscrubbers, and biotrickling filters), yet they are differentiated by the equipment configurations that are used to achieve the biodegradation. The fact that contaminants can be biodegraded by microorganisms has been established for quite a while for wastewater and solid waste. However, biofiltration has only been initiated to emerge as a cost-effective and viable air treatment method few decades ago. A biofilter contains a static filter bed that consists of a porous media or packing material, which acts as a host to a bacteriological population. These microbes, which form biofilms on the surface of the media breakdown pollutants within a contaminated air which flow through the filter bed (Soccol et al. 2003). A broad array of materials can be employed as biofilter media, organic materials such as
soil, peat and compost, and synthetic materials. Both media can offer elevated removal efficiency of different pollutants of over 90% (Shareefdeen et al. 2005, Islam et al. 2006).

2.3.1 Biofilter mechanism:

The mechanism of this air treatment includes complex types of processes, which can be divided into two main categories: physical-chemical processes, which are representative in the adsorption and sorption of the gas into the surface of biofilm, and biological process, which is the degradation of the pollutants by the microorganisms.

![Diagram of a biofilter](image)

**Figure 2-2: The core mechanism of a biofilter (Devliny et al., 1999).**

To eliminate the VOCs and odorous gases from the air, the pollutant stream should first transfer from the gas phase to aqueous phase (Darracq et al. 2009). That occurs when contaminants attach and colonize on the media surface and absorb into the moist biofilm, which is known as absorption or adsorption interactions (physical treatment). The biological treatment occurs when microbes in the biofilm degrade and transfer contaminants through their metabolic process to
other substances with less health and environmental impact such as CO₂ and H₂O. The mechanism of air treatment in a biofilter is elucidated in Figure 2-2. As microbial activity predominantly occurs under aerobic condition, oxygen plays an essential role in the biotransformation. Among the several types of reactions that occur simultaneously with the air biological treatment, the oxidation reaction is considered as the basis for this type of treatment:

\[
\text{Organic Pollutant} + O_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O} + \text{Biomass}
\]

The biological air treatment systems commonly have a limited input of nutrients, and as result, the energy can be derived from three different ways (i) using pollutants as a source of nutrients and energy (as ATP) for growth and maintenance of microbial activity, which yields additional biomass and CO₂, H₂O, sulfate, and nitrate as by-products; (ii) recycling part of the formed biomass as in the case of VOCs, where autotrophic microorganisms drive energy from the oxidation of the accumulated organic compounds and use CO₂ which is included into the biomass as a carbon source; and (iii) using an external supply of other nutrients such as nitrogen, phosphorus, minerals, and trace elements, which are usually added to incoming water as traditional supports for microbial growth in biofilters as presented in Figure 2-3. However, this method is not preferred because excess growth could occur when nutrients are constantly supplied, and unwanted plugging might occur (Revah et al. 2005; Datta et al. 2005; Sercu et al. 2006)
2.3.2 Type of biofilters

Biofilters are classified based on their configuration into either open- or closed-bed systems, as well as based on the flow sequence (horizontal or vertical flow).
Open biofilters with single-bed systems, which are used frequently to control pollution from animal facilities, were the predominant design in the past. Figure 2-4 shows the structure of an open biofilter that contains a 1 m-sized deep room filled with packing material such as soil or compost (biofilter media), and is open to the atmospheric conditions. However, recently, some modifications have been applied to this type of biofilter such as roofs, which can offer some weather protection. Because of the simplicity of the open biofilter design, it is considered less expensive than in the case of the closed system.

Figure 2-5: Schematic diagram illustrates the structure of a closed biofilter,

(Shareefdeen et al. 2005)

Closed systems have become a more popular air treatments because of the necessity to fulfill the emission monitoring fundamentals. A closed system controls both the biofilter outlet and inlet gas streams in contrast with an open system, which discharges treated gas directly to the atmosphere. As shown in Figure 2-5, a closed system consists of a humidifier and a packed filter bed inhabited with microorganisms through which a waste airstream is passed. Influent air
is pre-humidified to keep sufficient moisture in the filter bed. This type of biofilter tends to be a more engineered system that allows for a better contaminant loading over a certain footprint area, and also grants more accurate control of biofilter function and moisture. However, both types of biofilters are sometimes provided with a sprinkling system, which may contain the required nutrients for the growth of microorganisms. Additionally, they include a distribution system containing perforated pipes underneath the bed to guarantee an equal flow of gas through the porous bed of the biofilter (Datta et al. 2005, Janni 2011).

**2.3.3 Factors affecting biofilter performance failures and pollutant release**

The overall efficiency of a biofilter is determined by its critical operational and performance parameters, which include:

- **Packing media:** As mentioned earlier in this chapter, two types of materials can be used for the media, which are organic materials such as soil, peat and compost, and synthetic materials. Both types of media should be designed to include certain properties to provide optimal performance, which include a high surface area for microorganism growth, long-standing physical stability, low pressure drop, good moisture holding, pH buffering, and nutrients (Datta et al. 2005, Devinney et al., 1999).

- **Moisture content:** The moisture content of the biofilter bed has a great influence on its performance because the drying of bed could occur due to a low moisture content, which leads to a decline in pollutant degradation by microorganisms, and to a varying gas distribution. For this reason, it is important to provide the biofilter with a sprinkler system for direct water supply (Datta et al. 2005, Khammar et al. 2003)
• **Temperature**: Temperature control is also very critical to biofilter performance. The recommended temperature range for a biofiltration system is between 15 and 40 °C and for microbial population from 20 to 35 °C (Leson and Winter 1991; Bohn 1992). However, some studies show that the temperature could be expended to the range of 0 to 70 °C, and a biofilter can work efficiently under this new range (Giggey et al. 1994; Kong et al. 2001; Datta et al. 2004).

• **Oxygen content**: Oxygen is vital to this air treatment system since the major microorganisms employed in biofilters are aerobic; oxygen is required for their metabolic activities. Although oxygen can be easily supplied within the incoming airstream when a biofilm is relatively thin, a limitation could occur due to the overloading of biofilm, which results in the formation of acidic and other intermediaries (Datta et al. 2005).

• **pH**: The optimum pH range for microorganism activities is between 7 and 8. Maintaining the pH of a biofilter can occur at the beginning of air treatment by adding solid buffer agents to the packing media. Also, when the buffering capacity is drained, the biofilter bed is replaced with new material (Datta et al. 2005).

• **Nutrients**: Organic packing materials such as peat, and compost include nutrients to enhance biomass growth; however, nutrients should be provided for enhanced performance in the case of inorganic packing material because low nutrient levels have an inhibitory effect on the removal pollutant rate as shown in some studies (Weckhuysen et al. 1993; Morgenroth et al. 1996; Yang et al. 2002).

• **Pressure drop**: Pressure is a very critical factor in the design of biofilters. Structural stability and low biomass accumulation decrease the medium compaction potential which
would then cause channeling and increased pressure drop. In order to ensure that the operating pressure drop is low and to guarantee fluent gas flow, it is important to sustain interparticle void space between 40-80% (Datta et al. 2005, Kumar et al 2011).

2.3.4 Biofilter Failures and the Accidental Releases

Accidental releases can produce high ground-level concentrations of pollutants, even for a short period of time (U.S Environmental Protection Agency 2012). Discharges from a biofilter can occur when a drawback in the above biofilter parameters occurs, which causes a decline in its removal efficiency, hence causing harmful impacts on human health and environmental quality (Shareefdeen et al. 2005). It is believed that modeling accidental releases from industrial biofilters are required for the following reasons: (1) since biofiltration systems are emergent technologies and need long-term planning and development, modeling might be used to understand the outcomes of diverse accidental release situations, and thus assist to define the topography, meteorology and neighboring districts most appropriate to protect the residents from serious risk; and (2) modeling can help to identify the possible health effects of different pollutants when an accidental release does really occur, which means modeling can be used as a tool for risk assessment.

2.4 Air dispersion model

Air quality dispersion models are mathematical models of the behavior of air pollutants in the atmosphere. The fundamental aim of the dispersion models is to accurately estimate the pollutant concentration downwind of any source for a wide range of meteorological conditions
(Yu et al. 2011). There is a range of air dispersion models that have been used in different jurisdictions around the world to treat a wide array of modeling circumstances. They have been developed to assess various source types including point, area, and volume, various terrain (i.e., simple or complex), various locales such as urban, rural, various emission rates include plume, puff and various meteorological conditions. Air dispersion models have many features that cause them to be used in different investigations of air quality. They have the ability to elucidate the interactions of emission sources and the geophysical and meteorological conditions (Shewchuk et al. 2006). Moreover, using the dispersion models, it is possible to: determine whether a permissible facility is obeying with state or federal necessities, evaluating where the best location site for an air monitor that reads actual data, etc. (MDCA, Citizens” Guide to Air Dispersion Modeling, 2002), and finally, to estimate the possible environmental and health effects due to releases from industrial or trade locations (Shewchuk et al. 2006).

2.4.1 Models used in air dispersion modeling

There are two types of dispersion models used in air quality studies: steady state and non steady state.

2.4.2.1 Steady state model

Steady-state models are usually called Gaussian plume models. These are constructed on the mathematical approximation of the plume conduct and are the simplest models to use (Shewchuk et al. 2006). They estimate the pollutant concentrations for each hour, supposing that the meteorological conditions are even through the modeling domain. They assume that the
plume centerline moves straight to the end of the modeling region despite if it could really do that at the specified wind speed. For instance, if the wind velocity is 6 km/h, the plume has to tour a distance of 6 km in an hour simulation period. However, a plume dispersion model presumes that the traveling distance of plume to the end of the modeling location could be 20 or 30 km. They also do not have memory of former hour’s emission. Thus a plume traveling in a windy route over several hours cannot be simulated (Xing et al. 2006). As a result of the steady state, and straight-line features of these models, they obviously do not account for the bent plume trajectories and inconstant wind conditions that occur in complex flow circumstances. Furthermore, these models have a limited capacity to handle low wind speeds.

Although the limitations of the steady-state models, they can deliver realistic outcomes when used properly. Lately, superior methods of depicting the spatially changing turbulence and dispersion properties within the mesosphere have been developed. The recent dispersion models embrace an additional advanced way to describe dissemination and dispersion using the basic characteristics of the atmosphere instead of depending on general mathematical calculation. This allows for better management of challenging circumstances such as steep rugged topography and far transportation (Steyn et al. 2010). There are numerous steady-state models that are commercially accessible for air dispersion model such as ISCST3, AUSPLUME, and AERMOD.

2.4.2.2 Non-steady state models

Non-steady state dispersion models are usually called puff models advanced models (unsteady-state models). Puff models can handle the two drawbacks of plume models (Xing et al. 2006). Puff models discharge emissions independent of the source, allowing the puff to counter
the meteorology directly around it. This also permits puffs to be traced through multiple testing periods until they have either totally diluted or have been tracked throughout the entire modeling area and out of the computational zone. In addition, they can describe the accumulation of pollutants during tranquil conditions, the bent paths of plumes, and the effects of causality (where the former location of the plume is accounted for to define the present plume location). Although these models have the advantage of permitting meteorological conditions (winds, turbulence, vertical temperature construction) to alter across the modeling domain, they demand more computing power because they trace puffs that represent incoherent quantities of pollutants over time. In this way, puff models have a more accurate display of dispersion than plume models. There are models that treat emissions as a series of puffs such as the CALPUFF model and advanced model (puffs) (Figure 2-6) (Xing et al. 2006).

Figure 2-6: A graphic describing the tracing differences of a puff and a plume model (Lakes Environmental Website)
2.4.2 Factors affecting air dispersion

Odor dispersion is affected by many factors that include: 1) meteorological conditions; 2) geography; 3) source of odor release; 4) the position of the receptors to the source including distance and direction; and 5) the odor sensibility and the acceptance of the receptors (De Nevers, 1995, El-Harbawi 2013). However, the weather conditions, including, wind speed; wind direction; temperature; and atmospheric stability classes, and the topography of area are the dominant factors for air dispersion. Because the weather condition is variable and an essential input of air dispersion models, it attracted scientists’ attention when performing researches associated to odor dispersion.

There are several studies that have been conducted using atmospheric dispersion models to investigate the effect of weather parameters on the dispersion of different contaminants. Abdul-Wahab et al (2013) used the CALPUFF model to investigate the effect of geophysical and meteorological conditions on the dispersion of nitrogen dioxide (NO₂). Jeong et al (2012) identified the impact of the meteorological variability on O₃ and SO₄²⁻–NO₃⁻–NH₄⁺ concentrations in East Asia using the 3-D global chemical transport model (GEOS-Chem).

Schmitz et al (2004) explained the role of turbulence on the carbon monoxide (CO) pollutant distribution in their study; they used the Chilean Air Pollution Dispersion Model (CADM). Also, Melo et al (2012) evaluated the performance of two dispersion models AERMOD and CALPUFF to examine the impact of wind direction on the odor dispersion around a pig farm-building complex. However, very limited studies have been performed to investigate either the dispersion of pollutant emissions that accidently release from biofilters or the impact of the atmospheric and topographic conditions on the pollutant concentration.
Chapter 3: Material and Methods

3.1 Case studies:

To meet the objectives of this thesis, two industrial biofilters installed in Ontario, Canada were selected: One of the biofilter was installed at a printed circuit manufacturing facility for removal of VOCs and other was at a meat rendering facility to remove highly odorous pollutants such as di-methyl sulphide, ammonia etc.

3.1.1 Printed Circuit Board Factory (Toronto)

A Printed Circuit Board factory is located in the Greater Area of Toronto, and it emits Volatile Organic Compounds (VOCs) namely Propylene Glycol Monomethyl Ether Acetate (PGMEA), di-Propylene Glycol Monomethyl Ether (di- PGME), and 1-3-5triazine-2-4-6triamine. Although these compounds are considered safe and not causing any serious health effects, they have been regulated at the country level in Canada due to their strong smelling that cause inconvenience to the residents in the surrounding areas (Shareefdeen et al 2002, PGMEA Sigma-Aldrich SDS). Nevertheless, theses pollutants can cause many symptoms such as nausea, eyes, nose, or skin irritation, and headaches (Shareefdeen et al 2002). Table 3-1 shows the permissible exposure limit to PGMEA and the potential health symptoms associated with overexposure to this pollutant (Sigma-Aldrich SDS- PGMEA MSDS 2004). For this reason, the BIOREM Company (Guelph, ON, Canada) installed a 7500 cfm capacity commercial biofilter in this facility to control the VOCs emissions in August 2000. This biofilter system has two types of media organic wood based (Biomix) with a pollutant removal efficiency of 94%, and synthetic (BIOSORBEN) media that can remove the pollutants with 99% efficiency (Shareefdeen et al 2002).
Table 3-1: The health symptoms and permissible exposure limit of PGMEA pollutant (PGMEA Sigma-Aldrich SDS- PGMEA MSDS 2004)

<table>
<thead>
<tr>
<th>Exposure limit</th>
<th>Basis</th>
<th>Overexposure Health Symptoms</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 ppm</td>
<td>Canada. British Columbia OEL</td>
<td>Irritation eyes, skin, nose, throat;</td>
</tr>
<tr>
<td>75 ppm</td>
<td></td>
<td>Headache, nausea, dizziness, drowsiness,</td>
</tr>
<tr>
<td>50 ppm 270 mg/m3</td>
<td>Canada. Ontario OELs</td>
<td>Incoordination; vomiting, diarrhea</td>
</tr>
</tbody>
</table>

3.1.2 Meat Rendering Plant (Hickson)

A 15000 cfm capacity biofilter was installed in 1998 in a Meat Rendering facility that is located in Hickson (Ontario), to control air pollution. The significant pollutants from this facility are ammonia (NH₃), hydrogen sulfide, methanethiol, ethylamine, and dimethyl sulfide. There are many health effects associated with high concentrations of these pollutants in the atmosphere. For instance, the main concern of ammonia (NH₃) is the possibility of rising health risks because of a growth in PM₂.₅ linked with ammonium nitrate (Toro et al 2014), leading to heart attacks and strokes, and premature death (Wang et al 2013). As the hydrogen sulfide H₂S is an extremely toxic odor; high concentration could cause loss of consciousness and death (U.S. EPA 2003). Although Methanethiol (CH₄S) is considered to be relatively non-toxic, high concentration and long exposure affects the nervous system, and can cause convulsion and narcosis (Wei-jinag et al 2013). Similarly, inhalation of Ethylamine (CH₃CH₂NH₂) with high concentration causes nose and throat irritation as well as headaches (AEGLs 2008). The strong garlic odor of the dimethyl sulfide (CH₃)₂S causes headache, nausea and irritation to the eyes and respiratory system (MSDS
for DMS 2004). Table 3-2 represents the possible health effects associated with different concentrations of these compounds according to Canadian Council of Ministers of the Environment and United States Environmental Protection Agency.

**Table 3-2: The Health effects associated with different concentrations of pollutants emitted from this biofilter (CCME, U.S EPA)**

<table>
<thead>
<tr>
<th>Ammonia</th>
<th>Health effects</th>
<th>Hydrogen Sulfide</th>
<th>Health Effects</th>
<th>Methanethiol</th>
<th>Health Effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exposure limit (mg/m³)</td>
<td>Exposure limit (mg/m³)</td>
<td></td>
<td></td>
<td>Exposure limit (mg/m³)</td>
<td></td>
</tr>
<tr>
<td>25-300</td>
<td>- Eye, nose and throat irritation - Coughing</td>
<td>10-30</td>
<td>- Eye, nose and throat irritation - Headache, - Fatigue - Dizziness</td>
<td>20-50</td>
<td>- Irritation in eyes, skin, respiratory system - Narcosis</td>
</tr>
<tr>
<td>300-400</td>
<td>- Increases of blood pressure and pulse rate - Chronic lung disease</td>
<td>30-150</td>
<td>- Muscle fatigue - Dryness of nose and throat - Eye tissue damage - Lung disease</td>
<td>50-100</td>
<td>- Cyanosis - Convulsions</td>
</tr>
<tr>
<td>400-1200</td>
<td>- Immediate eye injury possible</td>
<td>150-200</td>
<td>- Nervous system depression - Fluid accumulation in the lungs</td>
<td>&gt;150</td>
<td>- Damage to the lungs, and the central nervous system</td>
</tr>
<tr>
<td>&gt;1200</td>
<td>- Chest pain - Pulmonary edema - Laryngospasm</td>
<td>200-500</td>
<td>- Muscle cramps - Low blood pressure - Paralysis</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3600-4500</td>
<td>- Fatal within 30 minutes</td>
<td>&gt; 500</td>
<td>- Death after exposure of 30 to 60 minutes</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Ethylamine</th>
<th>Health Effects</th>
<th>Dimethyl Sulfide</th>
<th>Health effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exposure limit (mg/m³)</td>
<td>Exposure limit (mg/m³)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25-100</td>
<td>Slight visual disturbances</td>
<td>30-300</td>
<td>- Severe inflammation - Necrosis of the eyes, mouth, and respiratory tract</td>
</tr>
<tr>
<td>100-300</td>
<td>- Transient mucous membrane irritation</td>
<td>300-700</td>
<td>- Severe damage to the lungs - Injures the liver, kidneys, heart, and central nerves system.</td>
</tr>
<tr>
<td>&gt;300-700</td>
<td>- Irritation of skin, eyes and upper respiratory tract with conjunctivitis sore throat, and coughing</td>
<td>&gt;700</td>
<td>- Coma and death</td>
</tr>
</tbody>
</table>
3.2 Description of models involved in this project:

In this thesis, we used the following three dispersion models:

3.2.1 Gaussian model:

The Gaussian dispersion theory is one of the oldest plume dispersion models (circa 1936). Also, it is a more preferable computational way to calculate the pollutant concentration at a certain point. The Gaussian theory connects average steady-state concentration of pollutant to many factors such as the wind speed, effective stack height and atmospheric conditions (Figure 3-1).

This model is based on assumptions, which are: (1) the emission rate of the pollutant is constant for a minimum average duration; (2) wind velocity is invariable in both time and altitude; (3) the contaminant is not exposed to degeneration or participant chemical interaction; and (4) the terrain is open and comparatively even (El-Harbawi, 2013; Banerjee et al. 2011).

![Gaussian dispersion](image)

**Figure 3-1**: Imagining of a Gaussian air pollutant dispersion plume (Shende et al 2013)

- Gaussian distribution equation:

This equation (1) depends on two dispersion parameters (i.e. $\sigma_y$ and $\sigma_z$) which are functions of wind speed, temperature, and cloud cover. In the other words, they can be estimated depending
on five different stability classifications which are stable, unstable, neutral, conditionally unstable, or conditionally stable (El-Harbawi et al. 2013, Shende et al. 2013).

\[ c(x, y, z) = \frac{Q}{2\pi \sigma_y \sigma_z u} \exp \left[ -\frac{1}{2} \left( \frac{y^2}{\sigma_y^2} + \frac{(z-H)^2}{\sigma_z^2} \right) \right] \]  

(1)

Where \( C = \) pollutant concentration (g/m\(^3\)); \( Q = \) emission rate (g/s); \( \sigma_y \) and \( \sigma_z \) = horizontal and vertical dispersion coefficients respectively, \( u = \) average wind speed (m/s), \( H = \) effective stack height, \( X = \) downwind distance, \( Y = \) distance in the horizontal direction, and \( Z = \) distance in vertical direction.

### 3.2.2 SCREEN3 model

SCREEN3 is a steady-state plume model that was developed by U.S. EPA to provide an easy-to-use method of obtaining maximum ground-level concentrations for different types of sources (point, area, flare, and volume), as well as concentrations in the hollow area, and during inversion breakup and shoreline fumigation. SCREEN3 is a screening version of the ISC3 model. The model focuses mainly on calculating hourly average concentrations from a single source. Also, it can be used for an initial assessment of fumigation events. Also, the SCREEN3 model can be used to: 1) identify the maximum ground-level pollutant concentrations downwind under any meteorological conditions; 2) simulate dispersion in country and town areas; 3) evaluate the effects of building downwash and; 4) assess the terrain effects (El-Harbawi, 2013, Bokowa et al 2010).
- **Input data requirement**

1- **Location of the sources (x, y, z)**

The pollutant concentrations and odor levels were identified within a 5 km radius of the plants.

2- **Stack physical height (m)**

The stack height was estimated from a reference of a similar biofilter.

3- **Pollutant emission rate (g/s)**

The pollutant emission rates for the study cases were obtained from (Shareefdeen et al., 2002).

4- **Wind speed (m/s)**

The average wind speeds were obtained from the environment Canada website (http://www.ec.gc.ca/dccha-ahcccd/default.asp?lang=en&n=71CB3873-1)

5- **dispersion parameters (σ_y and σ_z)**

The dispersion parameters were estimated based on stability classes and wind speed.

### 3.2.3 CALPUFF model:

CALPUFF is non-steady-state meteorological puff dispersion model that has been improved by the U.S. Environmental Protection Agency. This model can simulate the effects of temporally and spatially varying meteorological conditions on pollutant transport, transformation and removal. CALPUFF is planned for use on modeling areas from tens of meters to hundreds of kilometers from a source. It is the most appropriate model for assessing mesoscale transport of pollutants and their dispersion in near field complex terrain settings. Also, this model has the capability to characterize wet and dry deposition of the pollutants beside adapting point, area, and volume source emissions. CALPUFF model includes algorithms for nearby-source effects such as transitional plume height, partial plume permeation, sub-grid scale topography interactions,
building downwash in addition to long-range effects such as pollutant elimination, chemical conversion, vertical wind speed shear, over water transportation, and coastal interaction effects. Most of the algorithms include options to deal with the physical operations at different stages of details based on the model purpose. Terrain can be included into the simulation. The modeling system contains three major modules, CALMET, CALPUFF, and CALPOST. CALMET is the meteorological pre-processing package includes a set of processors for geophysical, and meteorological data (surface, upper air, precipitation, and overwater). CALPUFF is a Gaussian puff model with different effects such as chemical removal, wet and dry deposition, and complex terrain algorithms. CALPOST is the post-processing package, which is used to process the output models generated by CALMET and CALPUFF respectively (Figure 3-2) (www.src.com; Cui, 2011; U.S EPA 2013, Xing et al. 2006).

![CALPUFF Modeling System Diagram](image)

Figure 3-2: Diagram of CALPUFF modeling systems (U.S EPA 2013)
3.3 Required Model Setup Data:

First step in processing the models is by identifying the meteorological domain information for two case study regions (Table 3-3).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Toronto</th>
<th>Hickson</th>
</tr>
</thead>
<tbody>
<tr>
<td>Map Projection</td>
<td>LCC</td>
<td>LCC</td>
</tr>
<tr>
<td>Latitude of origin</td>
<td>43.776687</td>
<td>43.225033</td>
</tr>
<tr>
<td>Longitude of origin</td>
<td>79.488337</td>
<td>80.851565</td>
</tr>
<tr>
<td>False Easting</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>False Northing</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Continent/Ocean</td>
<td>Global</td>
<td>Global</td>
</tr>
<tr>
<td>Region</td>
<td>84</td>
<td>84</td>
</tr>
<tr>
<td>DATUM Code</td>
<td>WGS-84</td>
<td>WGS-84</td>
</tr>
<tr>
<td>X (Easting)</td>
<td>25 km</td>
<td>25 Km</td>
</tr>
<tr>
<td>Y (Northing)</td>
<td>25 km</td>
<td>25 Km</td>
</tr>
<tr>
<td>Number of X grid cells</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>Number of Y grid cells</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>Grid spacing</td>
<td>1 Km</td>
<td>1 Km</td>
</tr>
<tr>
<td>Number of vertical layers</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Number cell face heights (m)</td>
<td>0, 20, 40, 80, 160, 320, 640, 1200, 2000, 3000</td>
<td>0, 20, 40, 80, 160, 320, 640, 1200, 2000, 3000</td>
</tr>
</tbody>
</table>

3.3.1 Surface data

The hourly surface observations for the two locations -Toronto, and Hickson- were acquired from the historical weather records in the Canadian government website (climate.weather.gc.ca). The surface stations were chosen based on the closeness from the point source and upper air stations. For each station, each hourly record contains the date and the time, temperature, wind speed, wind direction, ceiling height, cloud cover, and station pressure. The hourly data for four modeling periods from (i) December 30, 2012 at 0000h to February 2, 2013 at 2300h; (ii) April
30, 2013 at 0000h to June 2, 2013 at 2300h; (iii) June 30, 2013 at 0000h to August 2, 2013 at 2300h, and (iv) August 30, 2013 at 0000h to October 2, 2013 at 2300h were extracted and organized in a certain layout that is suitable for use in SMERGE to create a formatted file SURF.DAT, which is compatible to be used with CLAMET. The information of the surface meteorological station selected in each of the two regions of study is shown in Table 3-4.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Toronto Buttonville A</th>
<th>Kitchener/Waterloo</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Station Name</strong></td>
<td><strong>Toronto</strong></td>
<td><strong>Hickson</strong></td>
</tr>
<tr>
<td>Latitude</td>
<td>43 51 44</td>
<td>43 27 39</td>
</tr>
<tr>
<td>Longitude</td>
<td>79 22 12</td>
<td>80 22 43</td>
</tr>
<tr>
<td>Elevation</td>
<td>198.1</td>
<td>321.6</td>
</tr>
<tr>
<td>Climate ID</td>
<td>615HMAK</td>
<td>6144239</td>
</tr>
<tr>
<td>WMO ID</td>
<td>71639</td>
<td>71368</td>
</tr>
<tr>
<td>TC ID</td>
<td>YKZ</td>
<td>YKF</td>
</tr>
</tbody>
</table>

**3.3.2 Upper air data**

The upper air meteorological information for the two locations was obtained from the radiosonde station records in the NOAA/ESRL radiosonde database (esrl.noaa.gov/raobs/). These data records contain station ID number, date and time, and information of sounding level followed by pressure, temperature, elevation, wind direction, and wind speed for each sounding level. The hourly data for two regions - Toronto, and Hickson- was taken from one radiosonde station, that is close to these two cities, for the three modeling periods mentioned above and was then prepared a format suitable to use in READ62 to generate the UP.DAT file that will be used later in the CALMET program. Table 3-5 lists information about the radiosonde station from which upper air meteorological data were extracted.
Table 3-5: Radiosonde stations information.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Toronto</th>
<th>Hickson</th>
</tr>
</thead>
<tbody>
<tr>
<td>Station Name/Location</td>
<td>Moosone PQ</td>
<td></td>
</tr>
<tr>
<td>UTM latitude</td>
<td>51.27</td>
<td></td>
</tr>
<tr>
<td>UTM longitude</td>
<td>80.65</td>
<td></td>
</tr>
<tr>
<td>X location on grid</td>
<td>808.3 km</td>
<td></td>
</tr>
<tr>
<td>Y location on grid</td>
<td>1 km</td>
<td></td>
</tr>
<tr>
<td>Elevation</td>
<td>10 m</td>
<td></td>
</tr>
<tr>
<td>WBAN</td>
<td>15803</td>
<td></td>
</tr>
<tr>
<td>WMO ID</td>
<td>71836</td>
<td></td>
</tr>
</tbody>
</table>

3.3.3 Geophysical data:

The geophysical data, including land use and terrain were obtained from the Geographic Information Systems Resource website (www.webgis.com) and used as input files in CTGPROC and TERREL to produce LU.DAT and TERREL.DAT respectively. This data is then compressed together by a MAKEGEO program to generate output file GEO.DAT, which can later be used in the CALMET program.

3.3.4 Emission rates and source parameters:

The pollutant emission rates for the two case studies were obtained from the reference (Shareefdeen et al., 2002). Table 3-6 and 3-7; contain the values of source parameters, and emission rates of pollutant at 90% removal efficiency of biofilter, respectively. These values were used in the CALPUFF model and specified for the four modeling periods.
Table 3-6: Source parameters information for the two case studies

<table>
<thead>
<tr>
<th>Source Parameters</th>
<th>Toronto</th>
<th>Hickson</th>
</tr>
</thead>
<tbody>
<tr>
<td>X Coordinate (km)</td>
<td>620.98</td>
<td>511.94</td>
</tr>
<tr>
<td>Y Coordinate (km)</td>
<td>484.99</td>
<td>478.61</td>
</tr>
<tr>
<td>Base Elevation (m)</td>
<td>198.4</td>
<td>353.6</td>
</tr>
<tr>
<td>Stack Height (m)</td>
<td>14</td>
<td>14</td>
</tr>
<tr>
<td>Stack Diameter (m)</td>
<td>0.31</td>
<td>0.31</td>
</tr>
<tr>
<td>Exit Velocity (m/s)</td>
<td>25.05</td>
<td>25.05</td>
</tr>
<tr>
<td>Exit Temperature (K)</td>
<td>308</td>
<td>308</td>
</tr>
</tbody>
</table>

Table 3-7: The emission rates of pollutants for the two case studies

<table>
<thead>
<tr>
<th>Location</th>
<th>Toronto</th>
<th>Hickson</th>
</tr>
</thead>
<tbody>
<tr>
<td>Species</td>
<td>VOCs</td>
<td>NH₃</td>
</tr>
<tr>
<td>Emission Rates (g/s)</td>
<td>0.507</td>
<td>0.13</td>
</tr>
</tbody>
</table>

2.3 Steady- State Meteorological Conditions

Under the steady-state condition, climatic elements were investigated by varying one parameter at a time while maintaining the others fixed to detect the changing of the model’s output depending on the alteration of this parameter. Weather parameters including wind speed, wind direction, temperature, mixing height, and atmospheric stability classes were examined. Table 3-8 illustrates the given values of these parameters that were used in the modeling runs.
Table 3-8: The assigned values for climatic parameters under steady state conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Wind speed (m/s)</th>
<th>Wind direction (degree)</th>
<th>Temperature (K)</th>
<th>Stability class</th>
<th>Mixing height (m)</th>
<th>Pressure (mb)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Variable values</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind speed (m/s)*</td>
<td>2, 4, 6, 8, 10</td>
<td></td>
<td>280</td>
<td>D</td>
<td>200</td>
<td>988</td>
</tr>
<tr>
<td>Wind direction (degree)</td>
<td>50, 100, 150, 200, 250, 300, 350</td>
<td>6</td>
<td>298</td>
<td>D</td>
<td>200</td>
<td>988</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>270, 285, 298, 308</td>
<td>6</td>
<td>280</td>
<td>D</td>
<td>200</td>
<td>988</td>
</tr>
<tr>
<td>Stability class*</td>
<td>A, B, C, D, E, F**</td>
<td>2</td>
<td>280</td>
<td>293</td>
<td>200</td>
<td>988</td>
</tr>
<tr>
<td>Mixing height (m)</td>
<td>100, 500, 1000, 1500, 2000</td>
<td>2</td>
<td>280</td>
<td>298</td>
<td>D</td>
<td>988</td>
</tr>
</tbody>
</table>

*These only parameters can be investigated by Gaussian equation.

** Very unstable (A), unstable (B), slightly unstable (C), neutral (D), stable (E), and slightly stable (F).

Each variable value of each parameter was examined in a distinct run.

2.4 Variable meteorological conditions

To study the effect of variable climatic conditions on PGMEA dispersion, we used the required surface meteorological data, and upper air meteorological data for the following modeling periods (i) January 14, 2013 at 0000h to January 16,2013 at 2300h; (ii) May 14,2013 at 0000h to May 16, 2013 at 2300h; and (iii) September 14, 2013 at 0000h to September 16 at 2300h.
Chapter 4

Results and Discussion

4.1 Identify Concentration of Released Pollutants

In order to estimate the concentration of pollutants, we used in this research three dispersion models: two steady-state models (Gaussian, SCREEN3), and a non-steady state (advanced) CALPUFF model. Also, we chose a month of each season _January, May, July, and September_ as modeling periods.

4.1.1 Using Gaussian and SCREEN3 models

Using the mathematical dispersion model (Gaussian) and screening model (SCREEN3) allowed for a prediction of the density of the pollutants as a function of wind speed, atmospheric stability, height of stack, as well as a different removal efficiency of the biofilter. The maximum average concentration of Propylene Glycol Monomethyl Ether Acetate (PGMEA), which was emitted from a printed circuit board factory (Toronto), at three stability classes – unstable, slightly unstable, and neutral- is shown in Figure 4-1. When using the Gaussian model, the highest levels of PGMEA observed for January, May, July, and September were 5.2 mg/m$^3$, 5.8 mg/m$^3$, 5.5 mg/m$^3$, and 0.23 mg/m$^3$ respectively at slightly unstable condition. However, when using SCREEN3 model, the concentrations of PGMEA were 16.54 mg/m$^3$, 18.52 mg/m$^3$, 17.7 mg/m$^3$, and 19.45 mg/m$^3$ for _January, May, July, and September_ respectively at a stability class of neutral, thus indicating that the highest concentration of PGMEA obtained in September as the wind speed in this month was the lowest (3.7 m/s). All of the observed PGMEA concentrations
are considered within the allowed limit for exposure as shown in Table 3-1, and they do not cause any health effects in this range.

![Graph showing PGMEA concentration by month](image)

**Figure 4-1**: PGMEA concentration by month [Gaussian (bars)-Screen (lines)] during three different stability classes (B-unstable, C-slightly unstable, and D-neutral) at a distance of 300 m from the biofilter stack.

In the Hickson case, the following pollutants; ammonia (NH₃), hydrogen sulfide (H₂S), methanethiol (CH₄S), ethylamine (CH₃CH₂NH₂), and dimethyl sulfide (CH₃)₂S are emitted. However, estimating the concentration of these pollutants shows that the dimethyl sulfide compound has the higher concentration in the airstream where the concentration of other compounds (NH₃), (H₂S), (CH₄S), and (CH₃CH₂NH₂) were very low and do not cause any health concerns. Figure 4-2 demonstrates the concentration of (CH₃)₂S for the study modeling periods in three different stability conditions. Similarly, the highest level of dimethyl sulfide was observed in the September month, where it reached (in the case of using the Gaussian model) 74.9 mg/m³ in a slightly unstable condition, and 480 mg/m³ when using the SCREEN3 model in neutral weather. According to Table 3-2, the maximum concentration of (CH₃)₂S, which was
observed using the Gaussian model in the four months can cause severe inflammation - necrosis of the eyes, mouth, and respiratory tract. Yet, in the case of using SCREEN3, the concentration of dimethyl sulfide can lead to severe damage of the lungs and injure the liver, kidneys, heart, and central nervous system.

![Figure 4-2: (CH3)2S concentration by month [Gaussian (bars)-Screen3 (line)] during three stability classes (B-unstable, C-slightly unstable, and D-neutral) at a distance of 300 m from the biofilter stack.]

The reason for the higher observations of The SCREEN3 model is that this model was designed to calculate the worst-case scenario and to be more precautionary than other dispersion models. Thus SCREEN3 includes an alternative mixing height algorithm, which uses the maximum predetermined mixing height or a value altered a little higher than the plume altitude, based on stability class (Brode, 1991). This leads to overstated concentrations compared to those predicted by the US EPA’s full Gaussian dispersion models (Drew et al. 2008).

4.1.2 Using CALPUFF model
The CALPUFF model was used to predict the concentration of pollutants released from the biofilters, as well as to simulate the transport and dispersion of these pollutants. The CALPUFF model was run for the same modeling periods, which are January, May, July, and September. Then, the CALPOST postprocessor was used to show the spatial distribution of predicted concentrations. Figure 4-3 represents the characteristics of both study areas. In this figure, the capability of the CALPUFF model to simulate the geographical condition of the area of interest can be seen. Table 4-1 illustrates the maximum monthly PGMEA average concentrations, and the coordinates when the biofilter has a 90% removal efficiency of pollutants.

Figure 4-3: The Characteristics of the study area (1) Toronto (A) google map (B) elevation, (2) Hickson (A) google map (B) elevation.
Table 4-1: The highest monthly average concentrations of PGMEA for four modeling periods for 90% removal efficiency of biofilter

<table>
<thead>
<tr>
<th>Modeling Period</th>
<th>Highest Average Monthly Concentration (mg/m³)</th>
<th>Coordinates (Km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>January</td>
<td>0.534</td>
<td>1, 2.5</td>
</tr>
<tr>
<td>May</td>
<td>0.369</td>
<td>0.2, 2</td>
</tr>
<tr>
<td>July</td>
<td>0.48</td>
<td>0.2, 0.5</td>
</tr>
<tr>
<td>September</td>
<td>0.423</td>
<td>2, 1.5</td>
</tr>
</tbody>
</table>

Figure 4-4: The dispersion of PGMEA emissions for modeling periods A) January B) May C) July D) September

The maximum monthly average concentration of PGMEA in January was 0.534 mg/m³ as shown in Table 4-1, occurring at the location of 1 km around the plant location. The PGMEA
plume distributed significantly on the north and east sides as seen in Figure 4-4 (A). In May, the highest monthly average concentration of PGMEA was 0.369 mg/m³, and was observed at the location of 0.2 km from the source (Table 4-1). Also, the pollutant dispersed in all directions, especially in the northwest direction as seen in Figure 4-4 (B). For the July month, the maximum monthly concentration was 0.671 mg/m³ at the distance of 0.2 km from the source. As displayed in Figure 4-4 (C), the plume dispersed significantly toward the northwest and northeast directions. Table 4-1 shows maximum monthly average concentration of PGMEA obtained in the month of September reached 0.423 mg/m³ within 2 km northeast of the source. The dispersion of PGMEA was heading drastically in the south and northeast direction as presented in Figure 4-4 (D), thus affecting people in that area.

In light of the above results, the monthly average concentrations of PGMEA for all four periods - January, May, July, and September - are considered under the allowable limit and do not pose any health symptoms (Table 4-1).

For Hickson’s study case, Tables 4-2 illustrates the highest monthly average concentrations of (CH₃)₂S, and the coordinates for the 90% removal efficiency of pollutants for the four modeling periods.

<table>
<thead>
<tr>
<th>Modeling Period</th>
<th>Highest Average Monthly Concentration (mg/m³)</th>
<th>Coordinates (Km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>January</td>
<td>5.57</td>
<td>2.5, 1</td>
</tr>
<tr>
<td>May</td>
<td>23.6</td>
<td>2.0, 2</td>
</tr>
<tr>
<td>July</td>
<td>22.1</td>
<td>1.5, 0.2</td>
</tr>
<tr>
<td>September</td>
<td>13.5</td>
<td>2.5, 0.2</td>
</tr>
</tbody>
</table>
The highest monthly average concentration of \((\text{CH}_3)_2\text{S}\) in January was 5.57 mg/m\(^3\) as seen in Table 4-2, occurring at the location of 2.5 km east of the plant. The pollutant plume dispersed pointedly on the north and east sides as shown in Figure 4-5 (A). In May, the highest monthly concentration of \((\text{CH}_3)_2\text{S}\) was found to be 23.6 mg/m\(^3\), and was observed at a coordinate 1.5 km from the source (Table 4-2). The pollutants accumulated around the source as shown in Figure 4-5 (B). The highest average concentration for the entire month of July was 22.1 mg/m\(^3\) at distance
1.5 km from the plant location, and the plume dispersed around the source as shown in Figure 4-5 (C). Table 4-2 shows the highest monthly average concentration of \((\text{CH}_3)_2\text{S}\) obtained in September 2013, as shown in Table 4-2, reached 13.5 mg/m\(^3\) within 2.5 km south of the source. The dispersion of \((\text{CH}_3)_2\text{S}\) was heading in the northeast and south directions as indicated in Figure 4-5 (D).

The highest monthly average concentration of \((\text{CH}_3)_2\text{S}\) for all periods are between 13.5 to 23.6 mg/m\(^3\). According to (Table 3-2), no health symptoms are associated with this range of concentration values.

### 4.2 Meteorological Condition Effects

#### 4.2.1 Steady state conditions

Analysis on the effect of climatic parameters including mixing height, ambient temperature, atmospheric stability class, wind speed, and wind direction on dispersion of accidental releases from a biofilter was carried out in this research. Air dispersion models (steady-state models such as Gaussian, and SCREEN3 or non-steady state such as CALPUFF) can determine the impact of these parameters on the downwind pollutant concentration and discover the dominant ones. However, the Gaussian and SCREEN3 models only allow investigating the effect of wind speed and stability classes on the concentration because of the limitations on the available climatic parameters that can be used as input in these models. In this part, an investigation was conducted under steady-state meteorological conditions by varying one
climatic parameter while maintaining other parameters fixed to detect the changing of the model’s output depending on the alteration of this parameter.

4.1.1 Wind Speed

The wind speed is considered a primary factor in odor dispersion and as the most climatic element that could affect the level of pollutant concentration in the atmosphere. The influence of wind speed on the pollutant concentration is shown in Figure 4-6. Series of runs were conducted under different wind speeds, which are 2, 4, 6, 8, and 10 m/s under neutral atmospheric stability (for Gaussian and SCREEN3 models), at a constant temperature of 293 K, a wind direction of 280 degree, mixing height of 200 m, and a pressure of 988 mb (for the CALPUFF model). Figure 4-6 shows that the highest level of PGMEA was obtained when the wind speed was 2 m/s, and the lowest observed was with a wind speed of 10 m/s for all three models. This result shows an agreement with the theory, which says there is a reverse relationship between the wind speed and pollutant concentration. As the wind speed increases, the concentration decreases because of the turbulence that is linked with wind speed, and which leads to a dilution of pollutants into the ambient air (Kgabi et al. 2009, De Nevers, N. 1995)
4.1.2 Atmospheric stability class

Atmospheric stability is the atmosphere tendency to suppress or boost vertical motion and hence turbulence. Generally, it can be categorized to stable, unstable, or neutral, which are calculated depending on the knowledge of the wind speed, solar radiation, and cloud coverage as developed by Pasquill in 1961. Atmospheric stability was classified to very unstable (A), unstable (B), slightly unstable (C), neutral (D), stable (E), and slightly stable (F). To study the effect of stability classes on the pollutant dispersion, the maximum PGMEA concentration was examined under these six stability classes. Here, wind speed was set to 2 m/s (for all models), the temperature to 293 K, the wind direction to 280 degree and the pressure to 988 mb as shown in Table 3-8. Figure 4-7 presents the average maximum PGMEA concentration at these stability classes using three models (Gaussian, SCREEN3, and CALPUFF). As seen in Figure 4-7, the concentration of the PGMEA pollutant obtained from SCREEN3 under the unstable atmospheric
conditions (A, B, and C) was less than neutral and stable conditions by 72% and 92%, respectively. The CALPUFF model shows similar observations; the stable and neutral conditions yield a higher downwind concentration of PGMEA pollutant than unstable conditions by 132% and 78%, respectively. These results seem to fit with a hypothesis that the mechanical turbulence resulting from strong winds in unstable conditions lead to increased dispersion and yields low pollutant levels (Guo et al 2006). However, the results from the Gaussian model were the opposite of other models. In three unstable conditions (A, B and C), the highest obtained level of PGMEA reached 5.3, 9.4, and 8.6 mg/m³, respectively. They are higher than neutral and stable conditions by 70% and 99%, respectively. This result goes against the fact that the neutral and stable atmosphere discourages the dispersion of pollutants and increases their ground level concentration due to their minimal atmospheric turbulence (Guo et al 2006, Alessandro D 2005). The possible reason behind this is because the Gaussian model cannot predict the concentration under stable conditions E and F as the observations have a skewed distribution (shown in Figure A-1), which is in contrast to the fundamental assumption of the Gaussian model. Zhu (1999) reported a similar observation when he used the INPUFF-2 model based on the Gaussian model theory to study the effects of stability classes on the performance of air dispersion models to predict agricultural odor transport. He concluded that the stability classes E and F are not suitable for use in the Gaussian models to predict agricultural (a short transport) odor.
Figure 4-7: Maximum PGMEA concentration vs. stability class (1) A, (2) B, (3) C, (4) D, (5) E, (6) F

4.1.3 Wind direction

To study the effect of wind direction on concentration, we used the CALPUFF model because this option is only available in CALPUFF model. The maximum concentration of PGMEA was obtained when the wind direction was set to the following values of 360 (N), 310 (NW), 220 (SW), 180 (S), 140 (SE), and 50 (NE) degrees, while the temperature, wind speed, and pressure were kept constant at 298 K, 6 m/s, 988 mb, respectively. As shown in Figure 4-8, it is difficult to determine the relationship between the pollutant concentration and wind direction variables since the result is not linear and is displayed in a random pattern.
4.1.4 Temperature

The CALPUFF model was conducted on different temperatures including 270, 285, 298, and 308 K. As shown in Figure 4-9, no change in PGMEA concentration occurs when the temperature changes from 270 to 308 K, which indicates that temperature has no impact on pollutant concentration for the range of temperature considered.
4.2.5 Mixing height

Mixing height is the height of a close layer of atmosphere to the ground where mechanical or turbulent mixing of air takes place. The CALPUFF model was conducted to analyze the effect of this factor on pollutant concentration. Mixing height was set to values of 100, 500, 1000, 1500, and 2000 m, and where other factors were not changed, wind speed was kept at 2 m/s, ambient temperature at 298 K, pressure at 988 mb, and the selected wind direction was 280 degree. The simulation outputs show that the mixing height has no influence on the CALPUFF model predictions as shown in Figure 4-10. That may be because the accidental releases from the biofilter generally have a low concentration, compared to emissions from industrial plants that release directly into atmosphere with high concentration, which therefore, are likely to be transported just a few meters above the ground.

![Graph](image)

*Figure 4-10: The effect of mixing height on modeled maximum PGMEA concentration*
4.2.2 Variable meteorological conditions

CALPUFF model can simulate the effect of varying spatial and temporal meteorological conditions on pollutant concentration, transport, transformation, and removal, thus CALPUFF was used to examine the PGMEA concentration under variables weather conditions. The CALPUFF model was performed for the three modeling periods, which are January 15, 2013 from 0000h to 2300h; May 15, 2013 from 0000h to 2300h; and September 15, 2013 from 0000h to 2300h. Since the area of this study is considered even, the geographic variations in the domain have a slight effect on the wind nature.

Wind field vectors in the model domain for the three periods were examined. During modeling time in January, a significant change in the wind direction and velocity occurred between 1500 and 2300 hours as the wind vectors altered their direction from northeast to south, and that happened specifically at 1500h and 1600h. Likewise, at 2000h, and 2200h the wind vectors traveled in the southwest direction, and during these hours, the speed became calmer and lighter. During the period in May, the wind vectors heading southeast and northeast directions most the time. However, the wind vectors at the early hour of the nighttime were blowing in a northwest direction (0000h). Lastly, on September 15, 2013, a change in wind direction and velocity happened at 1500 and 1600 hours, the wind changed direction from east to the north and west respectively, and the speed of the wind lessened. Table 4-3 illustrates the maximum hourly and daily PGMEA average concentrations for the three modeling periods.
Table 4-3: The highest hourly and daily average concentrations of PGMEA for three modeling periods

<table>
<thead>
<tr>
<th>Modeling Period</th>
<th>Highest Average 1h Conc. (mg/m³)</th>
<th>Time (HH:MM)</th>
<th>Coordinates (Km)</th>
<th>Highest Average 24h Conc. (mg/m³)</th>
<th>Time (HH:MM)</th>
<th>Coordinates (Km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>January 15, 2013</td>
<td>15.4</td>
<td>16:00</td>
<td>1, 0.5</td>
<td>0.776</td>
<td>00:00</td>
<td>2.5, 1</td>
</tr>
<tr>
<td>May 15, 2013</td>
<td>21.14</td>
<td>00:00</td>
<td>1, 0.25</td>
<td>0.964</td>
<td>00:00</td>
<td>2, 0.2</td>
</tr>
<tr>
<td>September 15, 2013</td>
<td>16.1</td>
<td>16:00</td>
<td>0.5, 0.25</td>
<td>1.49</td>
<td>00:00</td>
<td>2.7, 0.2</td>
</tr>
</tbody>
</table>

The maximum hourly average concentration of PGMEA on January 15, 2013 was 15.4 mg/m³ as displayed in Table 4-3. The wind speed of the observed concentration time was 2.10 m/s, which is used along with the B atmospheric stability class and considered as an unstable condition. As mentioned before, there is a reverse relationship between the wind speed and pollutant concentration. The concentration decreases while the wind speed increases due to the dilution effect by the ambient air. The contour plot of wind field vectors and highest hourly average concentration of PGMEA on January 15, 2013 at 1600h is shown in Figure 4-11. This figure displays that the plume of PGMEA emission distributed in the direction of wind toward the south, affected the residents existing in that area. Furthermore, the maximum daily average concentration of PGMEA on this date was 0.776 mg/m³ as shown in Table 4-3, occurring at the location of 2.5 km around the plant location. The PGMEA plume distributed sharply on the north and east sides as seen in Figure 4-12.
Figure 4-11: The wind field vectors and the maximum hourly average (PGMEA) concentration on January 15, 2013 at 1600h

Figure 4-12: The wind field vectors and the maximum daily average (PGMEA) concentration on January 15, 2013
On May 15, 2013, the maximum 1h average concentration at each receptor in the domain was 21.1 mg/m³, which estimated at 0000 h in the distance of 1 km of the point source in Table 4-3. The wind velocity in this hour was 2.2 m/s, which is used along with the D atmospheric stability class and is considered a Neutral condition. The contour and the hourly average concentration of PGMEA are shown in Figure 4-13. This Figure explains the plume distribution at 0000h of this day headed in the same wind direction to the northwest. On the other hand, the highest 24h average concentration of PGMEA was 0.97 mg/m³, and observed at the location of 0.5 km from the source (Table 4-3), and the pollutant dispersed in all directions, except the southwest as seen in Figure 4-14.

Figure 4-13: The wind field vectors and the maximum hourly average (PGMEA) concentration on May 15, 2013 at 0000h
Table 4-3 shows the maximum hourly concentration of PGMEA obtained at 1600h on September 15, 2013, was 16.1 mg/m$^3$ at a distance of 0.5 km from the source. Although the hourly concentration during the September period is close to that of January, the plume dispersion in these two periods is different. As seen in Figure 4-15, the pollutant accumulated around the source at 1600h because of the stable atmospheric condition at that hour (based on stability classes table and Figure 4-15). The maximum 24-h average concentration of PGMEA was obtained in the middle of September 2013, as shown in Table 4-3, and it reached 1.49 mg/m$^3$ within 1.5 km northeast and 1.5 km southwest of the source. The dispersion of PGMEA was heading toward the southwestern direction as elucidated in Figure 4-16, hence affecting people in that region.
Figure 4-15: The wind field vectors and the maximum hourly average (PGMEA) concentration on September 15, 2013.

Figure 4-16: The wind field vectors and the maximum daily average (PGMEA) concentration on September 15, 2013.
4.3 The Effect of Stack Height and Building Downwash:

4.3.1 Building downwash

Since some biofilters could be installed in urban areas as in the Toronto case study, the obstacle or building’s effect on pollutant concentration should be examined. The CALPUFF and SCREEN3 models were applied to simulate this effect. Figure 4-17 exhibits that when using the CALPUFF model, the concentration of PGMEA is higher in the presence of buildings seven times more than without buildings (3.44 mg/m$^3$ and 0.493 mg/m$^3$), when we assume there are five buildings around the source with height between 30 and 45 m. Also, the SCREEN3 model displays a marked increase in PGMEA concentration when we assume a building with a height of 45 m is close to the source. The possible reason behind that, is because buildings or other solid structures could have an impact on the flow of air near a source and may produce regions of robust turbulence and eddies on the downwind side of a building, which is known as building downwash.

![Figure 4-17: Modeled maximum PGMEA concentration vs. building presence around the Source](image)

Figure 4-17: Modeled maximum PGMEA concentration vs. building presence around the Source
4.3.2 Stack height effect

To study the effect of stack height on pollutant concentration, we chose Hickson’s case study as an example. As shown in Figure 4-18, the heights of the stack were chosen to be 15, 25, and 35 m and two dispersion models were chosen to conduct this analysis. The results from both dispersion models confirm that there is reverse relationship between stack height and observed concentration, which may be because the effective plume rise is enhanced with an increase of the stack height that stimulates the buoyancy produced dispersion.

Figure 4-18: Modeled maximum PGMEA concentration vs. biofilter stack height

4.4 Relationship Between Biofilter Performance and Concentration and the Health Effects

As formerly cited in this thesis, any deficiency of biofilter parameters could cause an inadequacy in biofilter performance and hence more release of pollutants into the atmosphere. The CALPUFF model has been used to predict the concentration of pollutant, assuming that the
removal efficiency of the biofilter declined to 50% and 20%. In order to evaluate the health effects on the individuals who reside around the biofilter location; the domain of both study cases was selected to be 25 by 25 km of the source, with the source at the center of this area.

4.4.1 Toronto case study

The location of the plant in this case study is the Greater Toronto Area, which is defined as the central city of Toronto with a population of 6,054,191 according to the 2011 census of Canada. Since the monthly concentration of July was higher than other months for this case study (Table 4-1), we chose this month to conduct this analysis and to evaluate the maximum health concerns that could be associated with it.

Table 4-4: The highest hourly, daily, and monthly average concentrations of PGMEA for 20, and 50% removal efficiency of biofilter.

<table>
<thead>
<tr>
<th>Removal Efficiency (%)</th>
<th>Highest Average 1h concentration (mg/m³)</th>
<th>Highest Average 24h concentration (mg/m³)</th>
<th>Highest Average 720h Concentration (mg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>58.1</td>
<td>4.7</td>
<td>1.0</td>
</tr>
<tr>
<td>20</td>
<td>145.0</td>
<td>11.8</td>
<td>2.5</td>
</tr>
</tbody>
</table>

Table 4-4 illustrates the maximum concentrations of PGMEA for average period of 1, 24, and 720 hours in July, when the biofilter removes the pollutant with 50% efficiency. As seen the Table 4-4, the highest average daily and monthly concentration are within the permissible exposure limit of 270 mg/m³, and are not causing any health effects. At 20% removal efficiency of the biofilter, the release of PGMEA increases to the surrounding air, and therefore the concentration will increase. However, because the maximum average daily and monthly concentrations of PGMEA are within the allowed limit exposure, there are no health effects
associated with these concentrations as indicated in Table 3-1.

4.4.2 Hickson case study

The plant of this study is located in Hickson, which is a village in Southwestern Ontario, Canada with a population of around 12,000 according to the 2011 census of Canada. May was selected as a modeling period to assess the health concerns linked to releases of the \((\text{CH}_3)_2\text{S}\) pollutant.

Table 4-5: The highest hourly, daily, and monthly average concentrations of \((\text{CH}_3)_2\text{S}\) for 20, and 50% removal efficiency of biofilter.

<table>
<thead>
<tr>
<th>Removal Efficiency (%)</th>
<th>Highest Average 1h concentration (mg/m³)</th>
<th>Highest Average 24h concentration (mg/m³)</th>
<th>Highest Average 720h Concentration (mg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>1712</td>
<td>231</td>
<td>47.11</td>
</tr>
<tr>
<td>20</td>
<td>4280</td>
<td>578</td>
<td>118</td>
</tr>
</tbody>
</table>

Table 4-5 represents the highest hourly, daily, and monthly concentrations of \((\text{CH}_3)_2\text{S}\) in May, when the biofilter removes the pollutant with 50% efficiency. When the biofilter has 50% removal efficiency, the highest hourly concentration of \((\text{CH}_3)_2\text{S}\) for this month was 1712 mg/m³. According to the United States Environmental Protection Agency (Table 3-2), this hourly concentration exceeded the permissible exposure limit range 25 mg/m³, and may cause serious health issues. Moreover, the highest daily and monthly concentrations, which are 231 and 47.11 respectively, exceeded the permissible exposure limit. The exposure to these concentrations can cause severe inflammation, and necrosis of the eyes, mouth, and respiratory tract. On the other hand, no health symptoms are associated with the highest average monthly concentration of
(CH$_3$)$_2$S for this period, which is considered within the exposure allowed limit. In addition, Table 4-5 represents the highest concentrations of (CH$_3$)$_2$S for the average period of 1, 24, and 720 hours when the biofilter removes the pollutant with 20% efficiency. As indicated in Table 4-5, the exposure to the highest hourly average (CH$_3$)$_2$S concentration, which are predicted to be 4280 mg/m$^3$, increase the risk of death and a coma. Moreover, the highest 24-hour average concentration of (CH$_3$)$_2$S, which was 587 mg/m$^3$, can cause severe damage to the lungs and injuries to the liver, kidneys, heart, and central nervous system. Lastly, the average monthly concentration could cause severe inflammation and necrosis of the eyes, mouth, and respiratory tract, according to the Canadian Council of Ministers of the Environment.

4.5 Comparison Between Dispersion Models Performance

Although air dispersion models have the ability to predicate ground-level pollutant emission from different sources, evaluating the performance of these models is a very important step to guarantee the high accuracy of observations. As we used three dispersion models Gaussian, SCREEN3, and CALPUFF, it is important to compare their performance and outcomes. The Gaussian type models are the most used of the mathematical models to represent the muddled nature of the atmospheric transport and the dispersion of pollutants. However, the accuracy of these models has some limitations. These include the difficulty of satisfying the assumption of the steady state, homogenous atmosphere, and the uncertainty of the source emission rate and plume release parameters (El-Harbawi 2013). Also, the Gaussian equation is unable to estimate the recirculation effects around buildings or at crossroads. Furthermore, this type of model is only designed to simulate the dispersion under high wind conditions or at
locations far from the source (i.e. distances greater than 100m). While the SCREEN3 model overcomes the limitations of the Gaussian model, however this model cannot determine the maximum concentration from multiple sources. On the other hand, The CALPUFF model is considered to be more accurate model because it can handle low wind speed cases, stagnation, coastal, complex terrain and flow reversals. Figure 4-19 illustrates the difference of the Gaussian and SCREEN3 results to the CALPUFF model for Hickson case study. The percentage differences between the Gaussian and CALPUFF predictions several thousand fold higher. Since the % differences between models are very high, selection of one of these models to estimate the accidental emission from a biofilter requires model comparison with biofilter field measurements, which may be collected by using field olfactometer.

![Figure 4-19](image)

**Figure 4-19:** differences (%) on \((\text{CH}_3)_2\text{S}\) concentration between Gaussian and SCREEN3 models to the CALPUFF model
Chapter 5

Conclusions and Future Work

The following conclusions can be drawn from this study:

1) Accidental releases from a biofilter, especially at low removal efficiency, can yield high concentration of pollutants, which can cause serious health problems.

2) Wind speed and atmospheric stability classes are the main factors affecting the pollutant dispersion and concentration; however, not all the models considered present the same reaction to the stability factor. When using the Gaussian model, PGMEA concentration was higher in unstable conditions rather than stable, and that does not correspond with the fact that stable weather has minimal turbulence, and therefore increases the level of pollutant concentration.

3) Although the wind direction has a direct impact on the pollutant plume path, for the wind direction range considered, no evidence in the observed results shows the relationship between the wind direction and the maximum concentration (randomly distributed).

4) For the range of temperature and mixing height considered, neither temperature nor mixing height has an impact on the maximum concentration.

5) As expected, both the stack height of the biofilter, and presence of buildings have an effect on the pollutant concentration where the increase in the stack height of biofilter decreases the concentration, while the presence of buildings can increase the concentration of pollutant.
For future work, it is recommended to investigate following aspects:

1) Conduct sensitively analysis to examine the accuracy of models by comparing the results to the actual plume measurements in the field.

2) As the dispersion models prove their validity to apply on biofilter systems, the same can be applied to investigate failure of other air pollution control systems such as bioscrubbers, and biotrickling filters.

For future installation of biofilters in industrial sites, it is recommended to:

1) Install biofilters away from buildings and residential areas to protect people from the effects of building downwash and serious health effects.

2) Construct the biofilters on elevated places to increase the dilution of pollutants, and therefore, decrease the health effects of accidental emissions from biofilters.

3) In any regulatory permitting process for biofilter installations, accidental release should be considered. Biofilters should have secondary units such as activated carbon bed as polishing unit to avoid any unexpected release.
Appendix A

To calculate sigma y and z, we used the following formulas (Caraway):

\[
\sigma_y = cx^b \\
\sigma_z = ax^d
\]

Where \( x \) is the downwind distance from the source.

The \( b \) & \( c \) values were obtained from the following table (Caraway):

<table>
<thead>
<tr>
<th>Stability Class</th>
<th>Downwind Distance in meters ( x &lt; 10,000 )</th>
<th>Downwind Distance in meters ( x \geq 10,000 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( C )</td>
<td>( B )</td>
</tr>
<tr>
<td>A</td>
<td>0.495</td>
<td>0.873</td>
</tr>
<tr>
<td>B</td>
<td>0.310</td>
<td>0.897</td>
</tr>
<tr>
<td>C</td>
<td>0.197</td>
<td>0.908</td>
</tr>
<tr>
<td>D</td>
<td>0.122</td>
<td>0.916</td>
</tr>
<tr>
<td>E</td>
<td>0.0934</td>
<td>0.912</td>
</tr>
<tr>
<td>F</td>
<td>0.0625</td>
<td>0.911</td>
</tr>
</tbody>
</table>
The a & d values were obtained from the following table (Caraway):

Table A-2: Power law exponents and coefficients for sigma z

<table>
<thead>
<tr>
<th>Stability Class</th>
<th>100 &lt; x ≤ 500</th>
<th>500 &lt; x ≤ 5000</th>
<th>5000 &lt; x</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>a</td>
<td>B</td>
<td>A</td>
</tr>
<tr>
<td>A</td>
<td>0.0393</td>
<td>1.281</td>
<td>0.0002539</td>
</tr>
<tr>
<td>B</td>
<td>0.1393</td>
<td>0.9467</td>
<td>0.04936</td>
</tr>
<tr>
<td>C</td>
<td>0.112</td>
<td>0.91</td>
<td>0.1014</td>
</tr>
<tr>
<td>D</td>
<td>0.0856</td>
<td>0.865</td>
<td>0.2591</td>
</tr>
<tr>
<td>E</td>
<td>0.1094</td>
<td>0.7657</td>
<td>0.2452</td>
</tr>
<tr>
<td>F</td>
<td>0.05645</td>
<td>0.805</td>
<td>0.193</td>
</tr>
</tbody>
</table>

Here are the calculated sigma y and z values that were used in Gaussian model:

Table A-3: The values of sigma y and z

<table>
<thead>
<tr>
<th>Downwind Distance (x)</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Sigma y</td>
<td>Sigma z</td>
<td>Sigma y</td>
<td>Sigma z</td>
<td>Sigma y</td>
<td>Sigma z</td>
</tr>
<tr>
<td>350</td>
<td>82</td>
<td>70</td>
<td>59</td>
<td>36</td>
<td>40</td>
<td>23</td>
</tr>
<tr>
<td>600</td>
<td>132</td>
<td>162</td>
<td>96</td>
<td>61</td>
<td>66</td>
<td>38</td>
</tr>
<tr>
<td>1000</td>
<td>206</td>
<td>470</td>
<td>152</td>
<td>108</td>
<td>104</td>
<td>61</td>
</tr>
<tr>
<td>2000</td>
<td>377</td>
<td>1998</td>
<td>283</td>
<td>235</td>
<td>196</td>
<td>116</td>
</tr>
<tr>
<td>3500</td>
<td>615</td>
<td>6430</td>
<td>468</td>
<td>438</td>
<td>325</td>
<td>194</td>
</tr>
<tr>
<td>5000</td>
<td>839</td>
<td>13546</td>
<td>645</td>
<td>652</td>
<td>450</td>
<td>270</td>
</tr>
</tbody>
</table>
Figure A-1: Maximum PGMEA concentration vs. downwind distance (m) at different wind speed using Gaussian model
Figure A-2: Maximum PGMEA concentration vs. downwind distance (m) at different stability classes using Gaussian model
Figure A-3: Maximum PGMEA concentration vs. downwind distance (m) at different wind speed using SCREEN3 model, (1- 2 m/s, 2- 4 m/s, 3- 6 m/s, 4- 8 m/s, 5- 10 m/s).
Figure A-4: Maximum PGMEA concentration vs. downwind distance (m) at different stability classes using SCREEN3 model, (1-A, 2-B, 3-C, 4-D, 5-E, 6-F).
Figure A-5: The contour plots of maximum PGMEA concentration at different wind speed using CALPUFF model, (1- 2 m/s, 2- 4 m/s, 3- 6 m/s, 4- 8 m/s, 5- 10 m/s).
Figure A-6: The contour plots of maximum PGMEA concentration at different stability classes using CALPUFF model, (1- A, 2- B, 3- C, 4- D, 5- E, 6- F).
Figure A-7: The contour plots of maximum PGMEA concentration at different wind direction using CALPUFF model, (1-360, 2-50, 3-140, 4-180, 5-220, 6-310).
Figure A- 8: The contour plots of maximum PGMEA concentration at different Temperature using CALPUFF model, (1- 270, 2- 285, 3- 298, 4- 308).
Figure A-9: The contour plots of maximum PGMEA concentration at different Mixing Height using CALPUFF model (1- 100, 2- 500, 3- 1000, 4- 1500, 5- 2000)
Journal papers submitted:


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