Air Force Institute of Technology

AFIT Scholar

3-2005

Optimal Sampling of a Chemical Hazard Area

Jennifer R. Plourde

OPTIMAL SAMPLING OF A CHEMICAL HAZARD AREA

THESIS

Jennifer R. Plourde, 2d Lt, USAF

AFIT/GOR/ENS/05-15

DEPARTMENT OF THE AIR FORCE
AIR UNIVERSITY

AIR FORCE INSTITUTE OF TECHNOLOGY

Wright-Patterson Air Force Base, Ohio

APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED.

OPTIMAL SAMPLING OF A CHEMICAL
HAZARD AREA

THESIS
Jennifer R. Plourde
2d Lt, USAF

AFIT/GOR/ENS/05-15

AFIT/GOR/ENS/05-15

OPTIMAL SAMPLING OF A CHEMICAL HAZARD AREA

THESIS

Presented to the Faculty

Department of Operational Sciences

Graduate School of Engineering and Management

Air Force Institute of Technology

Air University

Air Education and Training Command

in Partial Fulfillment of the Requirements for the

Degree of Master of Science in Operations Research

Jennifer R. Plourde, B.S.

2d Lt, USAF

March 2005

OPTIMAL SAMPLING OF A CHEMICAL HAZARD AREA

Jennifer R. Plourde, B.S.

2d Lt, USAF

Approved:

Dr. Jeffrey P. Kharoufeh	Date
Thesis Advisor	

Dr. James Moore	Date
Committee Member	

Abstract

This thesis proposes a methodology for optimally sampling a chemical hazard area subsequent to a chemical weapons attack. The objective is to identify the maximum number of areas that no longer require protective gear for safe operations. We model the area as an undirected graph and employ network analysis techniques to provide a methodological framework for identifying an optimal sampling sequence within a fixed time limit. We propose four models that characterize the secondary vapor concentrations: i) static and deterministic, ii) static and stochastic, iii) dynamic and deterministic, and iv) dynamic and stochastic. Comparisons of the static cases and their dynamic counterparts demonstrate the impact of temporal evolution of vapor concentrations on the optimal sampling path. We conclude that the number of safe areas may be either under- or over-estimated depending on the assumed nature of the secondary vapors.

Acknowledgements

Table of Contents

List of Figures

List of Tables

OPTIMAL SAMPLING OF A CHEMICAL

HAZARD AREA

1. Introduction

1.1 Background

The willingness of contemporary terrorist organizations to use asymmetric measures against their adversaries suggests the need for defending U.S. military installations and interests against chemical or biological attacks. According to [6], chemical and biological weapons (CBWs) are considered to be weapons of mass destruction (WMD) because they are capable of "high order destruction and/or of being used in such manner as to destroy large numbers of people." The devastation CBWs may cause, and the ease with which they may now be developed, stored, and transported has made protecting against them a primary concern for military installations. In the event of an attack on any United States military installation or interest, a method for identifying the most hazardous areas is required to protect human life and to restore operations to full capability as soon as possible.

The terrorist attacks on the United States on September 11, 2001 have dramatically altered the views of the American public and militaries. As noted in [6], the threats to U.S. targets, military combat personnel, and American military installations in foreign countries are very credible. However, steps have been taken to reduce the threat of chemical or biological attacks on groups or nations. The Chemical Weapons Convention (CWC) in 1997, and Biological Weapons Convention (BWC) were "adopted to stifle proliferation of chemical and biological weapons." However, there are shortcomings with the treaties. They do not focus on the small quantities that a terrorist group may employ, but on the large developmental pro-

grams of entire nations. Also, they do not regulate "dual use" items or chemicals such as Toxic Industrial Chemicals (TICs) that can double as weapons. These include chemicals such as methyl isocynate which was used in Bhopal, India (Dec 1984) that are not included in the schedules of chemicals listed in the CWC [6]. Due to these shortcomings, emergency response and assessment teams must be prepared to act following an attack.

The Department of Defense Chemical, Biological, Radiological, and Nuclear Defense Program (CBRNDP) Annual Report to Congress dated May 2004 [5] contains significant literature on the continuing need to defend against weapons of mass destruction (WMD) today. Among several other topics, the report includes information from an unclassified CIA report to Congress concerning the acquisition of technology that relates to WMD and advanced conventional munitions which states current threats to the United States and its assets. It also focuses on contamination avoidance as well as improving the individual protective equipment for the personnel who may be exposed to contamination.

According to the CBRNDP report, the CIA has provided evidence that several countries have an active interest in WMD. These countries include Iran, Iraq, North Korea, Libya, Syria, Sudan, India, and Pakistan and some of the key supplier countries are reported to be Russia, China, and North Korea. Disturbingly, many of the 33 "designated terrorist organizations" and other non-state actors across the world have shown interest in CBRN [5]. With all of these countries and organizations expressing interest in WMD, it is prudent for the U.S. to be concerned with defending against these weapons and to develop strategic policies that can be implemented in the event of such an attack to protect human life and to restore hazardous areas to full operational capabilities as quickly as possible.

Subsequent to a successful chemical attack on any fixed operational site, miliary or otherwise, vapor contamination can hinder operations for possibly a significant amount of time. The contamination results from persistent chemical agents that

deposit on various surfaces and then evaporate into the air, creating a hazardous vapor cloud. Atmospheric conditions may then cause this cloud to travel to parts of the site that may not have been directly hit and cause contamination, threatening the health of personnel in the area as well as their productivity. Decision makers must determine the level of mission-oriented protective posture (MOPP) for personnel in various work areas. The protective gear donned by personnel in (potentially) infected areas can be cumbersome and cause heat stress; therefore, commanders must take into account the specific threat, environmental conditions that affect the evaporation rates, work rates, the level of task difficulty, and mission requirements when deciding the appropriate MOPP level at any point in time following a chemical attack.

It is imperative to identify the areas of the site which can safely return to full operational capabilities as soon as possible. Knowing which areas of the site crews should sample first in order to identify where gear is (or is not) required is essential to restoring the site to full capabilities. At each sampled area, instrument readings must be obtained so that secondary vapor concentrations may be assessed.

Developing a strategy for prioritizing the areas to be searched that identifies the maximum number of areas in their optimal level of safety is the focus of this thesis. That is, by carefully choosing which areas to search to obtain actual vapor readings, a maximum number of areas can be reached within an allotted time while only searching those that are "critical." Critical areas are identified as those where the vapor concentration level has decreased below a fixed threshold that dictates the need for protective gear.

The basic problem can be viewed as a set covering problem. There exists a set of areas that need to be reached from some starting location while minimizing (or maximizing) some quantity. In this case, we seek to cover the maximum number of areas where protective gear is not required. This problem increases in complexity due to the addition of constraints, specifically a time constraint, forcing a feasible solution to the real world problem to satisfy these time restrictions. For example,

the solution must be a path through the site that does not allow subtours (disjoint paths) where the crew cannot move from one path to another.

The approach used in this thesis has not been previously applied to a problem considering the identification of secondary vapor contamination to an operational site subsequent to a chemical weapon attack. We model this problem as a network and employ operations research techniques to solve it. This approach also addresses the spatial and temporal dynamics of the real problem by incorporating them into the model. Though extensive research has been ongoing for defending against a chemical weapons attack, we focus our attention on obtaining a policy for the full restoration of operational capabilities as soon as possible should a chemical attack occur.

1.2   Problem Definition and Methodology

This thesis is primarily concerned with the development of a methodology for incorporating available vapor level data to "intelligently" assess the actual threat to personnel in areas throughout a fixed military installation. Thus, the problem of optimally sampling a chemical hazard area is our focus.

The dynamics of the problem may be described as follows. Following a chemical attack, detectors such as M-8 or M-9 paper are available for reading. They contribute a "yes" or "no" response as to whether or not a liquid drop of chemical has touched the paper. As the liquid begins to evaporate and enter the atmosphere, the wind carries it downstream and begins to disperse the hazardous vapors to other areas. Additionally, as time progresses, the concentration of the vapors begins to diminish and some areas may become safer. It is important to know when the areas begin to return to normal so that personnel may return to normal operations. Thus, methods for searching the site, with the objective of identifying the areas with a vapor concentration below a specific threshold, are considered.

This problem displays characteristics of several well-known problems. Part of the objective is the same as for the Travelling Salesperson Problem (TSP), where we seek to minimize the time to reach all cities on a tour. However, for this problem, the "salesperson" has a fixed amount of time to reach all of his or her destinations. Thus, it is possible that not all "cities" will be reached. Also we seek to maximize the reward for visiting "cities" and the "salesperson" does not have to return to the starting location.

Another well-known network problem similar to the one addressed here is the shortest path problem (SPP). The entity in the shortest path problem must find the path of minimum length (or time) from a starting location (source) to a specified destination (sink). Our problem strays from the SPP because we do not have a distinct sink node and we impose an upper bound on the length (time) of any path in our problem. It also varies from the SPP because we seek to sample as many areas as possible rather than simply finding a path of shortest length. There is a reward associated with reaching a node in our problem which is not necessarily included in the standard SPP.

This problem can also be viewed as a knapsack problem where a fixed amount of resource is available for use in maximizing the objective. In our problem, the resource is time, and we seek to maximize the reward. Contrary to the knapsack problem, the order in which the items are placed in the "knapsack" is important.

Since we seek to reach all the nodes, if possible, this problem shares a similarity with the minimum spanning tree problem. However, in the minimum spanning tree, each node must be connected but they may not form a connected path through the network. We seek a path that can be followed from beginning to end without reaching a dead end or becoming stuck in a cycle.

It is clear the problem of this thesis shares characteristics with several well-known optimization problems. However, new methodologies must be developed to

solve this particular problem. The proposed methodology incorporates aspects of each of those problems, but will be distinct from them in its formulation.

Our main contribution to the operations research literature is an optimal sampling procedure for a single crew to assess the current threat level at a fixed operational site in order to reduce MOPP levels as quickly as possible. We consider four distinct cases of this problem. First, we consider the case where vapor concentration levels are static and deterministic. Next, we assume the vapor concentrations evolve temporally, but remain deterministic. Third, we consider stationary probability distributions for the vapor concentrations and finally, we consider the case in which vapor concentrations evolve according to a time-variant probability distribution in each area. The methodologies as stated are progressively more complex. The ultimate solution is a time-adaptive policy directing the search crew through the site to maximize the number of areas identified to have vapor concentrations below the threshold. Thus, the maximum number of areas have fully restored operational capabilities.

1.3 Thesis Outline

Chapter 2 examines current literature in the areas of the ongoing threat of biological and chemical weapons to U.S. installations, domestic and foreign, as well as U.S. interests, and steps taken to defend against such an attack. Methodologies for formulating and solving problems, such as the one in this thesis, are also examined and discussed. In chapter 3, we formally define the problem and provide a mathematical programming formulation for each of the cases mentioned above. The first section describes the network model definitions and the second section states the model assumptions and defines each of the four cases. Chapter 4 presents numerical illustrations for each of the four cases and compares the results of the static cases with their dynamic counterparts. Finally, Chapter 5 provides some concluding remarks, recommendations, and directions for extensions and future research.

2. Relevant Literature

This chapter reviews relevant contributions to the area of emergency response subsequent to a biological or chemical attack, and a review of literature on network problems. Specifically, literature regarding stochastic, time-varying networks, time-adaptive route choice problems, and shortest path problems are reviewed.

2.1 Some Historical Perspectives

The use of *biological* weapons is not a modern idea. It has existed since 600 B.C. when the Athenians were known to contaminate rivers with skunk cabbage to incapacitate their enemies with a violent sickness [2]. During the 1300s, Tartarians utilized corpses infected with the plague by catapulting them over the city walls of Kaffa, possibly beginning the Black Death [19] and in America, blankets contaminated with smallpox were distributed to some Native American tribes in the 1700s [19]. Most recently, the 2001 introduction of Anthrax into the United States Postal Service reminded the American government and domestic population just how serious biological weapons are [20] and that they are a contemporary threat.

The first known manufactured *chemical* weapons date back to 1823 when mustard gas (levinstein mustard) was first synthesized. The first use of a chemical weapon dates back to 1914 when mustard gas was used during World War I by German forces [10]. More recently, the 1995 attack on a Tokyo subway by a Japanese cult employed sarin nerve gas killing twelve people and injuring thousands [3]. More notably, in March 1998, the Iraqi government used a "cocktail" of at least four chemical weapons (mustard gas, sarin, tabun, and VX) on Halabja, killing more than 5,000 individuals [7].

It is evident that, throughout history, both chemical and biological weapons have wreaked havoc on nations and communities. Currently, concerns about chemical weapons development and use are elevating for governments worldwide due to

scientific and technological advancements and the ease with which they can be obtained by adversaries and terrorists [6]. Today, they can be manufactured in the same factories that industrial or agricultural chemicals are made. Contemporary chemical weapons are easy to store as a liquid, which can be dispersed in vapor form (type of gas), or as an aerosol, (suspension of tiny liquid or solid particles in a gas) [15]. Chemical and biological weapons can be created using minimal technology; thus making them available to any terrorist group, country, or state who desires them. Advanced nations can produce more elaborate weapons with the use of chemical engineering, pharmaceutical, or biotechnology industries. More importantly, the globalization of these industries, scientific engineering, and technical personnel exchanges, have made sharing information much easier leading to even easier access to chemical and biological technology [6].

Contemporary terrorist groups are willing to use asymmetric measures to accomplish their goals, and therefore, threaten the use of chemical or biological weapons. Due to the absence of dominating global powers other than the United States, the threat is very real and alarming. Thus, chemical and biological defense has received much attention, especially the development of chemical sensors and instruments for detecting and quantifying chemical vapors. Other areas of focus include the development of emergency response strategies for affected regions and individuals, and restoration of a site subsequent to a chemical or biological attack.

2.2   Current and Developing Research Areas

The Department of Defense Chemical, Biological, Radiological, and Nuclear Defense Program (CBRNDP) Annual Report to Congress from May 2004 [5] stresses contamination avoidance including reconnaissance, detection, and identification. If a chemical agent release is unavoidable, these three areas are key to ensuring forces in the affected area assume the optimal level of mission oriented protective posture (MOPP) to sustain operations and restore military installations to full operational

capabilities as soon as possible. Currently, advanced technologies are being developed for chemical and biological standoff detection, early warning detection, miniaturization, and interconnectivity. There are other areas also receiving attention such as enhancements in detection sensitivity, interference rejection, logistics supportability, and affordability [5].

The CBRNDP report [5] states that contamination avoidance seeks "to provide a real-time capability to detect, identify, characterize, quantify, locate, and warn against all known or validated CBRN warfare agent hazards." The optimization of sensor technologies is being researched to meet near-term goals. Mid-term goals focus on developing improved tactical detection and identification capabilities for both chemical and biological warfare agents. The focus of far-term efforts is on multi-agent sensors for CBRN agent detection and remote/early warning CBRN detection. According to the CBRNDP Annual Report to Congress (2004), the goal of contamination avoidance is "direct integration of CBRN detectors as a single system into various platforms linked into command, control, communication, computer, and intelligence (C^4I) networks." Improvements in these technologies will ultimately lead to better detection of chemical agents and secondary vapors contaminating sites, making it easier to identify areas of the site that are operating in their optimal level of MOPP.

Focus in the area of contamination avoidance has several potential payoffs. CBRN detection systems to be developed will "provide the capability to detect, identify in real time, map, quantify, and track all known CBRN contamination in a theater or operations." Acquiring these capabilities will enable commanders of a targeted site to avoid contamination, determine the need for (and verification of) effective reconstitution procedures, as well as assume optimal protection that will enable sustainment of the mission and continuance of fighting with minimal performance degradation and casualties. An important payoff of the technologies being developed is in the dual use potential. Occupational Environment Health

Surveillance can use the developed technologies to monitor air pollution, noxious fumes inside enclosed areas, and municipal water supplies.

There exist several major technical challenges for advancing contamination avoidance science and technology. These include biological collection, detection and identification, improved agent discrimination and quantification, sample processing, interferent (i.e., false positive and negative alarms), and ambient biological background rejection. Also, it is challenging to reduce size, weight, and the power requirement for detectors, as well as power generation and consumption, development of integrated biological and chemical detection systems, and fusing sensor data with mapping, imagery, and other data for the near real-time display of events. The discrimination capability of standoff detection for biological materials have been improved in the two years prior to the publication of the 2004 CBRNDP annual report [5]. Clearly, the government recognizes the potential hostile use of biological or chemical WMDs on the domestic United States and/or foreign interests. However, the main focus of the research has been on avoiding CBRN hazards through the development of early detection devices and a warning system. The problem of this thesis focuses on procedures to be employed in the event of an attack that could not be avoided.

Should an attack occur on a military installation or other interest, it is important to have an effective response policy available. To do this, the nature of the weapons released over the site must be understood and the behavior of the released agent (e.g., biological or chemical) must be studied. Thus, an important aspect of studying chemical weapons attacks is understanding the spatial and temporal evolution of the chemical release. Several papers have been written regarding emergency response subsequent to a biological or chemical attack [20], forecast models [17], source release models [13], receptor models, and other topics concerning the behavior of pollution or a released chemical [9].

Extensive research has been conducted on anthrax attacks, specifically with regard to emergency response in populated areas. Wein, Craft, and Kaplan [20] compared various emergency responses to such an attack. They develop a mathematical model consisting of an atmospheric dispersion model, an age-dependent dose-response model, a disease progression model, and a set of spatially distributed two-stage queueing systems consisting of antibiotic distribution and hospital care. The paper covers the response to a biological weapon attack, specifically anthrax, but not a methodology for identifying areas that may become contaminated. They agree that a Gaussian plume model may be "too simplistic to monitor and predict the spatiotemporal anthrax concentrations" following an attack but they use the "downstream" portion with a more sophisticated atmospheric model to capture "atmospheric complexities" that are previously ignored. Thus, they model the evolution of anthrax through space and time but do not provide a methodology for searching an area to identify where people are vulnerable to inhaling potentially deadly spores.

Craft, Wein, and Wilkins [4] understand deterrence is not a reliable strategy for defense against terrorists, but the best security against an attack is in consequence management. That is, how the number of deaths can be minimized after an attack has occurred. Again, the focus is on treating individuals who suffer from anthrax inhalation and not on identifying a policy for searching the area to find where atmospheric conditions have spread the contamination and where time (or atmospheric condition) has reduced the risk of contamination to other areas.

Similar works have been published for the case of smallpox. Kaplan, Craft, and Wein [11] estimate the number of smallpox cases and deaths resulting from an attack in a large urban area. Specifically, they show that mass vaccinations following an attack result in "far fewer deaths and much faster epidemic eradication" than the interim policy of isolating symptomatic cases and performing traced vaccinations with mass vaccinations as a secondary plan if the first is infeasible. Kaplan, Craft, and Wein [12] also evaluate existing and alternative proposals for the emergency

response to a smallpox attack. Like the previously discussed papers, methodology for identifying contaminated areas and areas that are free of contamination is not considered.

Developing an optimal sampling procedure subsequent to a chemical agent release over a fixed operational site, is contingent upon reliable spatiotemporal concentration data. Research in fields such as weather forecasting, receptor models, atmospheric pollution, vapor dispersion, and other such areas is necessary for devising ways to obtain this information. According to Sofiev [17], a "demanding" application of short-term weather forecasting is the real-time emergency modelling of nuclear and chemical hazardous events. The paper presents an operational system developed to create a short-term forecast of potential risk areas, specifically in the event of a nuclear power plant accident. The framework developed in the work displays the capability of addressing inverse problems of working with an unknown source of release. This contribution is highly significant because the source of a chemical agent release is not likely to be known.

Researchers have published substantial works on estimating the source releaserate of atmospheric pollution [14]. Subsequent to a gas release, forecasting the concentration of the gas in the atmosphere depends on the rate and the location of the release. Thus, four distinct cases for a single point source of a released gas have been considered:

1. Instantaneous release from a known location,

2. Instantaneous release from an unknown location,

3. Extended release over a period of time from a known location, and

4. Extended release over a period of time from an unknown location.

According to Kathirgamanathan *et al.* [14], the first case is simple due to just a single parameter requiring estimation. The authors published a previous work [13] for the second case in which they present an inverse model to estimate

the parameters for the model simultaneously. Case three is the focus of [14] where the authors develop an inverse model using methods from groundwater modelling literature and identify factors that affect the accuracy of inverse model prediction. The authors state they will address case four in future papers.

A result of the work for case two in [13], yields the advection-diffusion equation for determining vapor concentration at specific points that we refer to in Chapter 3. This equation is an example of an expression used for determining the chemical concentration at specified points some distance from the point of release at specified times. It is important to note that in the event of a chemical attack, it is unlikely that the amount of chemical release, or the exact location of the release, will ever be known. Thus, even a formal mathematical model for determining the concentrations at points around the attack will have only limited value in discerning the actual concentration at those areas unless a reading is obtained through sensors or some other instrument.

Once methods for obtaining all data are developed, methods for determining optimal sampling procedures must be developed to incorporate real-time information into the methodology. In this thesis, we seek to identify an optimal sampling strategy for searching an area subsequent to a chemical attack. We model the real problem as a network and apply network analysis techniques to determine the optimal solution. Because network models are so critical to our approach to this problem, a review of rudimentary concepts is provided next.

2.3   Network Modelling and Analysis

Ahuja's text [1] provides a foundation for modelling various problems as network flow problems and developing algorithms to solve the models. This text provides the background that is necessary for understanding the models provided in Chapter 3 for determining an optimal sampling strategy.

A specific type of network flow problem important to this thesis is the shortest path problem. According to Ahuja [1], this problem is "perhaps the simplest of all network flow problems." However, that does not diminish the importance of the shortest path problem for our purposes. The objective of the basic problem is to find a path of minimum cost or length from a source node to a sink node where each has an associated cost or length. We seek to identify the shortest time path while simultaneously maximizing a reward (i.e., the number of areas safely operating without protective gear).

The notation of Ahuja [1] refers to a directed network $G = (\mathcal{N}, \mathcal{A})$ where $\mathcal{N}$ is the set of nodes and $\mathcal{A}$ is the set of arcs connecting those nodes. There is an arc length or cost, $c_{i,j}$ associated with each $(i, j) \in \mathcal{A}$. The source node s is where the flow (e.g., vehicle, computer data packet, etc.) originates and the sink node t is where the flow terminates. The term $A(i)$ is used to define the arc adjacency list of node i. That is the list of all arcs outgoing from node i into other nodes. The "length of a directed path" is defined to be the sum of the lengths of arcs in the path. It is assumed the network contains a directed path from the source to all other nodes in the network, otherwise, there would exist isolated nodes that could never be reached. Though there are several types of directed shortest path problems, finding the shortest path from each node to every other node is the type that is relevant to this problem. It is referred to as the "all-pairs shortest path problem."

A simple string model is used to aid in the understanding of a shortest path problem between a specified pair of nodes s and t. Ahuja [1] points out that this model can easily be extended to the shortest path problem with multiple destinations and nonnegative arc lengths. Assuming the string cannot be stretched, use the knots to represent nodes, where $c_{i,j}$ is the length of string joining the two knots i and j. Taking hold of the knot s in one hand and the knot t in the other and pulling the hands apart leaves one or more paths held tight. These represent the shortest paths

from node s to t since they are the lengths that are restricting the source and sink knot from being pulled farther apart.

Several important aspects of the shortest path problem can be taken from this string model [1]. The taut strings represent arcs on the shortest path and thus, the distance between any two successive nodes i and j on that path equal $c_{i,j}$ of the arc (i, j) between the nodes. Considering any two nodes i and j, that may not be successive, that are connected by arc (i, j) in $\mathcal{A}$, the shortest path distance from the source s plus $c_{i,j}$ is always as large as the shortest path distance from the source to node j. This composite distance may be larger because the string between knots i and j may not be taut (i.e. not in the shortest path).

According to Ahuja [1], there are two groups of algorithmic approaches to solving shortest path problems, both of which are iterative: label setting and label correcting. Each of these approaches assigns tentative distance labels to nodes at each step. These distance labels are estimates of the shortest path distances. In other words, they are upper bounds on the distances. The types of algorithms differ in their methods of updating distance labels from one step to the next and the class of problems they solve. Label setting algorithms work by designating one label as permanent (optimal) at each iteration and are applicable only to shortest path problems defined on acyclic networks. The more general label correcting algorithms consider all labels as temporary until they are made permanent at the final step. They are applied to all classes of problems but are less efficient than the label setting algorithm [1].

Integer programming (IP) is used to solve optimization problems where the variables are discrete or are restricted to integer values. Specifically, IP can be used to solve shortest path problems [21]. The basic formulation has an objective function that seeks to maximize or minimize some profit or cost. For example, consider the linear program $\max\{cx : \mathbf{A}x \leq b, x \geq 0\}$ where $\mathbf{A}$ is an m by n matrix, c an n-dimensional row vector, b an m-dimensional column vector, and x an n-dimensional

column vector of variables or unknowns. This becomes an integer program by adding the restriction that certain variables must be integers [21]. There are three different forms of integer programming. A mixed integer program (MIP) is one where some of the variables must be integer and others are not. When all of the variables are integer, it is an integer program (IP) and when all of the variables are restricted to values of 0 or 1, it is referred to as a binary integer program (BIP) [21].

The Travelling Salesperson Problem (TSP) is a common binary integer program in operations research and is very relevant to the models presented in this thesis. The original TSP is used to model and solve a problem where a single salesperson must visit n cities exactly once and return to his/her original location. There is a time (distance) $c_{i,j}$ associated with travelling from city i to city j. The objective of the TSP is to minimize travel time (distance) by identifying the optimal order in which the salesperson should visit each city and return to his/her starting point [21]. The TSP is directly related to this thesis problem where the salesperson represents a search crew, the cities represent the areas of interest, and the time corresponds to the time required to travel between the areas. However, several modifications must be made to accommodate the restrictions in this thesis problem and these will be discussed in the following chapter.

The binary knapsack problem is another well-known problem related to this thesis. Essentially, one has a "knapsack" and must fill it with some number of items. Each item has a cost (e.g., size) associated with it, and thus, using an item takes up some of the resource (e.g., space). The objective is to maximize the benefit of what goes in the knapsack while adhering to the resource constraint. The knapsack problem relates to the optimal sampling problem because we seek to maximize the reward of the search by choosing arcs (with associated times) without exceeding the available resource (time). However, the order in which the arcs are chosen matters to this problem since they must form a feasible path through the system.

Several algorithms have been developed for finding the least expected travel time path through a network. However, these work only for networks with deterministic time-dependent (or time-variant) travel times and for networks with random non-time dependent (or time-invariant) travel times [8]. Some fairly recent papers have studied networks with stochastic and time-variant (STV) travel times [16]. Miller-Hooks and Mahmassani [16] state that STV networks provide "a more appropriate representation" for use in making critical routing decisions than deterministic, static models.

Miller-Hooks and Mahmassani [16] present a methodology for determining paths with the least expected time (LET) through the network. The resulting set of paths are Pareto-optimal (or efficient). The results are Pareto-optimal since no other solution would be optimal to all objectives in this multi-objective problem. The method for determining LET paths for STV networks differs from the method for determining LET paths in networks with time-invariant travel times and is more difficult. For networks with random, time-invariant travel times, each random arc weight can be set to its expected value and solved using deterministic methods.

Thomas and White [18] model an anticipatory route selection problem as a Markov decision process (MDP). The objective of their problem is to find the "minimum expected total cost route from an origin to a destination that anticipates and then responds to service requests, if they occur, while the vehicle is en route." Their problem is important to mobile communication technologies that enable communication between dispatchers and drivers. Real-time information is used to determine the best route for a single pickup and delivery vehicle when the likelihood, as a function of time, that a potential customer will request a pickup, is known. The flexibility incorporated into the anticipatory routing problem allows dispatchers to contact a driver, who may be in the process of a pickup and delivery, and inform them of a new pickup request. The driver can then adjust his or her route to accommodate this new request. This attribute is important to other problems where the ability to

receive real-time information allows the entity (e.g., truck, person, crew) to adapt its route to accommodate the new information, thus optimizing the route [18].

The anticipatory routing problem which Thomas and White [18] consider involves a single, uncapacitated vehicle travelling along feasible arcs from a known origin to a known destination in a fixed amount of time. As a vehicle traverses an arc, it accrues a travel cost dependent on the arc (e.g., time, money, resource) and accrues a reward after visiting a node requiring a pickup. Clearly, if no pickup is requested, no reward is accrued. It is assumed each customer has a known distribution giving the probability that the customer will request a pickup at time t or before, for all t. Thomas and White [18] formulate the model of the road network as a MDP. The graph consists of a set of nodes and edges. An arc exists if and only if there is a road permitting travel between the two endpoints of the arc. They define a *successor set* containing the adjacent nodes for each node which includes the node itself (i.e., the driver can wait at a node). There is an origin and destination node in the set of nodes but they are not in the set representing customers who may or may not request service (i.e., requests cannot be made from the origin or destination node).

Decision epochs for the MDP occur when the vehicle arrives at a node and this is a *finite horizon* problem with the positive integer T indicating that action selection terminates no later than $T - 1$. A random variable Q represents the total number of decisions and $k^l(t)$ represents the state of customer l's current service request. The successor set is also the *action set* whose cardinality is necessarily finite. They also define *decision rules* at a time t as a function that selects an available action and a *policy* as a sequence of those decision rules and determine the structured cost function and policy structure results. The work is important to this thesis because it incorporates real-time information when making decisions by anticipating possible requests. The ability to incorporate real-time or near real-time information into decisions allows for optimal policies being developed when the problem is dynamic.

The main contribution of this thesis is an optimal sampling procedure for a single crew to assess the contamination level at various areas throughout a fixed operational site subsequent to a chemical attack. The objective is to identify the maximum number of areas that can safely operate without protective gear and to complete the search within an allotted time limit. We consider four cases, increasing in complexity, and formulate each one as a binary integer program to develop a methodology for optimally sampling the site in each case. First, we consider static and deterministic vapor concentrations and then we modify the problem to allow the vapor concentrations to behave according to a stationary probability distribution. Next, we incorporate temporal evolution into the deterministic model and develop an algorithm for identifying the optimal sampling procedure. Finally, we consider vapor concentrations that evolve according to a time-variant probability distribution and develop an algorithm that identifies the optimal sampling procedure based on the probability of obtaining a reward at a searched area. The final solution is a time-adaptive policy directing the search crew through the site to the maximum number of areas identified to have vapor concentrations below the threshold. Thus, the maximum number of areas in which personnel can safely operate without protective gear are identified.

3. Formal Mathematical Model

In this chapter, we present a mathematical model for optimally searching an operational site subsequent to a chemical attack. We consider three distinct cases before examining the fourth (and most realistic) case, ultimately developing a policy for searching the site, within an allotted amount of time, to find the maximum number of areas in which the level of protective gear can be safely reduced.

3.1   Model Description

Assume that a fixed site (e.g., a military installation) is situated on a Cartesian plane such that ordered pairs (x, y) may be used to identify and label critical locations such as the flight line, headquarters, and other operationally imperative areas. In Figure 3.1, such locations are indicated by an asterisk ($*$). Orienting the site on the positive quadrant of the coordinate system with the origin of the chemical agent release in the southwest corner, each area can be identified by the ordered pair (x, y), where x and y are the distances, in meters, from the origin in their respective directions to the point where vapor concentration readings will be obtained.

In this research, we represent the fixed operational site as a network in which the areas are considered to be the nodes of the network. Nodes are labelled by the
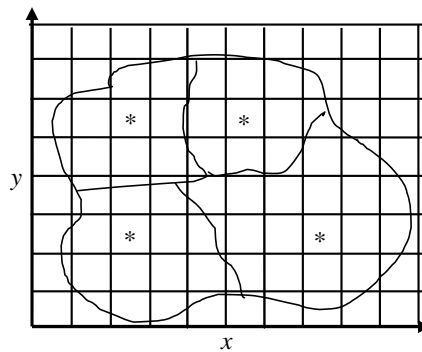
Figure 3.1   Graphical depiction of areas on an installation.

integers $1, 2, ..., N$, where N is the total number of areas. The network's arcs connect pairs of nodes to represent feasible travel between those nodes. It is important to note, that though the arcs are represented as line segments, the actual path between the areas may not necessarily be straight (or direct). The arcs simply represent feasible travel paths from one area to another.

Let $G = (\mathcal{N}, \mathcal{A})$, be a directed graph where $\mathcal{N}$ is the set of nodes, having cardinality N (i.e., $|\mathcal{N}| = N$), and $\mathcal{A} = \{(i, j) : i, j \in \mathcal{N}\}$ is the set of arcs connecting pairs of vertices i and j. An arc (i, j) is said to be *incident* to nodes i and j when the arc directly connects node i and node j [1]. A *directed* arc connecting nodes i and j indicates feasible travel between nodes i and j in the direction of the arc. *Undirected* arcs have no arrowheads on either end and imply travel is possible in both directions. That is, one may arrive at node j from node i and likewise, one may arrive at node i from node j. A *leaf* is a node with at most one arc incident thus allowing only one route in and the same route out. Arc weights denote *static* and *deterministic* travel times between two nodes and the cost (or reward) associated with each node is found from the vapor concentration at that node. The *in-degree* of a node is the number of arcs incoming to the node and the *out-degree* is the number of arcs emanating from the node. A node $j \in \mathcal{N}$ is said to be *covered* if it has been visited.
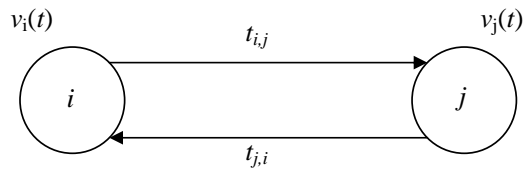
Figure 3.2   Graphical depiction of network definitions.

In Figure 3.2, arc (i, j) is incident to nodes i and j. The deterministic duration $t_{i,j}$ is required to travel from node i to node j. Finally, at time t, the vapor concentrations at nodes i and j are $v_i(t)$ and $v_j(t)$, respectively. If the vapor concentration level does not depend on time, the notation is simply v_i and v_j.

The primary focus of this thesis is the routing of a search crew through a fixed operational site in order to identify locations in which hazardous secondary vapors are present subsequent to a chemical weapons attack. In reality, this problem is both dynamic and stochastic in nature. That is, the vapor concentrations change over time, either increasing in some areas or decreasing in others. The problem is stochastic in that the hazardous vapor concentrations are random variables and are governed by some (time-variant) probability distribution which is assumed to be known. Due to the stochastic temporal and spatial evolution of the secondary vapors, it is necessary to obtain actual data through chemical vapor sensors and/or other such instruments. Technological capability to obtain such data will contribute to solving the problem by providing accurate, real-time information. However, in lieu of having such data, we assume known distributions in our model.

Due to the dynamic and stochastic nature of the vapor concentration levels, crews must intelligently search the site to obtain concentration measurements to determine the correct level of protection required for safe operations. Thus, they need to reach as many areas as possible within a fixed time window while ignoring non-critical areas or areas not likely to be contaminated. In order to approach this problem, we first consider the following three cases:

1. Static and deterministic vapor concentration levels;

2. Static and stochastic vapor concentration levels;

3. Dynamic and deterministic vapor concentration levels.

Once these three cases are formulated and solved, the fourth, and most realistic case, of dynamic and stochastic vapor concentrations, can be formulated and solved using the techniques and insights obtained from the previous three formulations.

In the next section, a number of problem assumptions are presented. Also, we present the four cases considered and the methodology for solving each one.

3.2 Model Assumptions and Cases

All four cases employ the following set of assumptions:

1. The weapon released is a chemical agent with known characteristics (e.g., chemical makeup and properties, effect on human life, evaporation rates, lifetime, etc.).

2. Only one crew is available to obtain instrument readings of vapor concentration levels.

3. The crew travels (either on foot or in a vehicle) at a constant velocity and experiences zero delays due to traffic, etc.

4. Travel times between nodes are static and deterministic.

5. Travel times between two nodes are symmetric (i.e., $t_{i,j} = t_{j,i} \; \forall (i,j) \in \mathcal{A}$).

6. Only one reading within each area is required to assess the correct level of protective gear required.

7. The time required to obtain an instrument reading is constant.

8. There is a fixed vapor concentration threshold v^* below which protective gear is not required and above which it is required.

9. Vapor concentrations evolve spatially (i.e., the level of contamination in an area depends on its distance from the initial release).

The first assumption implies that we focus on chemical weapons, as opposed to biological weapons. The next two assumptions regarding the search crew simplify the problem. The methodology we develop is based on a single crew available for the task that travels, either in a vehicle or on foot, at a constant velocity. Again, to reduce the number of stochastic elements in the problem, we impose the assumption of a fixed and deterministic amount of time required for obtaining instrument readings. This allows the instrument reading time to be added to the travel time. Also, we

assume symmetric travel times, thus implying travel from node i to node j requires the same amount of time as travelling from node j to node i. Research suggests a fixed vapor level exists, above which the vapor concentration is harmful to human beings and below which they can operate safely. Finally, we recognize the chemical vapor concentrations change as one moves farther from the source of release. This assumption attempts to capture the true behavior of chemical vapor concentrations considered when developing the methodology for each case.

In the following subsections we present the three cases mentioned in section 3.1. First, we consider the case where the vapor concentration level at each node is static and deterministic. This is a trivial case where the vapor concentrations can be computed at the initial time of the attack and do not change over time. Second, we examine the case in which vapor concentrations are static and stochastic. This is closer to the real world case because the vapor concentrations cannot be known with certainty until an instrument reading is obtained. The probability distributions for the vapor concentrations are assumed to not change over time. Third is the case considering dynamic and deterministic vapor concentrations. Time is incorporated into the mathematical formula and the vapor concentrations change (deterministically) as time progresses. Finally, the fourth case considers dynamic and stochastic vapor concentrations. Representative of the real world situation, the vapor concentration levels behave according to a time-variant probability distribution. There is a clear objective for each case and the result is a policy, in some cases time-adaptive, that directs a search crew through the site with the goal of identifying the maximum number of areas for which the level of protective gear can be safely reduced.

3.2.1 Static and Deterministic Vapor Concentration Levels

The first case considers a scenario, subsequent to a chemical agent release, in which the vapor concentrations at each area are static and deterministic quantities. That is, they do not change over time and can be determined via a mathematical

formula in which all of the parameters are known. An appropriate formula, such as those vapor dispersion models [14], can be used to determine the vapor concentrations, v_j, at each node. Figure 3.3 provides an example of the network representation for this case.
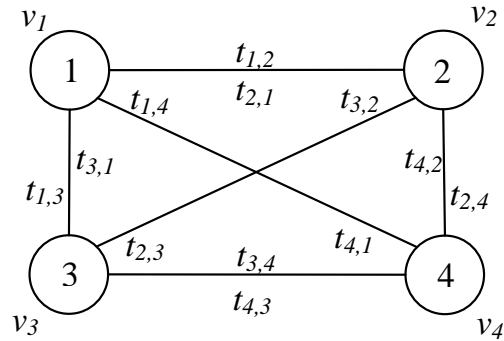
Figure 3.3   Network representation for a 4-node site in the static/deterministic case.

This is a multi-objective case where we seek to identify the shortest time path from the starting node s to the other nodes contained in the site while maximizing the number reached. The vapor concentration levels are calculated, at a fixed time t_0, from an equation such as the advection-diffusion Equation (3.2). The following parameters must be known to employ Equation (3.2) to compute v_j, when node j has coordinates $(x, y, 0)$:

$x, y, z \equiv$ Cartesian coordinate system with the x-axis oriented in the direction of the mean wind, the y-axis in the horizontal cross-wind direction, and the z-axis in the upwards vertical direction.

$k_x, k_y, k_z \equiv$ eddy diffusivities for the x, y, and z directions, respectively in m^{2}sec^{-1}

$q \equiv$ the total mass release in kg

$h \equiv$ height above the ground where the instantaneous gas release occurs in m

$u \equiv$ wind velocity in m/sec

The equation,

$$v_j = \frac{q}{8\pi^{\frac{3}{2}}(k_x k_y k_z)^{1/2}t_0^{3/2}} \exp\left[-\frac{(x-ut_0)^2}{4k_x t_0} - \frac{y^2}{4k_y t_0}\right] \times$$
$$\left(\exp\left[-\frac{(z-h)^2}{4k_z t_0}\right] + \exp\left[-\frac{(z+h)^2}{4k_z t_0}\right]\right), \qquad (3.1)$$

can be simplified to

$$v_j = \frac{q}{8\pi^{\frac{3}{2}}(k_x k_y k_z)^{1/2}t_0^{3/2}} \exp\left[-\frac{(x-ut_0)^2}{4k_x t_0} - \frac{y^2}{4k_y t_0}\right] \times$$
$$\left(2\exp\left[-\frac{h^2}{4k_z t_0}\right]\right), \qquad (3.2)$$

since we assume $z = 0$ (i.e., the x, y-plane lays on the ground). Thus, from this point forward, the ordered pair (x, y) is sufficient for denoting the coordinates of a node.

In the static case, t_0 denotes the elapsed time since the initial release when the vapor concentration for each node $j \in \mathcal{N}$ is calculated and it remains constant. Employing Equation (3.2) yields the vapor concentration for coordinates (x, y) corresponding to the graphical location of each node $j \in \mathcal{N}$, with specified parameters q, u, k_x, k_y, k_z, and h. From these concentrations, we define a reward r_j for each node j. For a fixed vapor concentration threshold, denoted v^*, the reward for each node is

$$r_j \equiv \begin{cases} 1, & v_j < v^* \\ 0, & v_j \geq v^* \end{cases}. \qquad (3.3)$$

The travel times are used to identify the optimal route the search crew must follow. The ordered set ψ contains the nodes found in the optimal path in the order in which those nodes should be searched. Following this path allows the crew to reach as many areas as possible in the minimum amount of time.

The mathematical programming formulation for the problem consists of a multi-objective function and several constraints. The objective function (3.4) seeks

to maximize the number of areas sampled where a reward is observed while also minimizing the time required to search the site. However, a time constraint (3.5) is imposed, where T is the allotted time for the search and $t_{i,j}$ is the time required to travel from node i to node j. Due to (3.5), the result may be a path that does not reach every node in the network. The optimal path identified as the solution is denoted, ψ. In the mathematical formulation, $x_{i,j}$ is a binary variable assuming a value of 1 if the search crew travels from node i to node j and 0 if node j is not reached from node i. The set $\mathcal{S} \subset \mathcal{N}$ is a set of nodes creating a subtour (i.e., a path not beginning and ending at the source node, s). For networks whose nodes have a minimum in-degree of 2, the formulation is

$$\max \sum_{i=1}^{N} \sum_{j=1}^{N} r_j x_{i,j}(opt), \quad \min \sum_{i=1}^{N} \sum_{j=1}^{N} t_{i,j} x_{i,j} \tag{3.4}$$

subject to

$$\sum_{i=1}^{N} \sum_{j=1}^{N} t_{i,j} x_{i,j} \;<\; T \tag{3.5}$$

$$\sum_{j=1}^{N} x_{s,j} \;=\; 1 \text{ for } s \in \mathcal{N} \tag{3.6}$$

$$\sum_{i=1}^{N} x_{i,j} \;\leq\; 1 \text{ for } j = 1, ..., N; j \neq i \tag{3.7}$$

$$\sum_{j=1}^{N} x_{i,j} \;\leq\; 1 \text{ for } i = 1, ..., N; i \neq j \tag{3.8}$$

$$x_{i,j} + x_{j,i} \;\leq\; 1 \text{ for all } (i,j) \in \mathcal{A} \tag{3.9}$$

$$\sum_{i \in \mathcal{S}} \sum_{j \in \mathcal{S}} x_{i,j} \;\leq\; |\mathcal{S}| - 1 \text{ for } \mathcal{S} \subset \mathcal{N}, 2 \leq |\mathcal{S}| \leq N - 1 \tag{3.10}$$

$$x_{i,j} \;=\; \begin{cases} 1, \text{ if } (i,j) \in \psi \\ 0, \text{ otherwise} \end{cases} \tag{3.11}$$

$$t_{i,j} \;\geq\; 0. \tag{3.12}$$

Clearly, Equation (3.6) requires that exactly one arc emanates from the source node s in the final solution. This ensures the search crew departs from its starting location. The next two equations, (3.7) and (3.8) restrict the number of incoming and outgoing arcs to at most 1. These constraints work for the case where the minimum in-degree of all nodes is 2, because the search crew cannot become stuck at a leaf of the network when an outgoing arc exists. Since there is no benefit for returning to a previously searched node when the rewards are static, these constraints hold and Equation (3.9) is included to prevent the crew from backtracking (i.e., using the same arc twice). Equation (3.10) eliminates subtours from the solution as illustrated in Figure 3.4 and finally, (3.12) restricts the times to nonnegative numbers.
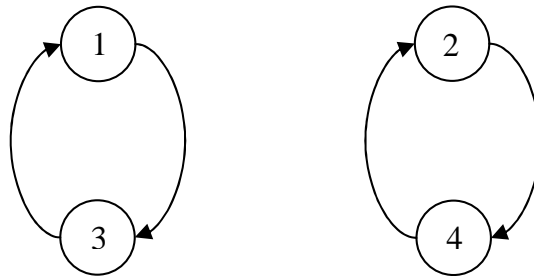
Figure 3.4   Network representation of a subtour.

The mathematical formulation bears similarity to the well-known Travelling Salesperson Problem (TSP). The objective function is to minimize some time (distance) and there is a subtour elimination constraint. However, due to the knapsack problem constraint (3.5), where time is the "resource," it is possible that not all nodes will be reached, a requirement of the TSP. Also, the crew does not have to return to the origin as required in the TSP. Hence, TSP solution procedures are not directly appropriate for solving the problem in this case.

For networks having a node whose minimum in-degree is 1, it is possible for the crew to become stuck at a leaf unless Equations (3.7), (3.8), and (3.9) are removed from the formulation. Removing those constraints allows the crew to backtrack along an arc should it become stuck at a leaf node. Equations (3.7) and (3.8) can

be replaced with

$$\sum_{i=1}^{N} x_{i,j} \leq 2 \text{ for } j = 1, ..., N; j \neq i$$

and

$$\sum_{j=1}^{N} x_{i,j} \leq 2 \text{ for } j = 1, ..., N; i \neq j,$$

respectively. These new constraints allow an arc to be included at most twice, allowing the crew to continue the search from a leaf node.

We have determined the best way to solve this case is by implicit enumeration. Beginning with the starting node s, each adjacent arc is examined. If the current time t plus the next travel time $t_{i,j}$ is greater than the allotted time T, the branch terminates at node i. Due to this time constraint, an upper bound can be found on the number of possible arcs in the optimal solution. This upper bound is given by

$$u.b. = \left\lfloor \frac{T}{\min_{(i,j) \in \mathcal{A}} \{t_{i,j}\}} \right\rfloor. \qquad (3.13)$$

Determining this upper bound reduces the size of the problem by providing a limit to the number of arcs in the optimal path. For example, if $T = 60$ minutes is allotted for the search, and the minimum travel time for all arcs was 5 minutes, the upper bound on the number of arcs in the optimal solution is 12. Hence, if there were more than 12 nodes in the network, not all of them could be reached in the optimal solution. Also, the size of the problem is further reduced by restricting backtracking unless necessary and by not allowing the same node to be searched more than once.

We define a *branch* as an ordered vector of nodes representing a feasible path with an associated time length, denoted τ_k. Each branch b_k for $k = 1, ..., B$, where B is the number of branches, is examined and if the cardinality of the branch equals the number of nodes in the network, the path of minimum time is chosen. That is, for all branches such that $|b_k| = N$, the optimal path ψ is the branch b_k^* with

minimal total search time

$$\tau_k^* = \min_k \{\tau_k\} \qquad (3.14)$$

If the maximum cardinality of all branches

$$b \equiv \max_k \{|b_k|\} \qquad (3.15)$$

is less than number of nodes, the branch of maximum cardinality (and shortest time) is optimal. That is, the optimal path $\psi = b_k^*$ is that path for which

$$\tau_k^* = \min_k \{\tau_k : |b_k| = b\}. \qquad (3.16)$$

Upon completion of the path specified by the optimal path ψ with total time τ_k^*, instrument readings are obtained for all nodes in the path (i.e., $\forall j \in \psi$). The term r_j, represents the indicator function, $I\{v_j < v^*\}$, and is 1 if $v_j < v^*$ and 0 otherwise. That is, if the vapor concentration at node j is, in fact, less than the predetermined threshold, then the indicator function will assume the value unity. For all nodes not in the path, $j \notin \psi$, the vapor concentration v_j obtained from Equation (3.2) is used to determine the reward value r_j for those nodes. The total reward r^* is the sum of all reward values, denoted by

$$r^* = \sum_{j \in \mathcal{N}} r_j. \qquad (3.17)$$

Next we consider the case in which the vapor concentrations are assumed to behave according to a known probability distribution that is time-invariant.

3.2.2 Static and Stochastic Vapor Concentration Levels

The second case considers a scenario in which the vapor concentration at each node is distributed according to some known (and time-invariant) probability dis-

tribution with a finite first moment. That is, the vapor concentration level at node j is not known, but rather the expected value of the vapor concentration at node j can be computed or estimated. The random variable V_j denotes the random vapor concentration at node j.

It has been shown by Hall [8] that the least *expected* travel time path through time-invariant stochastic networks can be solved using the same methods as those for time-invariant deterministic networks. Thus, in this static case the problem can be solved using implicit enumeration. Figure 3.5 is an example of the network representation of this case.
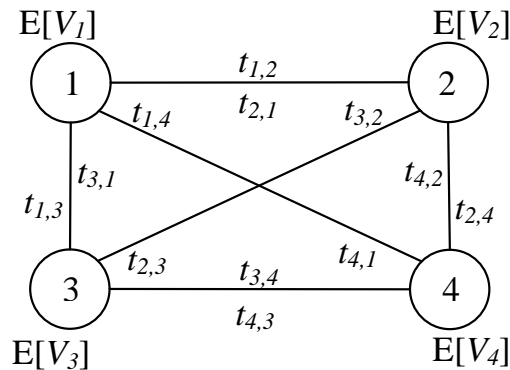
Figure 3.5   Network   representation   of   a   4-node   site   in   the static/stochastic case.

We seek to maximize the reward while minimizing the time required to travel through the network. This allows the crew to reach as many nodes as possible in the allotted time. The difference from the previous case is, before the search begins, vapor concentrations at each node j cannot be determined with an equation such as Equation (3.1), but the expected value can be computed through a known (stationary) probability distribution. Thus, using the *expected* vapor concentration,

the reward value for each node is determined by

$$r_j = \begin{cases} 1, & E[V_j] < v^* \\ 0, & E[V_j] \geq v^* \end{cases}.$$ (3.18)

Here, expected vapor concentrations are considered rather than deterministic values and *actual* vapor concentrations cannot be known until instrument readings are obtained.

Unlike the case in section 3.2.1, the initial r_j values are based on the expected vapor concentrations. Therefore, a realization of the vapor concentration as a result of the crew's search may reveal more areas below the threshold, or more areas above the threshold, than initially expected. Essentially, the true r_j values cannot be assigned to an area until the crew obtains the instrument reading for that area. Thus, the importance of searching as many areas in the allotted time is more notable for this case where the actual total reward can only be known following an instrument reading of every site. At time T, the end of the time allotted for the search, the decision makers will know the total reward r^* such that

$$r^* = \sum_{j \in \mathcal{N}} r_j.$$

In the next section we consider the case where the vapor concentrations are deterministic, but dynamic. We present an algorithm for determining the optimal policy that will maximize the reward while completing within the allotted time.

3.2.3 Dynamic and Deterministic Vapor Concentration Levels

The third case is distinct from the first two cases in that we now assume the vapor concentrations depend on time. The vapor concentration for each node can presumably be computed from known physical relationships but the values depend

on the time of the calculation. This is more representative of the real world case since chemical vapor concentrations do change over time (and space). Figure 3.6 provides an example of the network representation for this case.
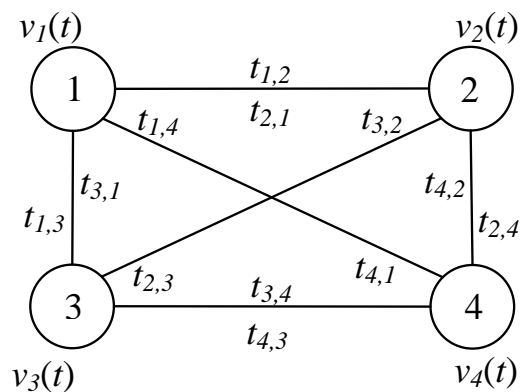
Figure 3.6   Network representation of a 4-node site in the dynamic/deterministic case.

As before, let $v_j(t)$ denote the vapor concentration at node j at time t. The advection-diffusion Equation (3.2) is an example of how one might calculate $v_j(t)$ where node j is located at coordinate (x, y). In this case, we allow t to vary, allowing the vapor concentration for each node $j \in \mathcal{N}$ to be updated at various times. Recall the equation

$$v_j(t) = \frac{q}{8\pi^{\frac{3}{2}}(k_x k_y k_z)^{1/2}t^{3/2}} \exp\left[-\frac{(x-ut)^2}{4k_x t} - \frac{y^2}{4k_y t}\right] \times$$
$$\left(2\exp\left[-\frac{h^2}{4k_z t}\right]\right), \qquad (3.19)$$

where t is updated to represent the time the crew will arrive at the next node j (i.e., $t = t + t_{i,j}$ when the current location is at node i). Using this equation, the search crew can calculate the vapor concentrations for all areas adjacent to their current location at the time of their arrival to that subsequent area.

Again, the decision maker's desire is to return the site to full operational capabilities as soon as possible. Thus, they need to know where and when the protective

gear requirement can be withdrawn and where and when it needs to be implemented. Therefore, we develop an algorithm that seeks to maximize the number of areas searched in which the protective gear is no longer required (i.e., where the reward value is 1).

The algorithm begins with an initialization step that commences at t_0, the time duration from when the chemical agent was released over the site to the completion of the first instrument reading. The crew uses an appropriate instrument for reading vapor concentrations to determine the concentration for the origin node s. Thus, the reward for node s is

$$r_s(t_0) = \begin{cases} 1, & v_j(t_0) < v^* \\ 0, & v_j(t_0) \geq v^* \end{cases}. \tag{3.20}$$

The algorithm then considers all areas adjacent to area s. Vapor concentrations are calculated for those areas using Equation (3.19) and the time it would be when the crew arrives there (i.e. the current time, t_0, plus the travel time from s to j, $t_0 + t_{s,j}$).

If an area has a future vapor concentration level *below* the threshold, it is a candidate for reduction. Each such area is then considered individually and the one with the minimum difference from the threshold is chosen (i.e., the node such that $v_j(t)$ is closest to v^*). We choose the area with the minimum difference below the threshold because it is the most critical area. That is, it is one that most demands an instrument reading since it is closest to being considered contaminated to a degree that is unsafe for personnel working in the area without protective gear. If there are no areas below the threshold, the node within the shortest amount of time (distance) is chosen. This is because the crew must leave its current location and if no adjacent node has a positive reward, choosing the closest node will advance the crew in a minimum amount of time so more nodes can be considered.

This method is repeated for all adjacent areas and the time t is updated appropriately until the allotted search time has expired. Previously searched nodes can be revisited if the vapor concentration at a later time is found to be below the threshold. As measurements are taken in each area, the value of r_j is assigned. When the search time expires, decision makers will know the exact number and location of areas operating safely without protective gear and those still requiring the gear for safe operations. The formal algorithm for solving the mathematical program is provided in what follows. The set $\mathcal{N}$ denotes the set of N nodes in the area to be searched and $\mathcal{N}_i$ is the set of nodes adjacent to node $i \in \mathcal{N}$. The set $\mathcal{R}$ is used to record nodes in the path with a reward value of 1 and the set ψ is the ordered set of nodes in the optimal path.

Initialization:

$\mathcal{N} = \{1, 2, ..., N\};$

$\mathcal{N}_i = \{j : (i, j) \in \mathcal{A}\};$

$\mathcal{R} = \emptyset;$

$\psi = \emptyset;$

$t \leftarrow t_0;$

$i = 1;$

Calculate current vapor level at node i, $v_i(t)$

If $v_i(t) < v^*$

$r_i(t) \leftarrow 1;$

$\mathcal{R} = \{i\};$

$\psi \leftarrow \psi \cup \{i\};$

Else

$r_i(t) \leftarrow 0;$

$$\psi \leftarrow \psi \cup \{i\};$$

End

Step 1

$\quad$ **Calculate** $v_j(t + t_{i,j}) \; \forall j \; \in \mathcal{N}_i$

$\qquad$ **If** $v_j(t + t_{i,j}) < v^*$

$$r_j(t + t_{i,j}) \leftarrow 1;$$

$\qquad$ **Else**

$$r_j(t + t_{i,j}) \leftarrow 0;$$

$\qquad$ **End**

Step 2

$\quad$ **For** each $j \in \mathcal{N}$ such that $r_j = 1$

$\qquad$ Choose j such that $v_j(t + t_{i,j}) = \arg\min_{j \in \mathcal{N}_i}\{v^* - v_j(t + t_{i,j})\}$

$$\mathcal{R} \leftarrow \mathcal{R} \cup \{j\};$$

$$\psi \leftarrow \psi \cup \{j\};$$

$\quad$ **End**

$\quad$ if $r_j(t + t_{i,j}) = 0 \; \forall \; j \in \mathcal{N}_i$

$\qquad$ Choose j such that $t_{i,j} = \min_j\{t_{i,j}\}\forall j \in \mathcal{N}_i$

$$\psi \leftarrow \psi \cup \{j\};$$

$\quad$ **End**

$$t \leftarrow t + t_{i,j};$$

Step 3

$\quad$ **If** $t \geq T$

$\qquad$ **STOP**

$\quad$ **Else**

$$i \leftarrow j;$$

Return to Step 1

End

This algorithm has been coded in the standard mathematical computing environment MATLAB® to determine a policy for searching the site when the vapor concentration levels are assumed to be dynamic and deterministic. The order in which the nodes are added to the set ψ is the order in which the site should be searched. Moreover, the cardinality of the set $\mathcal{R}$ is the number of areas where the protective gear is no longer required for the safety of the personnel working in those areas. Ultimately, the algorithm results in a time-adaptive policy that directs the crew to the maximum number of areas where it is critical to search while reaching as many as possible within the allotted time.

The next subsection considers the final and most realistic case in which the vapor concentration levels are both dynamic and stochastic. This more complicated case is approached in a manner similar to the one used in the previous case.

3.2.4 Dynamic and Stochastic Vapor Concentrations

Finally, the fourth case is most representative of the real world problem where the vapor concentrations at each node are denoted by time-dependent random variables. The solution to this final problem will also be a time-adaptive policy.

If a chemical agent is released over an area, the hazardous secondary vapors will continue to contaminate other areas and pose harm to the personnel working in the those areas. This case partially captures the true nature of those secondary vapors by not only incorporating time into the formulation, but also assuming a time-variant probability distribution to determine the probability that the vapor concentration at each area of interest is below the threshold level.

Figure 3.7 illustrates a possible network representation for this case. The label on each node, $V_j(t)$ denotes the random vapor concentration level at node j at time t and, as before, each arc weight represents the travel time from node i to node j.
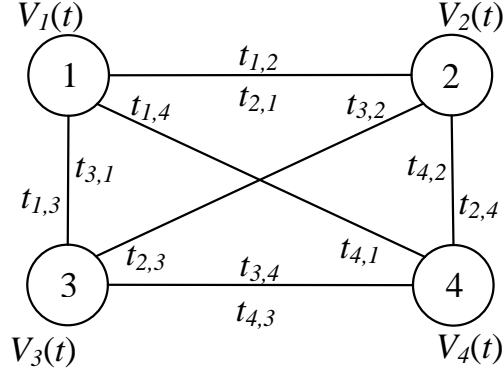
Figure 3.7   Network representation of a 4-node site in the dynamic/stochastic case.

We assume each node has an associated probability distribution that governs the behavior of the vapor concentration, over time, at that node. As time progresses, the parameters of the distribution change. In this work, we assume the concentration at each node is a random variable with an exponential distribution. Each node j will have an associated *rate* parameter at time t, namely, $\mu_j(t)$. The cumulative distribution function for $V_j(t)$ is

$$\pi_j(t) \equiv P(V_j(t) \le v) = \begin{cases} 1 - \exp(-\mu_j(t) \cdot v) & v \ge 0 \\ 0 & v < 0 \end{cases}. \tag{3.21}$$

Suppose the rate parameter for node 1 at $t = 420$ sec is $\mu_1(420) = 144.30$. The probability that node 1 is less than the threshold $v^* = 0.0006 mg/m^3$ at time 420 seconds is 0.0829. This probability is calculated by

$$\pi_1(420) = 1 - \exp(-144.30 \cdot 0.0006) = 0.0829. \tag{3.22}$$

Continuing in this fashion, the probability $\pi_j(t)$ that each node is less than the threshold can be determined for each time t. These probability values are used in the algorithm presented in this section.

The algorithm we developed for this case has a structure similar to that of the case assuming deterministic and dynamic vapor concentrations. It begins with an initialization step at time t_0 (the duration of time since the chemical agent release and the completion of the first instrument reading), and with the search crew located at node s (the starting point for the search). The crew obtains an instrument reading for its starting node and each node it searches. If $v_j(t)$ is below the threshold, the node receives a reward value at time $r_j(t)$ according to

$$r_j(t) = \begin{cases} 1, & v_j(t) < v^* \\ 0, & v_j(t) \geq v^* \end{cases}. \tag{3.23}$$

If $r_j = 1$, the set of reduced nodes $\mathcal{R}$ is updated by

$$\mathcal{R} = \mathcal{R} \cup \{j\}, \tag{3.24}$$

indicating the vapor concentration at node j has dropped below the threshold for time t.

For each adjacent node, the cumulative distribution function (c.d.f.) of the appropriate probability distribution is used to determine the probability that the next node to be searched will have a vapor concentration level below the threshold upon arrival. The crew then chooses the area with maximum probability of having a reward. This will direct them to the area where they are *most likely* to obtain a vapor concentration reading below the threshold at the next time step. Once the crew arrives at the area, it must obtain an instrument reading to determine the actual vapor concentration. In the algorithm, this is accomplished by drawing a value from the probability distribution as the realization $v_j(t)$ of the random variable $V_j(t)$. If

the vapor concentration is below the threshold, the reward value for that node, at time t, assumes a value of 1 and is added to the set $\mathcal{R}$.

There is a single stopping criterion terminating the algorithm. Once the time allotted for the search expires the search crew must cease searching the site and end at its current location. Upon termination, the set $\mathcal{R}$ contains, in order, the nodes searched where the vapor concentration was decreased. The set ψ contains the nodes, in order, to be searched within the allotted time to maximize the reward.

For nodes that remain uncovered, the expected value of the vapor concentration is used to determine the reward value. For uncovered nodes, the reward is

$$
r_j(t) = \begin{cases} 1, & E[V_j(t)] < v^* \\ 0, & E[V_j(t)] \geq v^* \end{cases}.
\tag{3.25}
$$

Thus, the final reward is

$$
r^*(\tau^*) = \sum_{j \in \mathcal{N}} r_j(t),
\tag{3.26}
$$

such that $t < T$ is the time of the last instrument reading and τ^* is the time length of the solution. This value, $r^*(\tau^*)$ is the total number of nodes that, according to actual instrument readings for $j \in \psi$ and the rewards for $j \notin \psi$ (determined from the expected vapor concentrations), no longer require protective gear.

Upon completion of the algorithm, decision makers will know which areas of the site are operating safely without protective gear, those that still require the gear for safe operations, those which are *expected* to not require the gear, and those *expected* to still require the gear. Below is the formal algorithm for solving the mathematical program. Recall, the set $\mathcal{N}$ denotes the set of N nodes in the area to be searched and $\mathcal{N}_i$ is the set of nodes adjacent to node $i \in \mathcal{N}$. The set $\mathcal{R}$ is used to record nodes in the path with a reward value of 1 and the set ψ is the ordered set of nodes in the optimal path.

Initialization:

$\mathcal{N} = \{1, 2, ..., N\};$

$\mathcal{N}_i = \{j : (i, j) \in \mathcal{A}\};$

$\mathcal{R} = \emptyset;$

$\psi = \emptyset;$

$t \leftarrow t_0;$

$i = 1;$

Obtain current vapor level $v_i(t)$

If $v_i(t) < v^*$

$r_i(t) \leftarrow 1;$

$\mathcal{R} \leftarrow \mathcal{R} \cup \{i\};$

$\psi \leftarrow \psi \cup \{i\};$

Else

$r_i(t) \leftarrow 0;$

$\psi \leftarrow \psi \cup \{i\};$

End

Step 1

Calculate $\pi_j(t + t_{i,j}) \equiv P\{V_j(t + t_{i,j}) < v^*\} \; \forall j \; \in \mathcal{N}_i$

Step 2

Choose j such that $\pi_j(t) = \max_{j \in \mathcal{N}_i} P\{V_j(t + t_{i,j}) < v^*\}$

Obtain instrument reading at this node.

If $v_j(t + t_{i,j}) < v^*$

$r_j(t) \leftarrow 1;$

$$\mathcal{R} \leftarrow \mathcal{R} \cup \{j\};$$

$$\psi \leftarrow \psi \cup \{j\};$$

$$t \leftarrow t + t_{i,j};$$

Else

$$r_j(t) \leftarrow 0;$$

$$\psi \leftarrow \psi \cup \{j\};$$

$$t \leftarrow t + t_{i,j};$$

End

Step 3

If $t \geq T$

STOP

Else

$$i \leftarrow j;$$

Return to Step 1

End

This algorithm differs from the previous algorithm due to the stochastic nature of the vapor concentration levels. It cannot be known with certainty whether or not an area has a vapor concentration below the threshold until it is searched by the crew and an instrument measurement obtained. Thus, the algorithm chooses which nodes to search based solely on the probability the vapor concentration level will be below the threshold upon the crew's arrival.

Since there exists a non-zero probability that a searched area will have a vapor concentration above the threshold, the algorithm allows the crew to search that area again by not removing it from the set of candidate nodes. The resulting policy can include searching a node more than once since the probability distributions change

over time, and the nodes are searched based on probabilities which may not be very high.

The next chapter provides several numerical examples to illustrate each of these four cases. We setup each case and employ the mathematical formulations and algorithms developed in this chapter to find an optimal sampling procedure for the site.

4. Numerical Results

In this chapter, the main results of Chapter 3 will be illustrated through four example problems. The algorithms developed in the previous chapter will be used to identify a policy that directs the search crew through the site in order to identify the maximum number of areas at which protective gear may be removed. We will compare the results for the static/deterministic with the dynamic/deterministic vapor concentration levels, as well as the results for the static/stochastic with the dynamic/stochastic vapor concentration levels to discuss the impact of excluding the dynamic nature of the secondary vapor concentrations when searching the site.

4.1   Generating Problem Instances

We randomly generate ten ordered pairs, $\{(x_i, y_i) : i = 1, 2, ..., 10\}$, to represent a site with ten critical areas. Plotting these coordinates depicts the location of the critical areas with respect to each other and the initial chemical agent release. From this plot, a network graph is drawn using nodes to represent the critical areas and arcs to represent feasible travel between pairs of areas.

We arbitrarily consider a rectangular area of the site 100 meters by 150 meters. A standard spreadsheet application was used to randomly generate the ten x-coordinates and ten y-coordinates recorded in Table 4.1. The points are distributed uniformly over the intervals $(5, 100)$ and $(5, 150)$, respectively, and the pairs are given in ascending order by the x value to assign node numbers to each area.

This example assumes all critical areas of the site lie to the northeast of the chemical agent release. If the release occurred elsewhere, the origin may be translated to the appropriate location without affecting the solution procedure. The areas are plotted in Figure 4.1.

Table 4.1 x, y-coordinates for example site.

Node	x (m)	y (m)
1	6.276	23.015
2	14.466	56.527
3	33.297	96.017
4	42.992	5.234
5	60.240	53.504
6	71.900	140.526
7	86.365	36.667
8	94.149	86.361
9	98.829	7.664
10	99.742	100.500

Creating a node for each point on the plot in Figure 4.1, and connecting pairs of nodes with arcs, generates the network representation for this example. Also assuming zero detours, the Euclidean distance from node i to node j, denoted $d_{i,j}$, can be computed as

$$d_{i,j} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}. \tag{4.1}$$

Assuming zero delays or obstacles, and a constant velocity of 26.8224 m/min (1 mi/h) we calculate the travel time for a search crew from one node to another. Five minutes are added to the time on each arc $(i, j) \in \mathcal{A}$ to account for the instrument reading at node j. Recall, the travel times are symmetric so that $t_{i,j} = t_{j,i}$ for all $(i, j) \in \mathcal{A}$.

Figure 4.2 depicts the network graph for the notional site. The following sections use this site as a template for each example. The appropriate methodology is applied in each section to obtain a path directing the search crew through the site to identify the maximum number of areas at which the protective posture level can be reduced.
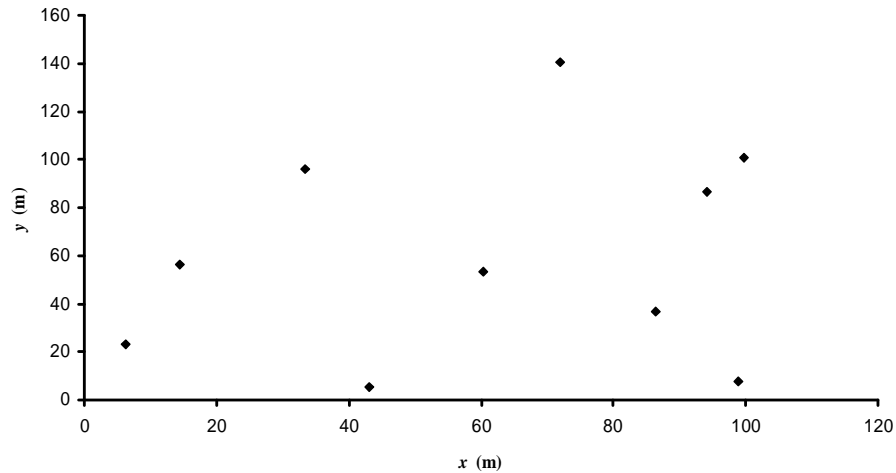
Figure 4.1   Plot of x, y-coordinates for the notional site.

4.2   Example 1: Static and Deterministic Vapor Concentrations

Recall for this case that vapor concentrations are time-invariant and can be calculated using a deterministic formula such as the advection-diffusion Equation (3.1) (see Chapter 3). We seek a policy ψ to identify the areas of the site where the vapor concentration has decreased below the threshold since the initial chemical agent release. A decrease below the threshold value v^* allows personnel in the area to carry out the mission safely without the cumbersome protective gear. The search crew will use this policy to search the site and obtain instrument readings for those areas.

We begin by calculating the vapor concentration level for each node at initial time t_0 (i.e., time since the chemical agent release). Parameters used in Equation (3.1) are tabulated in Table 4.3.

The calculated vapor concentration and reward value at each node is recorded in Table 4.4. The reward value is calculated as follows for threshold $v^* = 0.0006$ mg/m^3:

$$r_j = \begin{cases} 1, & v_j < v^*, \\ 0, & v_j \geq v^* \end{cases}.$$
(4.2)

4-3

Table 4.2   Distance and travel time between nodes.

Arc	Length(m)	Travel Time (min)
(1,2)	34.50	6.29
(1,4)	40.79	6.52
(1,5)	61.98	7.31
(2,3)	43.75	6.63
(2,5)	45.87	6.71
(3,4)	91.30	8.40
(3,5)	50.33	6.88
(3,6)	58.92	7.20
(4,7)	53.56	7.00
(4,10)	110.89	9.13
(5,7)	31.08	6.16
(5,8)	47.22	6.76
(6,8)	58.56	7.18
(6,9)	135.56	10.05
(7,10)	65.22	7.43
(8,9)	78.84	7.94
(8,10)	15.20	5.57

The travel times, in minutes, are calculated using the relationship

$$t_{i,j} = \frac{d_{i,j}}{\nu} + 300, \tag{4.3}$$

where ν denotes the constant velocity of the search crew (in m/sec) and five minutes (300 sec) required for the instrument reading is added to the travel time. These times are entered into the matrix $\mathbf{T} = [t_{i,j}]$, where a dash (-) for $t_{i,j}$ signifies travel is infeasible between nodes i and j. The times are symmetric and remain constant throughout the duration of the search.
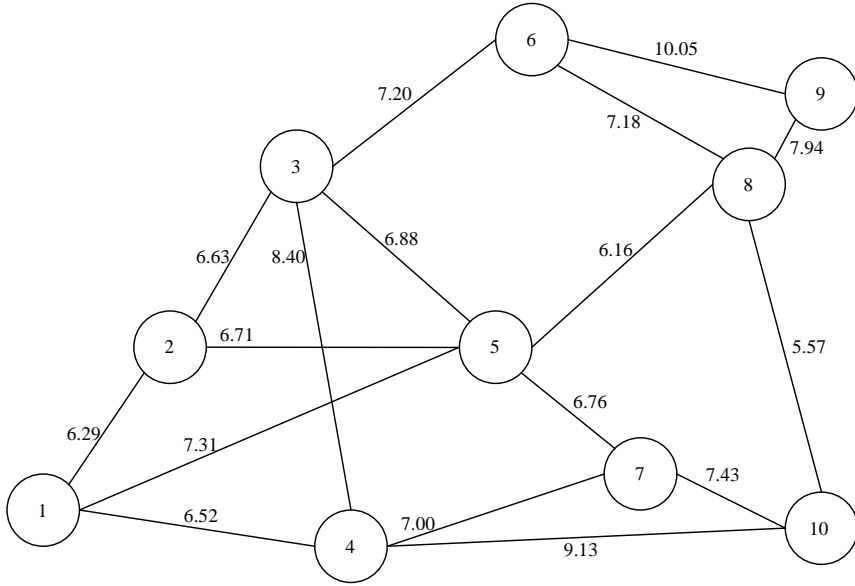
Figure 4.2   Network representation for the 10-node network.

$$
\mathbf{T} =
\begin{bmatrix}
- & 6.29 & - & 6.52 & 7.31 & - & - & - & - & - \\
6.29 & - & 6.63 & - & 6.71 & - & - & - & - & - \\
- & 6.63 & - & 8.40 & 6.88 & 7.20 & - & - & - & - \\
6.52 & - & 8.40 & - & - & - & 7.00 & - & - & 9.13 \\
7.31 & 6.71 & 6.88 & - & - & - & 6.76 & 6.16 & - & - \\
- & - & 7.20 & - & - & - & - & 7.18 & 10.05 & - \\
- & - & - & 7.00 & 6.76 & - & - & - & - & 7.43 \\
- & - & - & - & 6.16 & 7.18 & - & - & 7.94 & 5.57 \\
- & - & - & - & - & 10.05 & - & 7.94 & - & - \\
- & - & - & 9.13 & - & - & 7.43 & 5.57 & - & -
\end{bmatrix}
$$

The optimal path for this example problem was obtained using code written in the high-performance language MATLAB®. The code implicitly enumerates every feasible path that the search crew can complete in the allotted time of $T = 90$

Table 4.3   Parameter values for static/deterministic example.

Parameter	Description	Value
t_0	time since release	420 sec
q	amount of chemical agent released	1000 kg
k_x	eddy diffusivity	12 m^2/sec
k_y	eddy diffusivity	12 m^2/sec
k_z	eddy diffusivity	0.2113 m^2/sec
u	wind velocity	0.25 m/sec
h	height of release	50 m
v	vapor concentration threshold	0.0006 mg/m^3

Table 4.4   Vapor concentration and reward value for each node in the static/deterministic example ($v^* = 6.0 \times 10^{-4}$).

Node	v_j (x 10^{-3})	r_j
1	0.496	1
2	0.470	1
3	0.405	1
4	0.682	0
5	0.649	0
6	0.294	1
7	0.760	0
8	0.567	1
9	0.822	0
10	0.500	1

minutes to identify the policy ψ that maximizes

$$\sum_{i \in \mathcal{N}} \sum_{j \in \mathcal{N}} r_j x_{i,j}. \tag{4.4}$$

The solution to this problem, where we arbitrarily chose node $s = 5$ as the starting location is illustrated in Figure 4.3. This solution yields the integer reward of 6 which is the total number of areas whose vapor concentration is below the threshold level of $v^* = 0.0006$ mg/m^3. The path

$$\psi = \{5, 8, 10, 7, 4, 1, 2, 3, 6, 9\}$$

directs the search crew through the network and is able to reach each node exactly once in a total time of 62.85 minutes. There is a positive reward of 1 received from searching each of the nodes in the set

$$\mathcal{R} = \{1, 2, 3, 6, 8, 10\}.$$

No other path exists that reaches all ten nodes in less time. More importantly, the path ψ directs the crew through the site and reaches each of the critical areas where the level of MOPP can be reduced. The bold nodes in Figure 4.3 represent those areas of the site where protective gear is no longer required and the numbers on the arcs represent their order in the search. We provide an illustration for the static and stochastic case in the next section.
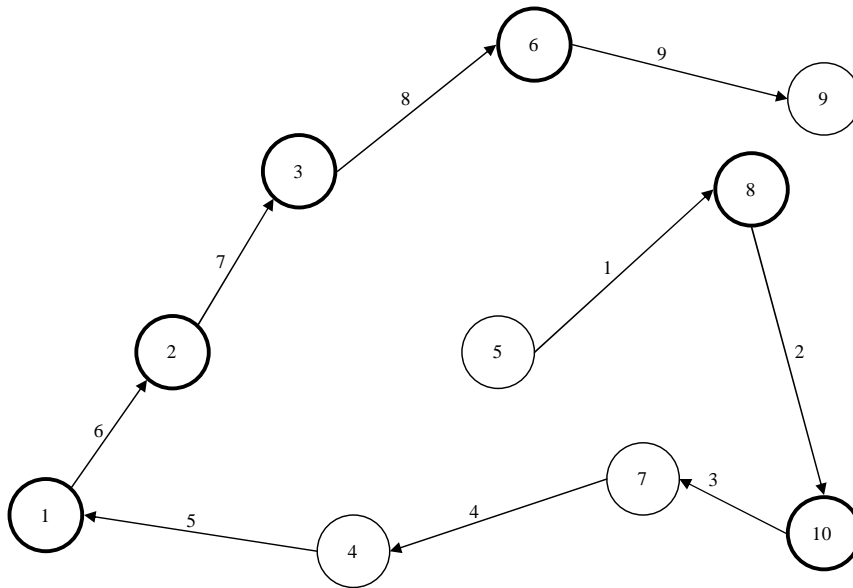
Figure 4.3   Optimal sampling path when concentrations are static and deterministic.

4.3 Example 2: Static and Stochastic Vapor Concentrations

For the case of static and stochastic vapor concentrations, the vapor concentration level at each node cannot be determined via a deterministic formula. Instead, we assume the concentration level is a time-invariant and continuous random variable.

We determine the expected value of the vapor concentration for each node at time t_0. Thus, time-invariant probability distributions and appropriate parameters are assigned to each node $j \in \mathcal{N}$. In this illustration, we use the continuous exponential distribution with rate parameter μ and cumulative distribution function (c.d.f)

$$F(x) = \begin{cases} 1 - \exp(-\mu x) & x \geq 0, \\ 0 & x < 0 \end{cases}.$$

The rate parameter for node j, μ_j, is recorded in Table 4.5.

Table 4.5   Rate parameters chosen for the exponential distributions used for example 2.

Node	μ_j
1	6666.67
2	1538.46
3	1322.75
4	1574.80
5	1754.39
6	10000.00
7	4347.83
8	2222.22
9	909.09
10	7692.31

The expected value of the random vapor concentration, $E[V_j]$ for each node $j \in \mathcal{N}$ is computed by

$$E[V_j] = 1/\mu_j. \tag{4.5}$$

These expected values are used to determine the reward value r_j for each node. Both of these values are recorded in Table 4.6.

Table 4.6   Expected vapor concentrations and rewards for example 2 ($v^* = 6.0 \times 10^{-4}$).

Node	$E[V_j](\times 10^{-4})$	r_j
1	1.50	1
2	6.50	0
3	7.56	0
4	6.35	0
5	5.70	1
6	1.00	1
7	2.30	1
8	4.50	1
9	11.00	0
10	1.30	1

Now that the expected value and expected reward for searching each node has been calculated, the same MATLAB® code used in section 4.2 is implemented to find the optimal path and total reward for sampling the areas. Again, since the algorithm seeks to find the path of shortest time throughout the site, the travel times have not changed, and the same starting node $s = 5$ is chosen. The optimal path is identical to the optimal path identified in the case of static and deterministic vapor concentrations. Thus, the solution is again

$$\psi = \{5, 8, 10, 7, 4, 1, 2, 3, 6, 9\}$$

with a total search time of 62.85 minutes. The solution is illustrated in Figure 4.4 where the bold nodes indicate locations containing vapor concentration levels below the threshold.

It is important to note the total reward has not changed from 6 but the six areas are not identical. This is due to the stochastic behavior of the secondary vapor concentrations at each node. Since the total reward in this case is based on expected values of the vapor concentrations, searching the site may, in fact, yield an actual reward value that differs from this reward. In this example, the areas in which a
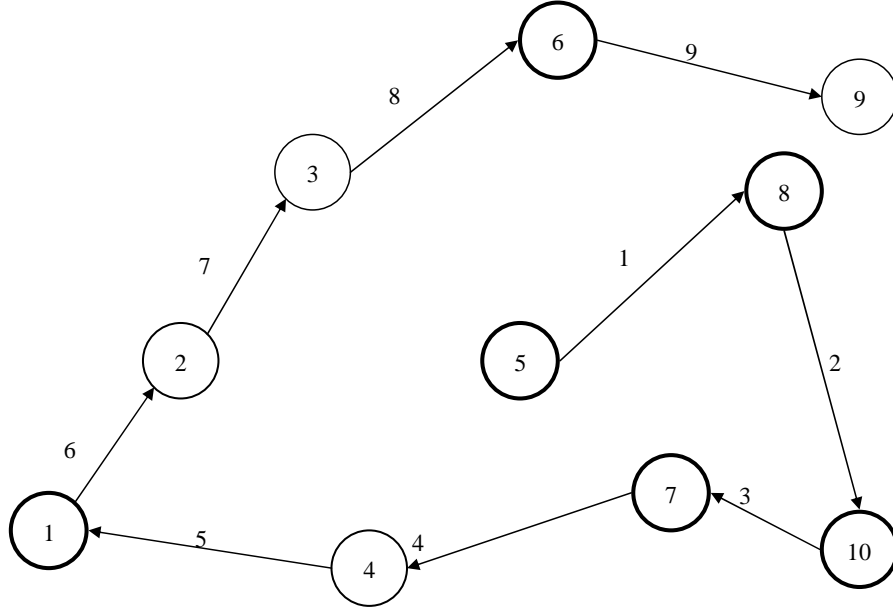
Figure 4.4   Optimal sampling path when vapor concentrations are static and stochastic.

reward is expected are

$$\mathcal{R} = \{1, 5, 6, 7, 8, 10\}.$$

The next section contains an illustration of the case with dynamic and deterministic vapor concentrations. Unlike the two previous examples, the vapor concentrations evolve over time, forcing the search crew to re-assess their route in a time-adaptive search.

4.4   Example 3: Dynamic and Deterministic Vapor Concentrations

Just as in the case of section 4.2, we assume vapor concentrations can be calculated at initial time t_0 using a deterministic formula. Using the same site and travel times from the previous two examples, we again use the advection-diffusion Equation (3.1) discussed in Chapter 3 to determine vapor concentrations for each area of the site.

Consider again the ten-node site depicted in Figure 4.2. Let the search crew begin at a node chosen arbitrarily, say node 5 (i.e., the starting node $s = 5$). Using Equation (3.1), the vapor concentration for the starting node $v_5(t_0)$ is computed using the initial time $t_0 = 7$ min (i.e., time since the chemical agent release).

Using the algorithm outlined in Chapter 3, subsection 3.2.3, and the time matrix $\mathbf{T}$, the initialization step yields the results in Table 4.7

Table 4.7   Results of initialization step for dynamic/deterministic example.

Node	t (sec)	$v_j(t)$	$r_j(t)$
5	420	0.00065	0

The set $\mathcal{R}$ remains empty and the set $\psi = \{5\}$. In step 2, the vapor concentration at nodes adjacent to node 5 are examined using the current time t_0 plus the travel time $t_{i,j}$ from node 5 to those adjacent nodes $j \in \mathcal{N}_i$ ($t = t_0 + t_{i,j}$). Recall, the time $t_{i,j}$ includes 5 minutes required for obtaining an instrument reading at node j. An indicator value of $r_j(t_0) = 1$ is assigned to node j if $v_j(t) < v^*$. The results of iteration 1 are displayed in Table 4.8. The anticipated reward of proceeding to each node adjacent to node 5 is 0 so the arc of shortest time is chosen (i.e., the arc from 5 to 8). The following updates are recorded:

$$
\begin{aligned}
t &= 420 + 369.6 = 789.6; \\
\mathcal{R} &= \emptyset; \\
\psi &= \psi \cup \{8\} = \{5, 8\}.
\end{aligned}
$$

Now the vapor concentration for each node adjacent to node 8 is calculated for $t = 789.6 + t_{8,j}$ for all $j \in \mathcal{N}_8$. Though the adjacent set $\mathcal{N}_8$ consists of the nodes $\{5, 6, 9, 10\}$, only nodes 6, 9, and 10 are considered since node 5 was previously sampled. That is, the crew cannot return to the node from which it has just departed.

Table 4.8   Results of iteration 1 for dynamic/deterministic example ($v^* = 6.0 \times 10^{-4}$).

Node	t (sec)	$v_j(t)$	r_j
1	858.6	0.0036	0
2	822.6	0.0035	0
3	832.8	0.0036	0
7	825.6	0.0064	0
8	789.6	0.0054	0

Table 4.9   Results of iteration 2 for dynamic/deterministic example ($v^* = 6.0 \times 10^{-4}$).

Node	t (sec)	$v_j(t)$	$r_j(t)$
6	1220.4	0.0048	0
9	1266.0	0.0080	0
10	1123.8	0.0070	0

After iteration 2, node 10 is chosen as the next node for the crew to search because the reward for all nodes adjacent to node 8 is 0 and the least time path is from 8 to 10. The nodes $\mathcal{N}_{10} = \{4, 7, 8\}$ are examined next. However, node 8 is momentarily excluded from consideration since it has just been searched. The algorithm continues for 12 iterations and terminates when the allotted time of 90 minutes (5400 seconds) is reached. The results of each iteration are recorded in Table 4.10 where the node in bold is the next node to be searched.

4-12

Table 4.10   Iterations 3-12 for dynamic/deterministic example ($v^* = 6.0 \times 10^{-4}$).

Node	t (sec)	$v_j(t)$	$r_j(t)$
	Iteration 3		
4	1671.6	0.0035	0
7	1569.6	0.0056	0
	Iteration 4		
4	1989.6	0.0024	0
5	1975.2	0.0028	0
	Iteration 5		
1	2413.8	0.00092	0
2	2377.8	0.0010	0
3	2388.0	0.0012	0
8	2344.8	0.0022	0
	Iteration 6		
6	2775.6	0.00091	0
9	2821.2	0.0013	0
10	2679.0	0.0014	0
	Iteration 7		
4	3226.8	0.00041	1
7	3124.8	0.00072	0
	Iteration 8		
1	3618	0.00016	1
3	3720.8	0.00017	1
7	3646.8	0.00033	1
	Iteration 9		
5	4052.4	0.00014	1
10	4092.6	0.00019	1
	Iteration 10		
4	4640.4	0.000050	1
8	4426.8	0.00011	1
	Iteration 11		
5	4796.4	0.000047	1
6	4857.6	0.000044	1
9	4903.2	0.000059	1
	Iteration 12		
6	5506.2	0.000017	1

The algorithm terminates after 12 iterations, yielding the path

$$\psi = \{5, 8, 10, 7, 5, 8, 10, 4, 7, 10, 8, 9\}$$

and reduced set

$$\mathcal{R} = \{4, 7, 8, 9, 10\}.$$

Area 6 would be the next area to search; however, the time required to travel to 6 and take the measurement exceeds the allotted time by 1.77 minutes so the algorithm terminates at node 9. The total reward for this example is 5, where areas not requiring protective gear are the nodes $j \in \mathcal{R}$. The total time required to complete the search (including obtaining instrument readings) is 81.72 minutes. Figure 4.5 graphically displays the search policy with bold nodes denoting those areas not requiring protective gear. The numbers along each arc indicate the order in which the arcs are added to the solution (i.e., the order of the sampling).
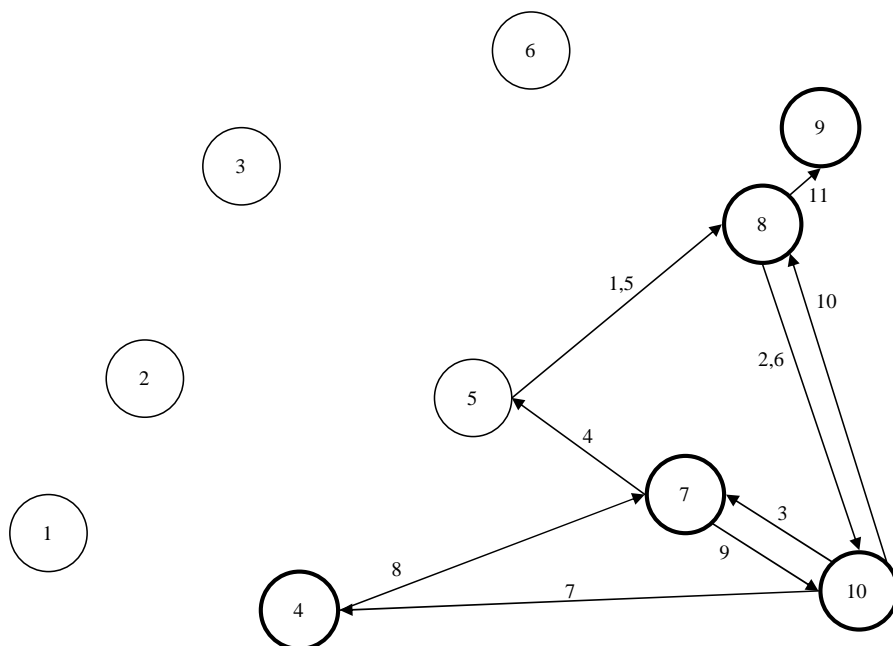
Figure 4.5   Optimal sampling path when vapor concentrations are dynamic and deterministic.

It is important to note the state of the system at the terminating time. Using Equation (3.1), the vapor concentration and reward value at each node is calculated for $t = 81.72$ min and these values are tabulated in Table 4.11. According to this information, all 10 areas of the site can safely operate without the protective gear. However, the search crew cannot reach all of those areas after the time when the vapor concentration decreases below the threshold and terminate the search within the allotted time of 90 minutes.

Table 4.11   Vapor concentration and reward for each node at algorithm's termination ($v^* = 6.0 \times 10^{-4}$).

Node	$v_j(81.72)$	$r_j(t)$
1	0.000023	1
2	0.000025	1
3	0.000030	1
4	0.000034	1
5	0.000040	1
6	0.000042	1
7	0.000052	1
8	0.000054	1
9	0.000059	1
10	0.000057	1

In the following section, we provide an example for the case of dynamic and stochastic vapor concentration levels. We employ the algorithm of Chapter 3, subsection 3.2.4 to identify a policy for directing a search crew through the site, by searching those areas *most likely* to have a vapor concentration below the threshold level.

4.5   *Example 4: Dynamic and Stochastic Vapor Concentrations*

Finally, we provide an illustration of the case of dynamic and stochastic vapor concentrations. More representative of the real-world problem, we allow the

secondary vapor concentrations to evolve over time according to a time-dependent probability distribution.

Consider the notional ten-node site depicted in Figure 4.2. Again, the time to travel from node i to node j remains fixed and the matrix of times $\mathbf{T}$ used for the previous examples is used here. Continuous probability distributions and parameters are assigned to each node $j \in \mathcal{N}$. For this example, we use the same distributions and initial parameters used in example 2 of section 4.3. Recall, we assume each node is governed by the exponential distribution with their initial rate parameters listed in Table 4.5.

In the case of dynamic and stochastic secondary vapor concentrations, the probability distributions change over time. Thus, for illustrative purposes, we choose the relationship

$$\mu_j(t + t_{i,j}) = (t + t_{i,j}) \times \mu_j^{-1}(t) \times 0.01 \tag{4.6}$$

to model the evolution of the distribution over time. Thus, at each iteration of the algorithm, the parameters are updated according to the time at which the search crew arrives at node $j \in \mathcal{N}$.

The algorithm presented in subsection 3.2.4 of Chapter 3 is implemented to find the path ψ for this case. As opposed to the algorithm employed in the previous section, it is the *probability* that a future node has a vapor concentration below the threshold that drives the solution identified at the termination of this algorithm. We again choose $s = 5$ as the starting location at time $t_0 = 420$ seconds. Using the probability distribution and parameter for node 5, a realization $v_5(420)$ of the random variable $V_5(420)$ is obtained by drawing a number from the appropriate exponential population (i.e., $V_5(420) \sim Exp(\mu_5(420))$).

Table 4.12 displays the results of the initialization step. At time $t_0 = 420$ sec, there is a 0.65 probability that the vapor concentration at node 5 is less than the threshold $v^* = 0.0006$ mg/m^3. The realization of the vapor concentration at node

5 at time 420 sec is 0.0011 mg/m^3. The realization value represents the instrument reading that will be taken at that time t in area 5 during the implementation of the path.

Table 4.12   Initialization step for dynamic/stochastic example.

Node	t (sec)	$\mu_j(t)$	$P(V_j(t) < v^*)$
5	420.0	1754.39	0.65

A reward value of 0 is assigned to node 5 for the current time and all nodes adjacent to node 5 are considered in the next step. The probability that the vapor concentration is below the fixed threshold for all nodes adjacent to node 5 is calculated. Based on these probabilities, recorded in Table 4.13, the next node is determined.

Table 4.13   Results of step 1 for dynamic/stochastic example.

Node	t (sec)	$\mu_j(t)$	$P(V_j(t) < v^*)$
1	858.6	775.19	0.372
2	822.6	186.92	0.106
3	832.8	158.73	0.091
7	825.6	526.32	0.271
8	789.6	281.69	0.155

The node chosen to be searched from node 5 is node 1 since it has the highest probability of having a vapor concentration below the threshold. Continuing in this fashion the algorithm terminates after twelve iterations. The resulting path is

$$\psi = \{5, 1, 5, 7, 10, 8, 6, 3, 5, 1, 4, 10\}$$

and this search is completed in 88.61 minutes.

Drawing random numbers from the family of exponential distributions for each node at each time, we determine the vapor concentration $v_j(t)$ for all $j \in \psi$ at the time they are searched. The values are recorded in Table 4.14.

4-17

Table 4.14   Vapor concentrations for nodes in ψ for dynamic/stochastic example ($v^* = 6.0 \times 10^{-4}$).

Node	t (sec)	$v_j(t)$	$r_j(t)$
5	420	0.0011	0
1	858.6	0.000012	1
5	1297.2	0.000106	1
7	1702.8	0.000172	1
10	2148.6	0.000103	1
8	2482.8	0.000113	1
6	2913.6	0.000172	1
3	3345.6	0.000179	1
5	3758.4	0.000609	0
1	4197.0	0.000693	0
4	4588.2	0.000803	0
10	5136.0	0.000001	1

Note, due to the dynamic and stochastic behavior of the secondary vapor concentrations, nodes that initially have concentrations below the threshold may become contaminated at later times. The total reward of this policy at the termination of the allotted search time is 5. Though the sum of the reward values in Table 4.14 is 8, one of those nodes (node 10) is repeated and two (nodes 1 and 5) have vapor concentrations that increase above the threshold v^* when searched again. Hence, the reduced set at the termination is

$$\mathcal{R} = \{3, 6, 7, 8, 10\}.$$

Thus, these 5 areas are the areas *most likely* to operate safely without protective gear.

Figure 4.6 is the graphical representation of the path ψ, where the bold nodes represent areas where protective gear is not required. The numbers along each arc indicate the order in which the arc is added to the solution.
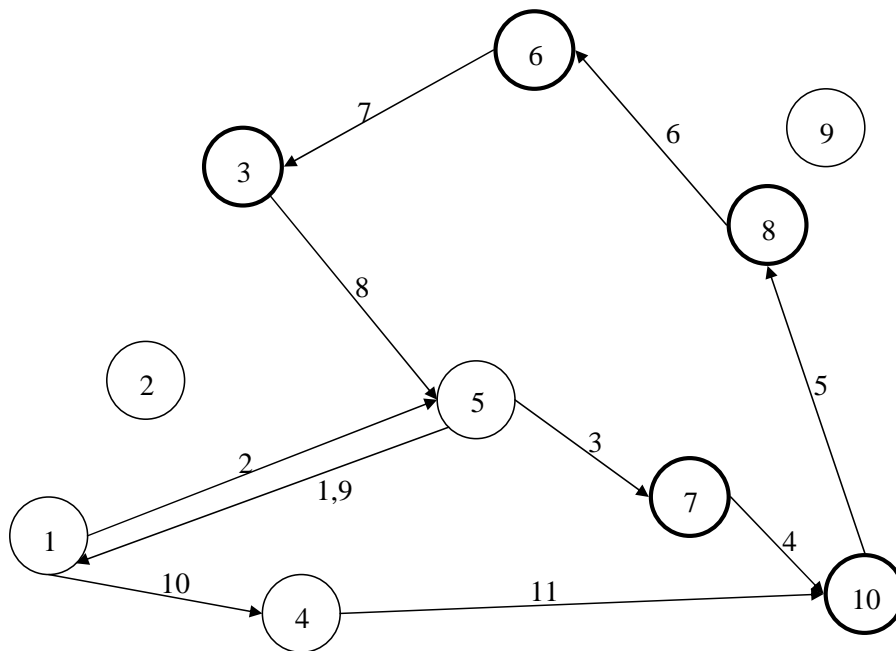
Figure 4.6   Optimal sampling path when vapor concentrations are dynamic and stochastic.

4.6   Comparison of Static and Dynamic Deterministic Solutions

The examples of sections 4.2 and 4.4 provide the basis for analyzing the impact of ignoring (or incorporating) time into the mathematical models developed in Chapter 3. We show there is a difference between the case where vapor concentration levels remain static and when they evolve over time.

Table 4.15 displays the solution to example 1 (static and deterministic) and example 3 (dynamic and deterministic). The optimal path for example 1

$$\psi = \{5, 8, 10, 7, 4, 1, 2, 3, 6, 9\}$$

directs the search crew through all ten nodes, reaching each one exactly once, in $\tau^* = 62.85$ minutes. The total reward, found from deterministically calculating the vapor concentration for each node $j \in \mathcal{N}$, is 6. They should find that nodes in the

reduced set

$$\mathcal{R} = \{1, 2, 3, 6, 8, 10\}$$

have vapor concentrations below the fixed threshold.

The optimal path of example 3,

$$\psi = \{5, 8, 10, 7, 5, 8, 10, 4, 7, 10, 8, 9\}$$

requires $\tau^* = 81.72$ minutes to complete, and never reaches nodes 1, 2, 3, or 6. The neglect of these nodes is due to the dynamic nature of the secondary vapor concentrations. In this case, the concentration of the node at the crew's arrival time drives the algorithm. For all nodes with a concentration below the threshold, the algorithm always chooses the vapor concentration closest to the threshold. If none of the nodes will have a concentration below the threshold, the algorithm chooses the closest (in distance or time) node. This also allows nodes to be searched if the vapor concentration decreases, even though it has been previously searched.

Note, in example 1 (static/deterministic vapor concentrations), 27.15 minutes remain in the time allotted for the search. We know vapor concentrations evolve over time, so those extra minutes are valuable in allowing the search crew to reach more nodes at later times to record any change in concentration, either positive or negative.

Figures 4.7 and 4.8 show the temporal evolution of the vapor concentrations for each node throughout the duration of the search for example 3. The vapor concentration from the static case in example 1 can also be seen on the plot. They are the vapor concentrations at time 420 seconds. It is clear that time directly impacts the vapor concentrations and thus, must be considered when developing a search policy that will optimally route a crew.

In example 3, only fifty percent of the nodes were found to have a vapor concentration less than the threshold, whereas in example 1, sixty percent of the

Table 4.15   Comparison of solutions to the static/deterministic and dynamic/deterministic examples.

Static		Dynamic	
Node	r_j	Node	$r_j(\tau)$
5	0	5	0
8	1	8	0
10	1	10	0
7	0	7	0
4	0	5	0
1	1	8	0
2	1	10	0
3	1	4	1
6	1	7	1
9	0	10	1
		8	1
		9	1
Total Time (min)	r^*	Total Time (min)	$r^*(\tau^*)$
62.85	6	81.72	5

nodes no longer required protective gear. However, only two of those nodes have vapor concentrations below the threshold in the example solutions. Thus, had the effect of time been ignored, personnel in areas 1, 2, 3, and 6 may have been harmed by not donning their protective equipment. The safe nodes of example 3 (nodes 4, 7, 8, 9, and 10) may be more accurate since they account for the evolution of the vapor concentrations over time.

In the next section, we compare the results of examples 2 and 4. This allows us to examine the impact of temporal evolution when we assume vapor concentrations are stochastic rather than deterministic.

4.7   Comparison of Static and Dynamic Stochastic Solutions

The comparison of examples 2 and 4 provide an interesting analysis of the effect of time of the secondary vapor concentrations when they are assumed to behave according to continuous probability distributions. In example 2, the probability
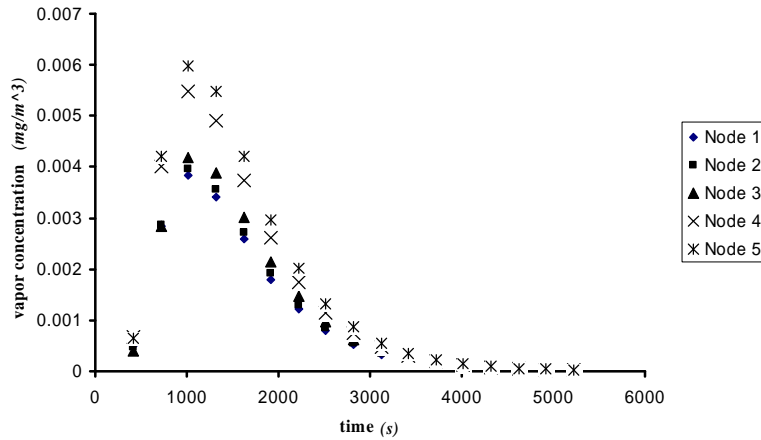
Figure 4.7   Evolution of vapor concentrations over time from example
3, nodes 1 through 5.

distributions are static and in example 4, they are time-variant. Recall, the result
of example 2 yields a path

$$\psi = \{5, 8, 10, 7, 4, 1, 2, 3, 6, 9\}$$

directing the search crew to all ten areas, reaching each one exactly once. In example
4, when time is incorporated into the methodology, the resulting path

$$\psi = \{5, 1, 5, 7, 10, 8, 6, 3, 5, 1, 4, 10\}$$

directs the search crew to just 8 of the 10 nodes. However, in example 4, the search
requires 88.61 minutes as opposed to the 62.85 required for example 2. The longer
search time in the dynamic case is a result of allowing previously searched nodes to
be searched again. Since the expected vapor concentrations are time-dependent there
exists a nonzero probability that the vapor concentration at a node may increase (or
decrease) over time. Thus, several of the nodes are searched more than once while
others are never searched at all.

In both examples, the vapor concentrations behave according to exponential
probability distributions. It is the probability that a vapor concentration is below
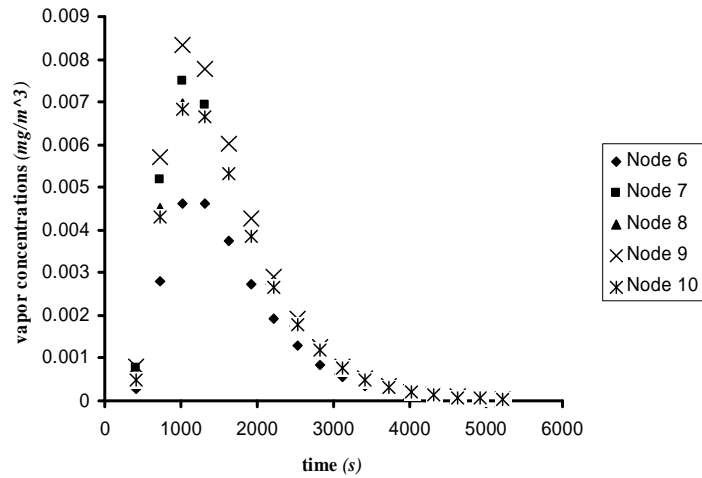
Figure 4.8   Evolution of vapor concentrations over time from example
3, nodes 6 through 10.

the threshold that drives the node selection in the algorithm in example 4. Thus, it
directs the crew as follows:

$$\psi = \{5, 1, 5, 7, 10, 8, 6, 3, 5, 1, 4, 10\}.$$

The reward for case 4 stems from searching nodes in the reduced set

$$\mathcal{R} = \{3, 6, 7, 8, 10\}.$$

Whereas the solution to example 2 is to search the nodes in the following order:

$$\psi = \{5, 8, 10, 7, 4, 1, 2, 3, 6, 9\}$$

with a reward for searching nodes

$$\mathcal{R} = \{1, 5, 6, 7, 10\}.$$

Table 4.16 Comparison of solutions to the static/stochastic and dynamic/stochastic examples.

Static		Dynamic	
Node	r_j	Node	$r_j(\tau)$
5	1	5	0
8	1	1	0
10	1	5	0
7	1	7	1
4	0	10	1
1	1	8	1
2	0	6	1
3	0	3	1
6	1	5	0
9	0	1	0
		4	0
		10	1
Total Time (min)	r^*	*Total Time* (min)	$r^*(\tau^*)$
62.85	6	88.61	5

The case assuming stochastic and dynamic vapor concentrations suggests that 50 percent of the nodes no longer require protective gear. If the policy for example 2 had been followed, they would believe that 60 percent of the areas can operate safely without protective gear; thus jeopardizing the personnel in those areas where the progression of time may cause the vapor concentrations to contaminate those areas that may have previously been deemed "safe."

4.8 Summary of Results

The four numerical examples provided in this chapter demonstrate the impact of increasing the complexity of the problem on the solution. In the first and most simplistic case, we determine that the optimal path is one that samples every node exactly once in the minimum amount of time. However, this case does not capture the true behavior of secondary vapor concentrations that are known to evolve over time and are subject to stochastic elements (e.g., wind, temperature, etc.). In the

real problem, it may be beneficial to re-examine an area if it is likely the vapor concentration has changed. Thus, the state of the system in the first example may not accurately represent the true state, resulting in a suboptimal solution of the real problem. The second case assumes vapor concentrations are governed by time-invariant probability distributions. The optimal path is identical to the path of the previous example, but the total reward is different due to the stochastic nature.

The last two numerical illustrations demonstrate the impact time has on the solution. In example 3, we assume the vapor concentrations can be computed by an equation that depends on time. The crew does not search every node in the optimal solution and searches some more than once. The solution procedure accounts for the evolution of the vapor concentrations over time and chooses where to direct the crew based on the calculated concentration at their time of arrival. Thus, the state of the system in example 3 is more representative of reality than either example 1 or 2. Finally, example 4 attempts to capture the true nature of the problem. The vapor concentration at each node evolves according to a time-dependent probability distribution. As time progresses, the probability a node has a vapor concentration below (or above) the threshold also evolves. Thus, in these illustrations, the resulting path accounts for the effect time has on the chemical agent as well as the effect time has on the probability distribution.

Consider the result of example 1, the case of static and deterministic vapor concentrations. The optimal path is one that reaches each node exactly once. Comparing this result with that of the dynamic and deterministic example emphasizes the impact of incorporating temporal evolution into the model. In example 3, the optimal path directs the search crew to some nodes more than once and others not at all. Due to the temporal evolution of vapor concentrations, some areas are more critical than others and require being searched several times, and those that will not change enough to warrant a search are excluded from the solution. Similar comparisons can be made with examples 2 and 4, the cases considering stochastic vapor

concentrations. Observing the results of both dynamic cases and comparing them with their static counterparts demonstrates that ignoring the temporal evolution of the vapor concentrations could lead to suboptimal results that overestimate (or underestimate) the number of areas operating safely without protective gear. For example, if the optimal path of example 1 is followed, four areas would be operating dangerously without protective gear because in example 3, those four areas are found to be hazardous at later times. Also, three of the areas would be inhibited by the cumbersome gear, when they could be operating safely without it. Likewise, the stochastic cases can be compared with a similar outcome.

It is important to note the examples in this chapter provide numerical illustrations based on several restrictive assumptions. A possible explanation for the results observed in these illustrations is that we assumed independent vapor concentration samples at each area over time. This may explain why we observed higher vapor concentrations in some areas at a point in time when it was previously below the threshold. In order to relax this assumption, we need a stochastic process in time and space describing the vapor concentration evolution. In the next chapter we provide a summary of this thesis, concluding remarks, and propose areas of future work.

5. Conclusions and Future Research

The threat of terrorist attacks with biological or chemical weapons has become a serious consideration for nations and their military forces. Modern research is underway for identifying emergency response procedures for specific biological weapons and for the incorporation of new sensor technologies and instruments for identifying and quantifying chemical contamination. However, methods for effectively sampling (in an optimal manner) chemical hazard areas subsequent to a chemical weapons attack lag far behind. This thesis has provided a methodological framework for incorporating real-time information for the purpose of optimally sampling a site contaminated by an initial chemical attack and hazardous secondary chemical vapor concentrations.

Three distinct cases of the problem were considered before the fourth (and most realistic case) was examined. These cases were: static and deterministic vapor concentration levels, static and stochastic vapor concentration levels, dynamic and deterministic vapor concentration levels, and dynamic and stochastic vapor concentration levels. For each of the four cases, the objective function and relevant constraints were defined and a solution methodology presented. The first two cases ignored the temporal evolution of vapor concentrations and focused on identifying the optimal path through a static system to maximize the reward (i.e., the number of areas no longer requiring protective gear). The final two cases incorporated temporal evolution of the chemical vapor concentrations to more accurately model the real world problem. The results of this thesis represent a significant contribution to the military operations research and bio-chemical defense communities by providing a method that can be implemented quickly and efficiently in response to a chemical attack on a military installation.

The methodology for each case was illustrated on four numerical example problems to identify the optimal path that results in the maximum reward within the

allotted time for the search. The parameters were defined, and the algorithm developed for each specific case was implemented to obtain those results. Finally, the result of the two static examples were compared with their respective dynamic counterparts to highlight the impact of the temporal evolution of vapor concentrations on the solution. It is clear that incorporating this evolution into the model resulted in solutions that captured more of the real problem's dynamics, thus maximizing the number of areas in an attacked site that can operate safely without the cumbersome protective gear. Ignoring the temporal evolution of the vapor concentrations may result in removing the protective gear requirement in areas that may subsequently become contaminated, thus exposing humans to an unnecessary hazard.

To realistically implement the techniques presented in this thesis, all of the parameters relevant to the methodology must be known. This thesis covers a small part of a much larger problem: estimating future downwind hazard areas when only detector/sensor data (e.g., human input, M-8/M-9 paper, etc.) is known and using those inputs to also estimate the source location and strength of the chemical agent release. The last part of the problem is to estimate the area of contamination. We assume this information is known *a priori*, allowing us to optimally direct a search crew through the site to sample areas likely to have vapor concentrations below a fixed threshold, indicating the area is safe.

Despite the fact that we assume the dynamics of the problem, the results of this thesis provide insight into data requirements for optimally sampling a chemical hazard area. For example, a model for estimating the spatiotemporal evolution of secondary vapor concentrations is critical to providing information regarding the concentration's probability distribution for each area. Employing a realistic model provides a means to identify areas likely (or unlikely) to be contaminated. These distributions may subsequently be applied to the stochastic cases of sections 3.2.2 and 3.2.4. Once the information is obtained, one can identify the areas that can safely operate without protective gear.

Another restrictive assumption of this thesis is the use of static and deterministic travel times between adjacent areas of the site. Traffic, obstacles, and other such impediments are likely to delay the search crew or prohibit it from taking a path altogether. Incorporating dynamic and stochastic travel times will result in solutions with a least expected time path with a maximum reward. Relaxing this assumption also leads to possible research in incorporating real-time information into the methodology. For example, as routes open or close due to unforseen circumstances, the solution path can be updated to accommodate these changes.

Relaxing the assumption of a single search crew would also result in different methodology. If more than one crew were available, a higher number of areas may be searched within the allotted time, resulting in more areas operating in the *correct* level of protective gear. Having a number of crews equal to the number of areas would be ideal because the problem would reduce to finding the shortest path from each crew's location to a specific area.

Finally, another area for future research involves incorporating real-time data into the methodology to better model the behavior of the secondary vapor concentrations. This is due to the temporal and spatial evolution as well as stochastic elements (e.g., wind direction and velocity, temperature, humidity, etc.) affecting the behavior. Once future downwind hazard areas can be identified and the inputs required for estimating parameters for those areas can be determined, they can be incorporated into the techniques developed in this thesis providing an optimal path.

The main results of this thesis reach far beyond military applications only. Hazardous vapor concentrations resulting from industrial accidents may contaminate surrounding communities, threatening the lives of civilians within some radius of the contamination. Having a procedure to optimally sample the affected area as quickly as possible (to identify which residents should be evacuated) is invaluable to saving lives. Also, should a chemical agent be released over a city or region, such a procedure

may directly help emergency crews identify contaminated areas and evacuate them in an efficient and timely manner.

Appendix A. Static/Deterministic Code

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%   Computing STATIC vapor concentrations for (x,y) coordinates      %
%                                                                    %
%    The purpose of this MATLAB code is to compute the static and    %
%    deterministic vapor concentrations for the network used in      %
%    this thesis.                                                    %
%                                                                    %
%    Author: Jennifer R. Plourde, AFIT/ENS GOR-05M                   %
%    Date: 1 Feb 05                                                  %
%    Last revised: 1 Feb 05                                          %
%    References:  Kathirgamanathan, P., McKibbin, R. and             %
%            R.I. McLachlan (2003). Source release-rate estimation   %
%            of atmospheric pollution from a non-steady point source %
%            - Part 1: Source ate a known location.  Res. Lett. Inf. %
%            Math. Sci. vol 5, 71-84.                                %
%                                                                    %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


%%%%%%%%%%%%%%%%%%%%%% VARIABLE DEFINITIONS %%%%%%%%%%%%%%%%%%%%%%%%%%%
%   Inputs required:                                                 %
%   nel: number of nodes                                             %
%   tm: (nel x nel)matrix of feasible travel times between nodes     %
%   X: (nel x 1) vector of x-coordinates                             %
%   Y: (nel x 1) vector of y-coordinates                             %
%   Z: (nel x 1) vector of z-coordinates (z = 0, for this thesis)    %
%   V: vapor threshold value                                         %
%   Q: total mass release (kg)                                       %
%   K_x, K_y, K_z: eddy diffusivities for x, y, z  (m^2s^-1)         %
%   H: height above the ground where release occurs (m)             %
%   U: wind velocity (m/s)                                           %
%                                                                    %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
clc;
clear;
format long;




%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Time matrix                                       %
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
tm =[ inf    6.29   inf    6.52   7.31   inf    inf    inf    inf    inf

      6.29   inf    6.63   inf    6.71   inf    inf    inf    inf    inf

      inf    6.63   inf    8.4    6.88   7.2    inf    inf    inf    inf

      6.52   inf    8.4    inf    inf    inf    7      inf    inf    9.13

      7.31   6.71   6.88   inf    inf    inf    6.76   6.16   inf    inf

      inf    inf    7.2    inf    inf    inf    inf    7.18   10.05  inf

      inf    inf    inf    7      6.76   inf    inf    inf    inf    7.43

      inf    inf    inf    inf    6.16   7.18   inf    inf    7.94   5.57

      inf    inf    inf    inf    inf    10.05  inf    7.94   inf    inf

      inf    inf    inf    9.13   inf    inf    7.43   5.57   inf    inf];


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% x, y coordinates                                     %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
X = [6.275673696

     14.46607868

     33.29676199

     42.99188208

     60.2395703

     71.90038759

     86.36478774

     94.14929655

     98.82869961

     99.741966];


Y = [23.01492355

     56.52684103

     96.01718192

     5.234534745

     53.50444044

     140.5256813

     36.6666158

     86.36143071

     7.663960692

     100.4998932];


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Parameters for sample advection-diffusion equation used %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
nel = 10;
Q = 1000;
K_x = 12;
```

```
K_y = 12;
K_z = .2113;
Z=0;
H=50;
U=.25;
V = 0.0006;
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

t = 7*60; % time since release
for i = 1:nel
    % Computes the vapor concentration (kg/m^3) for location (x_i,y_i)
    v(i) =  Q/(8*pi^(3/2)*(K_x*K_y*K_z)^(1/2)*t^(3/2))
            *exp(-(X(i)-U*t)^2/(4*K_x*t)-Y(i)^2/(4*K_y*t))*(2*exp(-(H)^2/(4*K_z*t))));
    % Converts units to mg/m^3
    v(i) =  v(i)*1000;
end

for i = 1:nel
    % If the vapor concentration at location i is below the threshold, a
    % reward value of 1 is assigned, else a value of zero is assigned
    if v(i) < V
        r(i) = 1;
    else
        r(i) = 0;
    end
 end
v
r
```

Appendix B. Dynamic/Deterministic Code

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%   Computing Dynamic and Deterministic                      %
%   vapor concentrations for (x,y) coordinates               %
%                                                            %
%   The purpose of this MATLAB code is to compute the dynamic and %
%   deterministic vapor concentrations for the network used in   %
%   this thesis.                                             %
%                                                            %
%   Author: Jennifer R. Plourde, AFIT/ENS GOR-05M            %
%   Date: 1 Feb 05                                           %
%   Last revised: 1 Feb 05                                   %
%   References:  Kathirgamanathan, P., McKibbin, R. and      %
%           R.I. McLachlan (2003). Source release-rate estimation %
%           of atmospheric pollution from a non-steady point source %
%           - Part 1: Source ate a known location.  Res. Lett. Inf. %
%           Math. Sci. vol 5, 71-84.                         %
%                                                            %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


%%%%%%%%%%%%%%%%%%%%%% VARIABLE DEFINITIONS %%%%%%%%%%%%%%%%%%%%%
%   Inputs required:                                         %
%   nel: number of nodes                                     %
%   tm: (nel x nel) matrix of feasible arc times between nodes (min) %
%   X: (nel x 1) vector of x-coordinates                     %
%   Y: (nel x 1) vector of y-coordinates                     %
%   Z: (nel x 1) vector of z-coordinates (z = 0, for this thesis) %
%   vt: vapor threshold value                                %
%   Q: total mass release (kg)                               %
%   K_x, K_y, K_z: eddy diffusivities for x, y, z  (m^2s^-1) %
%   H: height above the ground where release occurs (m)      %
%   U: wind velocity (m/s)                                   %
%   T: time allotted for search                              %
%   current: starting location                               %
%   R: set of nodes in the path                              %
%   reduced: set of nodes with reward of 1                   %
%   N: set of nodes 1:nel                                    %
%   Ni: set of node adjacent to node i                       %
%   tf: future time (t + t_i,j)                              %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


clc;
```

```
clear;
format long;


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% User Inputs                                               %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


nel = 10;
T = 90;
vt = 0.0006;
current = 5;
Q = 1000;
K_x = 12;
K_y = 12;
K_z = .2113;
Z=0;
H=50;
U=.25;


tm =[   inf     6.29    inf     6.52    7.31    inf     inf     inf     inf     inf
        6.29    inf     6.63    inf     6.71    inf     inf     inf     inf     inf
        inf     6.63    inf     8.4     6.88    7.2     inf     inf     inf     inf
        6.52    inf     8.4     inf     inf     inf     7       inf     inf     9.13
        7.31    6.71    6.88    inf     inf     inf     6.76    6.16    inf     inf
        inf     inf     7.2     inf     inf     inf     inf     7.18    10.05   inf
        inf     inf     inf     7       6.76    inf     inf     inf     inf     7.43
        inf     inf     inf     inf     6.16    7.18    inf     inf     7.94    5.57
        inf     inf     inf     inf     inf     10.05   inf     7.94    inf     inf
        inf     inf     inf     9.13    inf     inf     7.43    5.57    inf     inf];

    X = [6.275673696
        14.46607868
        33.29676199
        42.99188208
        60.2395703
        71.90038759
        86.36478774
        94.14929655
        98.82869961
        99.741966];


    Y = [23.01492355
        56.52684103
```

```
        96.01718192
        5.234534745
        53.50444044
        140.5256813
        36.6666158
        86.36143071
        7.663960692
        100.4998932];


reduced = [];
R = [current];


for i = 1:nel
    N(i) = 1;
end


% initial starting time
t = 7*60; % in seconds


%Initialization step
for i = current
    v(i) =  Q/(8*pi^(3/2)*(K_x*K_y*K_z)^(1/2)*t^(3/2))
            *exp(-(X(i)-U*t)^2/(4*K_x*t)-Y(i)^2/(4*K_y*t))*(2*exp(-(H)^2/(4*K_z*t)));
    v(i) = v(i)*1000;  %converts to mg
    if v(i) < vt & v(i) > 0
        r(i) = 1;
    else
        r(i) = 0;
    end
end


% If initial v < V, current is subtracted from set of nodes to visit
% Otherwise, it is still eligible to be searched


N(i) = N(i) - 1;


%%%%%%%End Initialization%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%   Step 1                                    %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


b = 0;
while t < 90*60
```

```
N;
for f = 1:nel
    if tm(current, f) == inf
        Ni(f) = 0;
    else
        Ni(f) = 1;
    end
end
Ni;
t = t/60; %return time units to minutes because of tm

%Calculate vapor concentration for each node j
for j = 1:nel
    tf = t + tm(current, j);
    tf = tf*60;   %converts to seconds
    v(j) = Q/(8*pi^(3/2)*(K_x*K_y*K_z)^(1/2)*tf^(3/2))
            *exp(-(X(j)-U*tf)^2/(4*K_x*tf)-Y(j)^2/(4*K_y*tf))*(2*exp(-((H)^2)/(4*K_z*tf)));
    v(j) = v(j)*1000; % converts to mg
end

for j = 1:nel
    if v(j) < 0
        v(j) = -v(j);
    end
end

false = 0;
used = false;

% Allow return to previously visited node if there is no other option
if max(N + Ni) <= 1
    ntmp = N;
    N = N + Ni;
    used = 1;
end

% If a node has been visited, set v < 0 so it won't be considered
for j = 1:nel
    if Ni(j) == 1
        v(j) = v(j);
    elseif Ni(j)
        v(j) = -v(j);
    end
```

```
    end


if b > 2
    temp = R(b - 1);


    if v(temp) > 0
        v(temp) = -v(temp);
    end
end


if used
    N = ntmp;
end
v
% If v < V, set r = 1 (MOPP reduced) o.w. r = 0
for j = 1:nel
    if v(j) < vt & v(j) >= 0
        r(j) = 1;
    else
        r(j) = 0;
    end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%    Step 2                                       %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


if r == 0
    for j = 1:nel
        if v(j) < 0
            ty(j) = inf;
        else
            ty(j) = tm(current,j);


        end
        M = min(ty);
    end
end


if sum(r) > 0


    for j = 1:nel
        if r(j) == 1
            M(j) = v(j);
```

```matlab
        else
            M(j) = 0;
        end
    end
end


P = max(M);
k = 0;


% Record j as the next node
for j = 1:nel
    if v(j) == P
        next = j ;
    elseif tm(current, j) == P
        next = j;
    end
end
for j = 1:nel
    if next == j
        if r(j) == 1
            k = j;
        end
    end
end
if k ~= 0
    reduced = [reduced, k];
end


% Remove j from further consideration
for j = 1:nel
    if j == next
        %  r(j) = 1;


        N(j) = N(j) - 1;
    end
end
%update time step
t = t + tm(current, next) ; % minutes
t = t*60;  %converts to seconds


if r(next) == 1
    N(next) = -1;
end
```

```
%Set next node as current and return to step 1


current = next;
if N == 0
    for j =1:nel
        if r(j) == 0
            N(j) = 1;
        else
            N(j) = 0;
        end
    end
end


R = [R, next];
b = length(R);
if N < 0
    break
end
ed = length(R);
edr = length(reduced);


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%   Step 3                                      %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
if t > 90*60

    over = length(R) - 1;
    R(over);
    time = t - tm(R(over),R(length(R)))*60;
    R(ed) = R(ed) - R(ed);
    reduced(edr) = reduced(edr) -reduced(edr);
    for j = 1:nel
        v(j) = Q/(8*pi^(3/2)*(K_x*K_y*K_z)^(1/2)*t^(3/2))
            *exp(-(X(j)-U*t)^2/(4*K_x*t)-Y(j)^2/(4*K_y*t))*(2*exp(-((H)^2)/(4*K_z*t)));
        v(j) = v(j)*1000; %mg
        for j = 1:nel
            if v(j) < vt
                r(j) = 1;
            else
                r(j) = 0;
            end
        end
    end
```

```
        end
      end
end

path = R;
path
edr = edr -1;

disp(['The number of areas in reduced MOPP is ' int2str(edr)])
disp(['These areas are ' int2str(reduced)])
disp(['The total time of the search is ' num2str(time/60) ' minutes.'])
```

Appendix C. Dynamic/Stochastic Code

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%    Computing Dynamic and Stochastic                           %
%    vapor concentrations for (x,y) coordinates                 %
%                                                                %
%    The purpose of this MATLAB code is to compute the dynamic and %
%    stochastic vapor concentrations for the network used in    %
%    this thesis.                                                %
%                                                                %
%    Author: Jennifer R. Plourde, AFIT/ENS GOR-05M              %
%    Date: 1 Feb 05                                              %
%    Last revised: 1 Feb 05                                      %
%    References:  Kathirgamanathan, P., McKibbin, R. and        %
%           R.I. McLachlan (2003). Source release-rate estimation %
%           of atmospheric pollution from a non-steady point source %
%           - Part 1: Source ate a known location.  Res. Lett. Inf. %
%           Math. Sci. vol 5, 71-84.                            %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%% VARIABLE DEFINITIONS %%%%%%%%%%%%%%%%%%%%%%%%%
%    Inputs required:                                           %
%    nel: number of nodes                                       %
%    tm: (nel x nel) matrix of feasible arc times between nodes (min) %
%    X: (nel x 1) vector of x-coordinates                       %
%    Y: (nel x 1) vector of y-coordinates                       %
%    Z: (nel x 1) vector of z-coordinates (z = 0, for this thesis) %
%    vt: vapor threshold value                                  %
%    Q: total mass release (kg)                                 %
%    K_x, K_y, K_z: eddy diffusivities for x, y, z  (m^2s^-1)   %
%    H: height above the ground where release occurs (m)        %
%    U: wind velocity (m/s)                                     %
%    T: time allotted for search                                %
%    current: starting location                                 %
%    R: set of nodes in the path                                %
%    reduced: set of nodes with reward of 1                     %
%    N: set of nodes 1:nel                                      %
%    Ni: set of node adjacent to node i                         %
%    tf: future time (t + t_i,j)                                %
%    mu: (1 x nel) vector of expected value of                  %
%        vapor concentration for each node                      %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
clc;
clear;
```

```
format long;

nel = 10;
T = 90;
vt = 0.0006;
current = 5;
Q = 1000;
K_x = 12;
K_y = 12;
K_z = .2113;
Z=0;
H=50;
U=.25;
mu = [ .00015 .00065 .000756 .000635 .00057 .0001 .00023 .00045 .0011 .00013];%EV's

tm =[inf    6.29    inf    6.52   7.31    inf    inf    inf    inf    inf
     6.29    inf    6.63    inf   6.71    inf    inf    inf    inf    inf
     inf    6.63    inf    8.4   6.88    7.2    inf    inf    inf    inf
     6.52    inf    8.4    inf    inf    inf    7      inf    inf    9.13
     7.31   6.71   6.88    inf    inf    inf    6.76   6.16    inf    inf
     inf    inf    7.2    inf    inf    inf    inf    7.18   10.05   inf
     inf    inf    inf    7     6.76    inf    inf    inf    inf    7.43
     inf    inf    inf    inf   6.16    7.18    inf    inf    7.94   5.57
     inf    inf    inf    inf    inf   10.05    inf    7.94    inf    inf
     inf    inf    inf    9.13    inf    inf    7.43   5.57    inf    inf];

    X = [6.275673696
        14.46607868
        33.29676199
        42.99188208
        60.2395703
        71.90038759
        86.36478774
        94.14929655
        98.82869961
        99.741966];

    Y = [23.01492355
        56.52684103
        96.01718192
        5.234534745
        53.50444044
        140.5256813
```

```
     36.6666158
     86.36143071
     7.663960692
     100.4998932];

reduced = [];
R = [current];


for i = 1:nel
    N(i) = 1;
end


%Time since release
t = 7*60 ;%seconds


rand('state', 135);


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%  Initialization                               %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
for i = current
        V(i) = expcdf(vt, mu(i));
        v(i) = exprnd(mu(i));
    if v(i) < vt & v(i) > 0
        r(i) = 1;
        reduced = [reduced, i];
    else
        r(i) = 0;
    end
end


N(i) = N(i) - 1;
%%%%%%%%End Initialization%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%   Step 1                                       %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
b = 0;
while t < 90*60
    for f = 1:nel
        if tm(current, f) == inf
            Ni(f) = 0;
        else
            Ni(f) = 1;
```

```
        end
end
t = t/60; %return time units to minutes because of tm

for j = 1:nel
    tf = t + tm(current, j);
    tf = tf*60;
    if Ni(j) == 1;
            mum(j) = mu(j)*.01*tf;
            V(j) = expcdf(vt, mum(j));
    else
        V(j) = 0;
    end
end
V
for j = 1:nel
    if V(j) < 0
        V(j) = -V(j);
    end
end

false = 0;
used = false;
% Allow return to previously visited node if there is no other option
if max(N + Ni) <= 1
    ntmp = N;
    N = N + Ni;
    used = 1;
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%   Step 2                                         %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% If a node has been visited, set v < 0 so it won't be considered
for j = 1:nel
    if Ni(j) == 1
        V(j) = V(j);
    elseif Ni(j)
        V(j) = -V(j);
    end
end

if b > 2
    temp = R(b - 1);
```

```
    if V(temp) > 0
        V(temp) = -V(temp);
    end
end

if used
    N = ntmp;
end

P = max(V);
mts = [];

for j = 1:nel
    if Ni(j) == 1;
        if V(j) == P
            mt = tm(current,j);

            if mt >0
                mts = [mts, mt];

                if tm(current, j) == min(mts)
                    next = j ;
                end
            end
        end
    end
end

for i = 1:nel
    v(next) = exprnd(mu(next));
end
for j = next
    if v(j) < vt & v(j) >= 0
        r(j) = 1;
    else
        r(j) = 0;
    end
end

if r(next) == 1
    k = next;
    reduced = [reduced, k];
```

```
        end
        t = t + tm(current, next) %minutes
        t = t*60;
        next
        if r(next) == 1
            N(next) = -1;
        end


        current = next;
        if N == 0
            for j =1:nel
                if r(j) == 0
                    N(j) = 1;
                else
                    N(j) = 0;
                end
            end
        end
        R = [R, next];
        b = length(R) ;
        v
        if N < 0
            break
        end
        ed = length(R);
        edr = length(reduced);
        if t > 90*60
            R(length(R));
            over = length(R) - 1;
            time = t - tm(R(over),R(length(R)))*60;
            R(ed) = R(ed) - R(ed);
            reduced(edr) = reduced(edr) - reduced(edr);
        end
    end
end
path = R;
path
S = sum(r);
disp(['The number of areas in reduced MOPP is ' int2str(S)])
disp(['These areas are ' int2str(reduced)])
disp(['The total time of the search is ' num2str(time/60) ' minutes.'])
```

Appendix D. Static Cases Enumeration Code

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%    Enumeration of all feasible paths in static/deterministic and    %
%    static/stochastic case                                           %
%                                                                     %
%    The purpose of this code is to find the optimal shortest         %
%    path of maximum reward for the static/deterministic and         %
%    static/stochastic case of this thesis.                          %
%                                                                     %
%    Author: Jennifer R. Plourde, AFIT/ENS GOR-05M                   %
%    Date: 10 Feb 05                                                 %
%    Last revised: 11 Feb 05                                         %
%    References: None                                                %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%%%%%%%%%%%%%%%%%%%% VARIABLE DEFINITIONS %%%%%%%%%%%%%%%%%%%%%%%%
%    Inputs required:                                                 %
%    tm: (nel x nel) matrix of feasible arc times between nodes (min) %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

clc;
clear;
t0 = clock;

tm =      [inf  6.29   inf   6.52   7.31    inf    inf    inf    inf    inf
           6.29   inf  6.63    inf   6.71    inf    inf    inf    inf    inf
            inf  6.63   inf   8.4    6.88   7.2     inf    inf    inf    inf
           6.52   inf  8.4     inf    inf    inf   7      inf    inf   9.13
           7.31  6.71  6.88    inf    inf    inf   6.76   6.16    inf    inf
            inf   inf  7.2     inf    inf    inf    inf   7.18  10.05    inf
            inf   inf   inf   7      6.76    inf    inf    inf    inf   7.43
            inf   inf   inf    inf   6.16   7.18    inf    inf   7.94   5.57
            inf   inf   inf    inf    inf  10.05    inf   7.94    inf    inf
            inf   inf   inf   9.13    inf    inf   7.43   5.57    inf    inf];

[jpath,jtime] = jenndykstra(tm)
t1 = clock;
etime(t1,t0)
```

D-1

```
%%%%%%%%%%%%%%%%%%%%%%%% Main Code %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%   Inputs required:                                               %
%   tm: (nel x nel) matrix of feasible arc times between nodes (min) %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

function [jpath,jtime] = jenndykstra(tm)


%building vectors

leftv = ones(1,size(tm,1));
%start at node 5
currv = [zeros(1, 4), 1, zeros(1,5)];
%currv = [1,zeros(1,size(tm,1)-1)];
prevv = zeros(1,size(tm,1));
maxtime = 90;
numbervector = [];
for i = 1:size(tm,1)
    numbervector = [numbervector,i];
end;
streamv = []; % current path

tims = 0; % accumulated time
%determine maximum size of path
maxsize = ceil(maxtime/min(min(tm)))+20;


%create tree and associated times
[masters,mastert] = steptree3(tm, leftv, currv, prevv, streamv,  tims, maxtime,
                    numbervector, maxsize);


%choose shortest time from the list
shortest = min(mastert);
found = 0;
i = 1;
% put rewards here

%identify the path associated with the shortest time
while found < 1
    if mastert(i,1) == shortest
        jpath = masters(i,:);
        jtime = mastert(i,:);
        found = 1;
    end;
    i = i + 1;
```

```
end;


i = 1;
while ((jpath(1,i) ~= 0) & (i < maxsize))
    i = i + 1;
end;


jpath = jpath(1,1:i-1);



%% this is the subroutine that is called recursively

function [masterss, mastertt] = steptree3(timem, leftv, currv, prevv, streamv,  tims,  maxtime,
                                numbervector, maxsize)

    masterss = [];
    mastertt = [];
    %update step
    if leftv*currv' == 1
        leftv = leftv-currv;
    end;
    tempstreamv = streamv;
    streamv = [streamv,currv*numbervector']; % where we're at


    leftv = logical(leftv);
    currv = logical(currv);
    prevv = logical(prevv);


    if sum(prevv) ~= 0
        temptims = tims;
        tims = tims + timem(prevv,currv);
    end;


    if ((sum(leftv) == 0) & ( tims <= maxtime))
        % if ((sum(leftv) == 0) | ( tims >= maxtime))
        masterss = [streamv,zeros(1,maxsize-size(streamv,2))];
        mastertt = tims;
    elseif ( tims > maxtime)
         masterss = [tempstreamv,zeros(1,maxsize-size(tempstreamv,2))];
        mastertt = temptims;


    else
        tempstring = timem(:,currv);
```

```
    run = 0;
    for i = 1:size(timem,1)
        if ((tempstring(i,1) <= maxtime) & (leftv(1,i) == 1))
            run = 1;
            nextstep = zeros(1,size(timem,1));
            nextstep(1,i) = 1;
            [temps, tempt] = steptree3(timem, leftv, nextstep, currv, streamv, tims,  maxtime,
                            numbervector, maxsize);
            if size(tempt,1) >=1
                masterss = [masterss;temps];
                mastertt = [mastertt;tempt];
            end;
        end;
    end;
    if run == 0 % called when stuck
        for i = 1:size(timem,1)
            if tempstring(i,1) <= maxtime
                nextstep = zeros(1,size(timem,1));
                nextstep(1,i) = 1;
                [temps, tempt] = steptree3(timem, leftv, nextstep, currv, streamv, tims,  maxtime,
                                numbervector, maxsize);
                if size(tempt,1) >=1
                    masterss = [masterss;temps];
                    mastertt = [mastertt;tempt];
                end;
            end;
        end;
    end;
end;
```

Bibliography

1. Ahuja, R., Magnanti, T., and J. Orlin (1993). *Network flows: theory, algorithms, and applications.* ed., Prentice Hall, Englewood Cliffs, NJ.

2. Benjamin, G. (2000). "Chemical and biological terrorism: planning for the worst - Health Policy Update." *Physician Executive.* 21 Feb 2005 http://www.findarticles.com/p/articles/mi m0843/is 1 26/ai 102340178/print.

3. Canadian Security Intelligence Service (1995). *The Threat of Chemical/Biological Terrorism.* Commentary No. 60. Ottawa, Ontario, CSIS/SCRS.

4. Craft, D., Wein, L., and A. Wilkins (2003). Analyzing bioterror response logistics: the case of anthrax. 21 Feb 2005 http://faculty-gsb.stanford.edu/wein/personal/Analyzing Bioterror Anthrax 11-03.pdf.

5. Department of Defense (2004). *Chemical, Biological, Radiological, and Nuclear Defense Program: Annual Report to Congress.* Washington, GPO.

6. Deputy Assistant to the Secretary of Defense for Chemical and Biological Defense (Oct 2001). *Chemical and Biological Defense Primer.*

7. Garmone, J. (15 Mar 2003). "Halabja: Symbol of Hussein's Inhumanity." *American Forces Information Service: News Articles.* 21 Feb 2005 http://www.defenselink.mil/news/Mar2003/n03152003 200303152.html.

8. Hall, R.W. (1986). The fastest path through a network with random time-dependent travel times. *Transportation Science*, **20**, 182-188.

9. Hsu, Y-K. and T. Holsen (2000). "The use of receptor models to locate atmospheric pollutant sources: PCBs in Chicago." (Unpublished). Clarkson University, Department of Civil and Environmental Engineering.

10. Hoenig, S. (2002). *Handbook of Chemical Warfare and Terrorism.* 2nd ed., Greenwood Press, Westport CT.

11. Kaplan, E., Craft, D., and L. Wein (2002). Emergency response to a smallpox attack: the case for mass vaccination. *Proceedings of the National Academy of Science*, **99**, 10935-10940.

12. Kaplan, E., Craft D., and L. Wein (2003). Analyzing bioterror response logistics: the case of smallpox. *Mathematical Biosciences*, **185**, 33-72.

13. Kathirgamanathan, P., McKibbin, R., and R.I. McLachlan (2002). Source term estimation of pollution from an instantaneous point source. *Res. Lett. Inf. Math. Sci.*, **3**, 59-67.

14. Kathirgamanathan, P., McKibbin, R., and R.I. McLachlan (2003). Source release-rate estimation of atmospheric pollution from a non-steady point source - Part 1: Source at a known location. *Res. Lett. Inf. Math. Sci.*, **5**, 71-84.

15. McLaughlin, S. (12 Sep 2003). "Toxic threat: how dangerous are chemical weapons of mass destruction?" *Current Science.* 21 Feb 2005 http://www.findarticles.com/p/articles/mi m0BFU/is 2 89/ai 108006635.

16. Miller-Hooks, E. and H. Mahmassani (2000). Least expected time paths in stochastic time-varying transportation networks. *Transportation Science*, **34**, 198-215.

17. Sofiev, M. (2002). "Real time solution of forward and inverse air pollution problems with a numerical dispersion model based on short-term weather forecasts." *HIRLAM Newsletter (Proc. of All Stuff Meeting of HIRLAM project)*, **14**, 131-138.

18. Thomas, B. and C. White (2004). Anticipatory Route Selection. *Transportation Science*, **38**, 473-487.

19. United States Army Medical Research Institute of Infectious Diseases. Medical Defense Against Biological Warfare Agents Course: History of Biological Warfare. *Encyclopedia of Bioethics*, 2545.

20. Wein, L., Craft, D., and E. Kaplan (2003). Emergency Response to an Anthrax Attack. *National Academy of Sciences*, **100**, 4346-3451.

21. Wolsey, L. (1998). *Integer Programming.* Wiley, New York.

1. REPORT DATE (DD-MM-YYYY) 21-03-2005	2. REPORT TYPE **Master's Thesis**	3. DATES COVERED (From – To) Apr 2004 – Mar 2005

4. TITLE AND SUBTITLE OPTIMAL SAMPLING OF A CHEMICAL HAZARD AREA	5a. CONTRACT NUMBER
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S) Plourde, Jennifer R., 2d Lt, USAF	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES(S) AND ADDRESS(S) Air Force Institute of Technology Graduate School of Engineering and Management (AFIT/EN) 2950 Hobson Street, Building 642 WPAFB OH 45433-8865	8. PERFORMING ORGANIZATION REPORT NUMBER AFIT/GOR/ENS/05-15
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFRL/HEPC Attn: Dr. W. Paul Murdock 2729 R. Street DSN: 785-3140 WPAFB OH 45433-5707 e-mail: William.Murdock@wpafb.af.mil	10. SPONSOR/MONITOR'S ACRONYM(S)
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT

APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

This thesis proposes a methodology for optimally sampling a chemical hazard area subsequent to a chemical weapons attack. The objective is to identify the maximum number of areas that no longer require protective gear for safe operations. We model the area as an undirected graph and employ network analysis techniques to provide a methodological framework for identifying an optimal sampling sequence within a fixed time limit. We propose four models that characterize the secondary vapor concentrations: i) static and deterministic, ii) static and stochastic, iii) dynamic and deterministic, and iv) dynamic and stochastic. Comparisons of the static cases and their dynamic counterparts demonstrate the impact of temporal evolution of vapor concentrations on the optimal sampling path. We conclude that the number of safe areas may be either under- or over-estimated depending on the assumed nature of the secondary vapors.

15. SUBJECT TERMS
Optimal sampling; chemical hazard area; optimal search

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Jeffrey P. Kharoufeh, Ph.D. (ENS)
a. REPORT	b. ABSTRACT	c. THIS PAGE	UU	108	19b. TELEPHONE NUMBER (Include area code) (937) 255-3636, ext 4603; e-mail: Jeffrey.Kharoufeh@afit.edu
U	U	U			

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39-18