EVALUATION OF WATER DISTRIBUTION SYSTEM MONITORING
USING A COMBINED SIMULATION-OPTIMIZATION APPROACH

by

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(ABSTRACT)

A simulation-optimization methodology was used to assess monitoring
strategies for a drinking water distribution network. Multiple simulation trials of
contamination events were used to create input data for an integer optimization
problem. A network model, based on the Blacksburg, VA water distribution system,
was used as the basis for a case study of contaminant transport under conditions of
uncertainty. The model was not calibrated due to the lack of reliable field data.

Optimization of monitoring plans was performed within the context event-
based simulation trials. This precluded the design of monitoring plans that were
directly compatible with requirements of water quality regulations. However, the
results of the optimization did provide information that may be of use to the broader
problem of compliance monitoring. Optimal plans were assessed in comparison with
several alternative plans using a separate set of simulation trials.

Optimization of monitoring plans derived from simulated source node
contamination events was generally effective at choosing points that provided better
detection of source node contamination than alternative plans based on random
sampling or judgement sampling. Optimal monitoring plans derived from simulated
random node contamination events were ineffective at detecting random node
contamination.

The results of optimization and the separate analysis of monitoring plan
performance indicated that the number of simulation trials may have been inadequate
to completely describe the stochastic behavior of the system. Additionally,
comparison of these results with those obtained from a previous simulation study
indicate that the results of any simulation of distribution system contamination may be
very sensitive to the level of contaminant loading and the size and layout of the
system.
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I. INTRODUCTION

A. Background

In accordance with the 1989 Safe Drinking Water Act, the Environmental Protection Agency (EPA) promulgated National Primary Drinking Water Regulations (NPDWR) that established maximum contaminant levels (MCLs) and monitoring requirements for a variety of contaminants (EPA, 1989a,b). Included in the NPDWR were specific requirements for monitoring drinking water distribution systems for coliform bacteria and the establishment of an MCL for total coliform. The coliform regulations were promulgated as "Total Coliforms (Including Fecal Coliforms and E. Coli); Final Rule" in the NPDWR (EPA, 1989b). The cost of complying with the drinking water regulations was estimated at $1.4 billion per year for the more than 200,000 public water utilities (Auerbach, 1994). This cost illustrates the need for efficient methods of regulatory compliance.

As discussed in greater detail in the literature review, the total coliform regulations specified a Presence-Absence (P-A) criteria for determining compliance with the MCL for coliform bacteria. In addition, guidelines for regular distribution system monitoring were established. These guidelines specified the reporting period to be one month and required a specific number of samples be collected and analyzed each month. The required number of samples was linked to the population served by
the system. An important characteristic of the regulations was the classification of system compliance. If the MCL for total coliforms was exceeded at any point in the system, then the regulations classified the entire system as out of compliance for the respective reporting period. In addition, supplementary sampling requirements were established for non-compliant systems, ostensibly to facilitate the distinction of isolated regulatory violations from more serious episodes indicating a failure in the treatment process or a breach of system integrity.

In establishing monitoring requirements, the regulations were less specific regarding where samples were to be collected within the distribution system and at what time samples should be collected. The only criteria for selecting monitoring points was the general guideline that the sampling be representative of the entire system and that samples be collected "at regular intervals throughout the month" (EPA, 1989b). It was mandated that a specific monitoring plan be filed and meet the approval of state authority. Thus, the manager of a water utility was left with few strict guidelines for establishing an effective monitoring program. An appropriate methodology for selecting the time and location of distribution system monitoring points was not established.

Ideally, the design of a monitoring plan would incorporate all available information concerning the occurrence of regulatory violations. In particular, information regarding the transport of contamination in the distribution network would allow the selection of monitoring points that provide the best opportunity for detection
of system non-compliance. Such information might be obtained from extensive empirical studies. Contamination events are usually infrequent, however. Therefore, obtaining enough empirical data to describe the transport of a contaminant under a variety of conditions is generally impractical.

An alternative is to incorporate information on the general behavior of contamination in distribution systems into a computer simulation of the specific system of interest. Using computer simulation, a wide variety of contamination events under a range of hydraulic conditions can be modeled. Monte Carlo experiments, based on multiple simulation trials with stochastic inputs, can be used to estimate the spatial and temporal distribution of contamination in the system. Simulation modeling has been widely used to study the hydraulic behavior of distribution systems (Clark and Males, 1986; Wood and Rayes, 1981) and dynamic hydraulic models have been linked to contaminant transport models to study contaminant propagation in distribution systems (Clark et. al., 1991; Deininger et. al., 1992; Grayman et. al., 1988). Jones (1992) used a dynamic constituent transport model named TRAK to evaluate sampling plan performance in a hypothetical distribution system. The use of Monte Carlo studies in the design of monitoring plans has been applied to the problem of locating optimal sites for groundwater monitoring wells (Meyer and Brill, 1988). This simulation-optimization methodology has been used in engineering design as well (Burn, 1989).
B. Research Objectives

The purpose of this research was to evaluate the use of a simulation-optimization approach in the design of a compliance monitoring plan for a realistic water distribution system. The constituent transport model TRAK was used to simulate contamination events in a water distribution network modeled after the Blacksburg, VA distribution system. The objective was not to construct a precise model of the Blacksburg system, but was to use the Blacksburg network as the basis for a realistic case study that would reflect the complexities of an actual water distribution system. This model was used to perform multiple Monte Carlo trials simulating contamination of the distribution system. The results of these simulations were then used to construct a mathematical optimization problem. The solution of the optimization problem provided a set of monitoring points that were optimal with respect to a prespecified measure of effectiveness. If Monte Carlo simulation provided a reasonable representation of the behavior of bacteriological contamination in the distribution system, then the optimal set of monitoring points should be superior to other monitoring plans in terms of the defined measure of effectiveness.
The specific objectives of this research were to:

1) use information from the Blacksburg, VA water distribution system and the constituent transport model TRAK to simulate the spatial and temporal distribution of a contaminant resulting from distribution system contamination events;

2) construct an optimization formulation for the design of a distribution system monitoring plan;

3) use the results of Monte Carlo simulation trials to determine an optimal monitoring plan for the distribution system being studied and assess the sensitivity of the optimal plan to selected parameters;

4) assess the adequacy of the Monte Carlo simulations for monitoring plan design and evaluation;

5) compare the calculated optimal plans with other sampling plans and assess their relative performance using an independent set of simulation trials;

6) evaluate the potential of the simulation-optimization methodology as a tool for the design of water distribution system monitoring plans.
Four sets of simulations were performed. Two sets represented source node contamination events and two sets represented transient node contamination events. One set of each type of contamination event was used in the design of optimal sampling plans and to evaluate the transport of contaminant in the system. The other two sets, one of each type, were used for independent evaluation of monitoring plan performance. These last two sets of trials were performed while the majority of the analysis was in progress, so the results of these were only available for the independent assessment of monitoring plan performance.

Calibration of the model using field data was not feasible for this research. When possible, actual data was used to construct the network model. However, the available hydraulic data was not sufficient to provide a meaningful calibration of the system flows and pressures. A field study was beyond the resources available for this research, so using a tracer study or an extensive sampling survey was not practical. The model algorithm was checked against manual calculations by Jones (1992) and was found to be reliable.
II. LITERATURE REVIEW

A. The Biological Quality of Drinking Water

1. Microbiological Contamination

The removal of pathogenic organisms has long been a primary goal of drinking water treatment. Procedures for pathogen removal, including filtration and sterilization by boiling, date back as far as 2000 B.C. (Culp, Wesner, and Culp, 1986 citing Baker, 1948). Even though the dangers associated with impure drinking water have been known a long time, it was not until 1854 that an epidemiological study explicitly linked an outbreak of disease to a contaminated source of drinking water. In that year, Dr. John Snow was able to identify the Broad Street pump in London as the source of contaminated water that caused the cholera epidemic in that city (Culp, Wesner, and Culp, 1986). In the United States, water treatment became a common practice in the early twentieth century. The process of building and improving drinking water treatment facilities accelerated rapidly following World War II (DeZuane, 1990).

The result of this effort was an apparent decline in the reports of waterborne disease outbreaks; at least until the last 20 years. Recent data have shown some startling trends in waterborne disease outbreaks. The Environmental Protection Agency (EPA) has reported that 427 outbreaks affecting 106,000 people were
confirmed between 1971 and 1983. Forty outbreaks were reported in 1983 alone (EPA, 1989). Craun reported that 248 outbreaks affecting 1,950 people occurred between 1981 and 1988 (Craun, 1990). For the years 1991-1992, 34 outbreaks affecting 17,464 people were reported (Moore et. al., 1994). Clearly, the improvements in water treatment technology over the last 50 years have not led to the elimination of waterborne disease in the United States.

The threat of waterborne disease outbreak has most likely been understated by the data on reported outbreaks. Although the Centers for Disease Control (CDC) and the EPA have been collecting data on the outbreak of waterborne disease since 1971, the reporting of an outbreak has been a voluntary process (DeZuane 1990). DeZuane (1990) cites an EPA sponsored study in Colorado as indicating that only 25 percent of the outbreaks of waterborne disease have been recognized and reported. Craun has been quoted to suggest that "outbreaks of waterborne disease are not identified unless at least 1 percent of the population in a community becomes ill within a few months" (Regli et al., 1991). The true extent of the problem of under-reporting is unknown. The problem has been attributed to a number of factors that are dependent on the nature and extent of the outbreak, the seriousness of the illness, and the awareness of state and local agencies (Moore et. al., 1994).

Outbreaks of waterborne disease have been attributed to a wide variety of organisms including pathogenic bacteria, viruses, protozoans, and helminths. Many of these organisms are transmitted through the fecal-oral route, so contaminated
drinking water is but one possible source of a disease outbreak (Tate, 1990). The most commonly identified cause of waterborne disease between 1971 and 1983 was the protozoan Giardia lamblia. Other identified pathogens include bacteria of the Salmonella species, the Shigella species, Campylobacter jejuni, Yersinia enterocolitica Pseudomonas sp, and enteropathogenic E-coli, and viruses such as Norwalk agents, Norwalk-like agents, rotaviruses, and hepatitis-A (EPA, 1989). Invertebrates such as crustaceans, nematodes, flatworms, water mites, and insect larvae have also been associated with waterborne disease. Many of these organisms are opportunistic pathogens and some act as hosts, protecting bacteria and viruses from treatment processes (Levy, Hart, and Cheetham, 1986). According to the EPA, no causative agent has been identified in about half of the reported outbreaks during the 1971-1983 period (EPA, 1989). In recent years, 1991-1992, the protozoan Cryptosporidium has been associated with a number of disease outbreaks and the E. coli 0157:H7 has also been recognized as an important waterborne pathogen (Moore et. al., 1994).

These studies show a persistence in the problem of controlling the biological quality of drinking water, even though there has been a dramatic increase in the level of technology and in regulatory oversight. The majority of identified disease outbreaks have been associated with inadequate or nonexistent treatment and with treatment deficiencies. Approximately 83 percent of outbreaks in non-community water systems from 1971 to 1980 were attributed to the use of untreated groundwater.
or groundwater with inadequate treatment. It has been estimated that 49 percent of outbreaks in community water systems were the result of treatment deficiencies (EPA, 1989). Cases of breakdowns or contamination of the treatment plant itself have been documented as the cause of contaminated drinking water (Weirenga, 1988; Burn, 1989). A deterioration of the source water can also lead to inadequate treatment. Population growth in urban areas has resulted in the increased use of poor quality water sources. This has been complicated by the pollution of drinking water sources by wastewater treatment plants, urban and rural runoff, feedlot discharge, and other human activity (AWWA, 1987). Deterioration of drinking water quality due to poor or degraded source water has been documented as the cause of disease outbreaks (Short, 1988; Stukel et. al., 1990).

The AWWA has promoted the concept of multiple barriers to ensure the quality of drinking water and protect against the spread of waterborne disease. The AWWA Committee on Bacteriological Sampling Frequency in Distribution Systems (AWWA, 1985) defined these barriers as:

- selection of high quality source;
- protection of the source;
- proper treatment and disinfection;
- maintenance of the integrity of the distribution system.

Outbreaks of waterborne disease have been the result of penetration of one or more of these barriers (AWWA, 1985). Numerous regulations have been instituted in an
attempt to strengthen each of these barriers. The Surface Water Treatment Rule (SWTR), for example, mandated that all utilities using surface waters of surface-influenced groundwater to provide filtration and disinfection as part of the treatment process (EPA, 1989a). This mandate was at least partially in response to the increasing evidence that microorganisms, particularly protozoans, were penetrating the treatment barrier in many systems. The final barrier before drinking water reaches the consumer is the distribution system. Contamination of water in the distribution system can result from external contamination entering the system as a result of backsiphon and cross-connection (AWWA, 1979; Brazos et. al., 1985; Craun, 1981; EPA, 1989). Typically, prevention devices are used to prevent these occurrences. DeZuane (1990) listed airgap separation, vacuum breakers, and backflow preventers as the most common devices for preventing flow from the users' plumbing back into the distribution system. These devices are intended to prevent a reversal of flow when low pressure or a vacuum exists in the distribution system pipe near a connection. Adherence to established standards for pipeline construction and repair was cited as an important barrier to distribution system contamination by Culp, Wesner, and Culp (1987). They specified the protection of new pipe sections, flushing, and disinfection as necessary practices for ensuring that pathogens do not enter the system at construction sites.

The growth and regrowth of organisms in the distribution system has been another problem. Bacteria that survive the disinfection process can colonize
distribution system surfaces forming biofilms. These colonies may grow in the presence of nutrients and periodically slough into the water (Geldreich, 1990). The presence of regrowth organisms may cause false positive tests that erroneously suggest a breakdown in treatment barriers or may mask the presence of indicator organisms in the event of an actual contamination episode (LeChevallier, 1990). Little progress has been made in controlling or monitoring the formation of biofilms, but the process of regrowth has been extensively studied (Herson et. al., 1991; LeChevallier, 1990; Martin et. al.,1982; Rice et. al., 1991).

2. Monitoring the Biological Quality of Drinking Water

The reliability of the multiple barriers to biological contamination can be viewed as the consistency of protection over time and area. The primary purpose of routine biological monitoring is to demonstrate the reliability of the overall system (AWWA, 1987). Monitoring with the purpose of identifying individual populations of pathogens is impractical in the routine analysis of drinking water. Specific pathogens may be present in small numbers, making them difficult to detect. The analysis required to identify individual organisms may not yield results in time for corrective action to be taken. For these reasons, it has been common practice to look for the presence of biological indicators in water samples (Tortora, Funke, and Case, 1992). Indicators are some class of organism that "provide evidence of recent fecal contamination from warm-blooded animals" (Tate, 1990). For an indicator to be
effective, a number of criteria must be satisfied. Specifically, microbiological indicators should be:

1) consistently present in human feces,
2) able to survive treatment barriers at least as well as pathogens,
3) detectable by simple tests that require little formal training in microbiology (Tortora, Funke, and Case, 1992).

Several indicators are available for the purpose of monitoring drinking water for biological quality. Turbidity and the disinfectant residual are important indicators for assessing treatment effectiveness (AWWA, 1987). High turbidity indicates the passage of particulate material through the filtration system. Residual disinfectant measures the adequacy of the disinfectant dosage. These two indicators provide direct information on the operation of the treatment process but do not provide a direct indication of the actual biological quality of the water. The most commonly used biological indicators are the Heterotrophic Plate Count (HPC) and the test for total coliform bacteria (Total Coliform Test).

The HPC provides an estimate of the number of bacteria that will develop into colonies during a period of incubation in a nutrient (DeZuane, 1990). It measures a broad group of microorganisms that includes pathogens and non-pathogens and is used as an indicator of the general bacteriological quality of the water (AWWA, 1987). However, there has been little correlation established between the HPC and the
probability of waterborne disease (Tate, 1990). Some systems appear to exhibit a higher than average background level of heterotrophic organisms without being at risk of an outbreak of disease (AWWA, 1987).

Total coliform bacteria are the standard indicator of biological quality in the United States. The AWWA considers it the "best available indicator of treatment effectiveness" (AWWA, 1987). Coliforms are not a specific type of bacteria in the taxonomic sense. The coliforms include several types of bacteria that exhibit certain characteristics that are common to many pathogenic organisms (Tortora, Funke, and Case, 1992). Coliforms may be detected using the multiple tube fermentation test or using a membrane filter (MF) test. The multiple tube fermentation technique results in an estimate of the Most Probable Number (MPN) of bacteria in the water sample based on the number of subsamples that exhibit gas production when incubated in a lactose broth (Tortora, Funke, and Case, 1992). The MF test allows the identification and enumeration of colonies that form on a culture media (DeZuane, 1990). These tests can be used to estimate the mean coliform density in a distribution system.

The standard practice is to use these tests to estimate the frequency-of-occurrence of bacteria in the system. This approach is often referred to as the Presence-Absence (P-A) approach and is based on determining the fraction of samples that are coliform-positive instead of estimating the coliform density (American Public Health Association, 1989). The P-A criterion for assessing water quality was found
to be more reliable than estimation of mean coliform density (Pipes et. al., 1987). The P-A approach also has the advantage of being a relatively straightforward test with clearly defined results (EPA, 1989; Pipes, 1986).

The total coliform indicator has several disadvantages as an indicator of the potential for waterborne disease. Coliform bacteria that grow in biofilms may be detected even though there has not been fecal contamination of the system (Tortora, Funke, and Case, 1992). In addition, protozoans such as *Giardia lamblia* and *Cryptosporidium* may be more resistant to disinfection than coliform bacteria (Tortotra, Funke, and Case, 1992). Recent studies (Moore et. al., 1994) have indicated that the coliform indicator may be inadequate for the detection of protozoa in drinking water. This presents a serious problem in view of the occurrence of protozoan-related disease outbreaks reported to the CDC. Additional problems with the total coliform test include the suppression of coliform populations by heterotrophic bacteria and seasonal variations in populations of non-pathogenic coliform bacteria (DeZuane, 1990).

Regardless of the deficiencies entailed with the total coliform test, it appears to be the best available indicator for evaluating the efficacy of treatment barriers in removing pathogenic organisms. For this reason, the EPA chose to use total coliforms as the standard for evaluating the biological quality of drinking water. The regulations establishing Maximum Contaminant Levels (MCL) for total coliforms were promulgated as part of the National Primary Drinking Water Regulations.
(NPDWR) in compliance with the 1986 Safe Drinking Water Act (SDWA).

Mandatory distribution system sampling and a strict Presence-Absence criteria for determination of compliance were established in the final rule for total coliforms (EPA, 1989b). The Final Rule set a Maximum Contaminant Level Goal at zero coliform bacteria. The enforceable MCL was defined using the P-A criterion and specified that:

- for systems analyzing 40 or more samples per month, no more than 5 percent of the monthly samples can be coliform-positive;
- for systems analyzing fewer than 40 samples per month, no more than 1 sample can be coliform-positive;
- systems serving more than 25 people must demonstrate compliance by routine sampling of the distribution system.

The regulations defined the compliance period to be one month. Demonstration of compliance is accomplished by sampling the distribution system; the number of samples collected each month is determined according to the population served. Table I shows the number of monthly samples to be collected by systems serving various populations. In the event of a coliform-positive sample, systems are required to take additional samples at points upstream and downstream from the point where the contaminated sample was collected. Ostensibly, the purpose of this additional
sampling is to help distinguish between an isolated incident and a more serious episode of system contamination. This approach would seem to indicate that non-compliance could be isolated to a portion of the distribution system, but the regulations were specific in attaching the condition of compliance\non-compliance to the entire system for the period during which coliform-positive samples were found. Compliance could then be achieved by monitoring during the next month.

No rationale has been clearly established for defining a one month monitoring period or for relating the number of samples to the population served. Pipes (1986) argued that sampling should be related to the persistence of microbiological quality but that further work is needed to establish a criteria for this approach. In modeling the bacterial populations of the Metz distribution system in France, the required number of samples for achieving a degree of precision was found to depend on the dispersion of bacteria in the system (Maul, El-Shaarawi, and Block, 1986). So, the criteria of basing the sample size on population is also questionable.
Table I: EPA requirements for distribution system monitoring based on the population served by the system.

<table>
<thead>
<tr>
<th>Population Served</th>
<th>Minimum Samples per Month</th>
</tr>
</thead>
<tbody>
<tr>
<td>≤ 1,000</td>
<td>2</td>
</tr>
<tr>
<td>1,000 - 5,000</td>
<td>5</td>
</tr>
<tr>
<td>5,000 - 10,000</td>
<td>12</td>
</tr>
<tr>
<td>10,000 - 20,000</td>
<td>24</td>
</tr>
<tr>
<td>20,000 - 40,000</td>
<td>40</td>
</tr>
<tr>
<td>40,000 - 70,000</td>
<td>75</td>
</tr>
<tr>
<td>70,000 - 110,000</td>
<td>100</td>
</tr>
<tr>
<td>110,000 - 160,000</td>
<td>120</td>
</tr>
<tr>
<td>160,000 - 220,000</td>
<td>140</td>
</tr>
<tr>
<td>220,000 - 300,000</td>
<td>170</td>
</tr>
<tr>
<td>300,000 - 500,000</td>
<td>200</td>
</tr>
<tr>
<td>500,000 - 800,000</td>
<td>250</td>
</tr>
<tr>
<td>800,000 - 1,200,000</td>
<td>300</td>
</tr>
<tr>
<td>1,200,000 - 1,600,000</td>
<td>350</td>
</tr>
<tr>
<td>1,600,000 - 2,000,000</td>
<td>400</td>
</tr>
<tr>
<td>2,000,000 - 2,500,000</td>
<td>450</td>
</tr>
<tr>
<td>2,500,000 - 4,000,000</td>
<td>500</td>
</tr>
<tr>
<td>≥ 4,000,000</td>
<td>600</td>
</tr>
</tbody>
</table>

Source: (DeZuane, 1990)
3. Distribution System Monitoring

The design of a distribution system monitoring plan involves the selection of a sampling frequency and the selection of the location of sampling sites (Geldriech, 1990). These decisions must be made in an environment of regulatory requirements, practical constraints on monitoring, and additional informational needs that the utility may have. Often, these multiple objectives may conflict with one another in the specification of a monitoring plan. The fundamental objective of distribution system monitoring has been stated as "to provide evidence of protection against the transmission of waterborne infectious disease" (AWWA, 1985). This objective is not very specific and provides little guidance in designing an effective monitoring plan. Geldriech (1990) described two types or "levels" of monitoring: routine compliance monitoring and special purpose monitoring. Routine compliance monitoring is intended to cover all major areas of the distribution system with the objective of demonstrating compliance with public health regulations. Special purpose monitoring addresses the need for the utility to understand the characteristics and performance of the system and allows the identification of problem areas that require corrective measures. The specific informational requirements of the utility were discussed in a workshop moderated by Geldriech (1988). During this discussion, LeChevelliard pointed out that routine compliance monitoring does not fully meet the monitoring objectives of a utility manager. "Definitive proof of contamination" including the identification of the nature of the problem (breakthrough at the treatment plant, cross
connection, regrowth, etc.), the significance of the problem as a public health threat, and the extent of the contamination in the system, was expressed by LeChevallier as the necessary information for decision making (Geldreich, 1988). Smith supported LeChevallier's assertion and emphasized the identification of the cause of a contamination problem as critical information (Geldreich, 1988).

The objectives of water quality monitoring have been classified by Valiela and Whitfield (1989) as being either "chronic" objectives or "acute" objectives. Acute objectives were described as defining "peak values of infrequent occurrence and short duration" while chronic objectives define "central tendency values of high frequency and/or long duration" (Valiela and Whitfield, 1989). The article also pointed out that most compliance monitoring is performed with acute objectives in mind and that such monitoring should focus on the frequency, magnitude, and duration of violations. The EPA (1989b) regulations for total coliform monitoring suggest an acute objective of identifying individual episodes of coliform contamination. However, the 5 percent rule for contaminated samples during a compliance period seems to indicate an accepted level of long term coliform density that should not be exceeded; this aspect of the regulation seems to fall into Valiela and Whitfield's classification of a chronic objective. Pipes (1986) suggested that monitoring should be related to the persistence of contamination. This would certainly indicate a view that supports an acute objective for compliance monitoring.

The EPA mandated monitoring requirements follow a protocol that is similar
to what Valiela and Whitfield (1989) define as "exceedence driven sampling" (EDS). This involves fixed frequency sampling (FFS), which entails sampling at regular intervals, with more intense sampling if exceedence is detected. Valiela and Whitfield (1989) found FFS to be appropriate for chronic objectives while EDS should be used only when acute objectives are involved. Criteria for determining the sampling frequency have been proposed by Casey et. al. (1983) and by Beckers et. al. (1972). Beckers et. al. (1972) proposed an objective of maximizing the expected proportion of violations detected with a fixed frequency sampling plan and labeled this parameter M. This criteria was criticized by Casey et. al. (1983) for not taking into account the dependencies among sampling points. In particular, they pointed out that multiple detection of a single violation was not considered in defining M. As an alternative, Casey et. al. (1983) proposed two measures derived from random sampling of a two-stage Markov process. Their first alternative measure, M', expressed the expected proportion of violated samples that will be detected with a variable sampling interval. Their second measure, M", considers the number of violated samples as a proportion to the expected number of violations. Using the second measure, they derived the optimal sampling interval for setting the expected number of violated samples equal to the expected number of violations.

The fixed frequency portion of the EPA requirements are defined with a one month monitoring period. Fixed frequency sampling within the compliance period was not explicitly defined in the regulations, however. Stukel et. al. (1987) compared
three sampling plans: once a month sampling at a fixed location, weekly sampling at a fixed location, and monthly sampling of a spatial cluster design. For the fixed point designs, weekly sampling was found to detect between 50 and 100 percent more incidents of contamination when used to monitor 15 small community water systems. Approximately 40 percent of the contamination incidents detected by the weekly sampling scheme were missed by the once monthly sampling scheme. The importance of spatial location of monitoring points was made apparent when the spatial cluster design was found to be more sensitive than weekly sampling even though the spatial cluster design was only sampled once a month.

Spatial allocation of sampling sites was investigated in depth by Maul et. al. (1986). This study used the results of an intensive sampling effort to assess the temporal and spatial distribution of heterotrophic bacteria in a section of the Metz, France distribution system. Bacterial densities were found to vary within the system; a non-hierarchial nearest-centroid clustering method was used to determine zones within which the mean bacterial density was constant. Seasonal variations in bacterial density were observed and were found to be of different magnitudes between zones. This study provided strong evidence for a systematic approach to sample site location and suggests that a single fixed point may not reflect the biological quality of the entire system. Lee, Deininger, and Clark (1991) suggested the concept of "coverage" as a criterion for the location of sample points. This objective is based purely on hydraulic behavior of the system with no assumptions made concerning the
distribution of contamination within the system. Their approach suggests that the water sampled at one point in the system may be used to infer the quality of water at points upstream of the sample point. In a complex system, a certain fraction of the water flowing to a particular point may flow through a particular pathway while the remainder of the flow at that point may arrive by other pathways. Using these calculations, a matrix of "water fractions", showing the fraction of water at a particular node that has passed through another node, is constructed. The approach allows the specification of a minimum water fraction that is required for a sample point to be representative of an upstream node. The water fraction matrix can then be used to determine the fraction of the system demand that is covered by a given sampling plan. This approach was applied to the Flint, MI water distribution system and the Chelshire, CT water distribution system (Lee, Deininger, and Clark, 1991). The effect of various sampling plans on the demand covered was assessed using hydraulic simulations for a variety of steady-state operational conditions. It should be noted that the coverage approach relies on the assumption that upstream water quality may be inferred from downstream water quality and does not explicitly take the process of dilution or decay of the constituent into account.

In practice, sampling locations have been generally chosen based on a combination of heuristic criteria and practical constraints. A survey conducted by the AWWA Committee on Bacteriological Sampling Frequency in Distribution Systems (AWWA, 1985) classified the sampling practices of 1796 utilities. The survey
indicated that public buildings, commercial buildings, and private residences were the most common locations for monthly sampling. Fewer than 30 percent of the respondents reported frequent sampling of storage tanks. Area representation was the most common criteria for selecting a sampling location with over 50 percent of respondents indicating that central and peripheral locations were chosen. The temporal allocation of sampling points varied according to the size of the utility. Large utilities were more likely to collect samples throughout the month on various days of the week and at different times of the day. There was a tendency, however, for all size utilities to favor sampling in the morning on weekdays. The issue of locating sampling points was discussed in a workshop moderated by Geldriech (1988). During this discussion, Pipes emphasized the importance of representing the major hydraulic zones of the system as well as incorporating randomization into the monitoring scheme. Many of the utility managers present indicated a preference for fixed monitoring locations, primarily as a matter of practicality. The conflict between the desire to employ a statistically logical monitoring strategy and the constraints that dictate what is practical in terms of sample collection were quite evident in this discussion.
B. Distribution System Models

1. Data Requirements and System Representation

a) Distribution network  Distribution systems have been modeled as a network of links and nodes. Nodes represent treatment plants, junctions, demand locations, storage reservoirs, and any location where water enters or leaves the system while the links between nodes represent the pipes in the system (Clark and Males, 1986; Males, Grayman, and Clark, 1988). Wood and Rayes (1981) classified nodes as being either junction nodes or fixed-grade nodes. Junction nodes are points where pipes join or where water enters or leaves the system. Fixed-grade nodes are points of constant head such as storage reservoirs and constant pressure regions. Pipes are divided into individual pipes of constant diameter and can be assigned to a closed circuit of pipes (Wood and Rayes, 1981). The set of all closed pipe circuits constitutes the primary loops in the system. Wood and Rayes (1981) offered the identity that the number of pipes in a system is equal to the sum of nodes and loops minus one. The specific pipe and node information required to fully model the system was listed by Epp and Fowler (1972). In order to solve a hydraulic model using their solution algorithm, the pipe diameters, lengths, and roughness coefficients; the elevations and demands at nodes; and information on reservoir elevations, pressure-reducing valves, and other fixtures are required.
b) Skelotonization In order to reduce the size of the hydraulic problem, it has been common practice to represent the system using a skelotonized network - a network of only the water mains and including only enough pipes to complete the major loops in the system. Often this may involve eliminating some pipes from the model, representing a series of pipes with one larger pipe, and consolidating demands at a fixed set of nodes (Culp, Wesner, and Culp, 1986). Metzger (1985) modeled a system using only 20 percent of the pipes in the network and achieved accurate hydraulic results. Clark et. al. (1991) modeled the propagation of a fluoride tracer in the Cheshire, Conn. system using fewer than 10 percent of the actual pipes in the system. The effects of skelotonization on hydraulic results has been found to be minimal, however, Hunt (1988) determined that skelotonization may affect the computed travel times for constituent transport models. Ferreira (1991) compared the computed travel times of a constituent for skelotonized and unskeletonized models of the North Penn distribution system. This study suggested that, in general, there is a divergence in the computed travel times that is more apparent for regions that contain numerous loops. The elimination of 4 inch pipes resulted in faster travel times, while the computed travel times were frequently greater when 6 inch pipes were also eliminated. Ferreira (1991) suggested that the elimination of 4 inch pipes resulted in more direct pathways for constituent travel while some of the direct pathways were eliminated when 6 inch pipes were also left out of the model.
c) **Water demands** Municipal water use may be classified into residential use, industrial use, commercial use, transportation use, public use, and loss (Hunke and de Mare’, 1984). Hunke and de Mare’ (1984) cite Howe and Linaweaver (1967) as indicating that residential water use comprises up to 50 percent of total use and is the most influential component in terms of demand variations. Jones (1991) cites Steel and McGee (1979) as indicating that water demands tend to follow hourly, daily, weekly, and seasonal cycles. Hourly demand has been found to reach 2 to 7 times the average hourly demand during peak use (Montgomery, 1985). Diurnal demand curves that typify hourly variations in demand have been published (AWWA, 1981). The diurnal demand cycle is common in municipal water systems (Hunke and de Mare’, 1984). Methods of allocating the demand to nodes in the system have been reviewed in numerous studies (AWWA, 1989; Cessario, 1980; Walski, 1983; Shawcross, 1985; Hirrel, 1986).
2. Hydraulic Models

a) Hydraulic equations The basic conditions for solving the flow in a network have been stated as:

1. flow into a junction = flow out of a junction;
2. each pipe must satisfy laws of pipe friction for flow in a single pipe;
3. zero total head loss around each loop (Daugherty et. al., 1985).

These conditions constitute a set equations that ensure continuity and conservation of energy. Wood and Rayes (1981) formulated these conditions in terms of unknown flow rates as the loop equations:

$$\Sigma Q_{in} - \Sigma Q_{out} = Q_e$$ (for j junction nodes) \hspace{1cm} (1)

This equation set (1) ensures that the inflow equals the outflow at each junction node.

The terms $Q_{in}$ and $Q_{out}$ refer to pipe flows into the node and out of the node, respectively. $Q_e$ refers to water demand or external inflow at the junction node.

$$\Sigma h_L = \Sigma E_p$$ (for 1 primary loops) \hspace{1cm} (2)

In this set of equations (2), $h_L$ refers to the energy loss in each pipe in the loop and $E_p$ refers to energy added to the loop by pumps. This equation ensures conservation of energy in each loop. If there are no pumps in the loop (ie., $\Sigma E_p = 0$), it can be seen to be equivalent to the third general condition of zero total head loss in a loop.
\[ \Delta E = \Sigma h_L - \Sigma E_p \quad \text{(for } f-1 \text{ pairs of fixed-grade nodes)} \quad (3) \]

The term \( \Delta E \) refers to the difference in energy between two fixed-grade nodes. This ensures conservation of energy between points of constant head. These three sets of equations, the number of equations equal to the number of pipes, comprise a set of simultaneous non-linear equations that can be formulated such that the solution provides the flows in each pipe. An alternative formulation, the node equations, represents the problem in terms of unknown head at junction nodes and unknown pump heads (Wood and Rayes, 1981). Both formulations are sets of non-linear equations that cannot be solved analytically.

b) Solution methods  Numerous solution methods have been developed for solving the hydraulic equations. The earliest method, developed by Cross (1936), is known as the Single Path Adjustment Method and is an iterative procedure for solving the loop equations by utilizing a first order expansion of the energy equations and solving for a correction factor for the flow in each loop (Wood and Charles, 1972; Wood and Rayes, 1981). This technique has been found to converge slowly or not at all in a number of cases (Wood and Charles, 1972). The analysis of hydraulic networks as a set of simultaneous linear equations was developed by Wood and Charles (1972). This method uses initial calculations of flowrates; the equations are then linearized using these approximate flowrates. These linear equations are then
solved to provide another calculation of flowrates. The procedure terminates when
the change in the calculated flowrate meets the convergence criterion (Wood and
Charles, 1972; Wood and Rayes, 1981). An improvement of the *Single Path
Adjustment Method* was the *Simultaneous Path Adjustment Method* which employs a
numerical method to solve the system of nonlinear equations simultaneously (Epp and
code that employed Newton's method to solve the system of nonlinear equations. The
program WATER (Municipal Hydraulics, 1990) is based on the Epp and Fowler
the node equations include the *Single Node Adjustment Method* and the *Simultaneous
3. Distribution Water Quality Models

   a) Steady-state and dynamic models  Distribution water quality models attempt to predict the location and magnitude (e.g., concentration) of some constituent within the distribution system, usually as a function of hydraulic conditions. Steady-state models rely on steady-state hydraulic predictions to determine the magnitude of the constituent at points in the distribution system. Clark and Males (1986) used steady-state modeling to assess the spatial distribution of costs for the long-run operation of the New Vienna, OH water distribution system. The steady-state approach has limitations with regard to the modeling of contaminant propagation. Males et. al. (1988) applied a steady-state model to predict concentration of total trihalomethanes in the North Penn Water Authority system. While the resulting model provided useful information for designing a pilot sampling study, the authors pointed out that the steady-state model was of very limited use in providing predictions of water quality at specific times and locations in the system (Males et. al., 1988). In order to obtain information on the travel time and concentration of a constituent under the changing conditions that are typical of distribution system operation, it is necessary to create a dynamic model of distribution water quality. Dynamic models provide predictions of water quality over time and may be used to assess the impact of tank hydraulics and demand fluctuations on contaminant concentrations (Grayman et. al., 1988; Jones, 1992). Dynamic models have usually been quasi-dynamic. They have relied on sequential steady-state solutions at discrete
time periods with the solution for one period providing the initial conditions for the next period (Grayman et. al., 1988; Jones, 1992; Males et. al., 1988).

b) Constituent transport models  Constituent transport models are numerical methods for calculating the change in water quality through a distribution system. Three processes have been identified in modeling distribution water quality: advection in the pipeline, mixing at pipe junctions, and decay or growth of the constituent (Liou and Kroon, 1987). Approaches to the problem have been suggested by Grayman et. al. (1988) and by Liou and Kroon (1987). The method employed by Grayman et. al. (1988) used discrete time increments, $\Delta t$, of constant duration. The algorithm divides each link in the network into a series of sub-links such that the travel time from one sub-node to an adjacent sub-node is approximately equal to $\Delta t$. Thus, the number of sub-links and sub-nodes may vary from link to link and from time period to time period. The concentration of constituent at each sub-node is the concentration at the upstream sub-node one period before, so this method was computationally fairly simple. At nodes where links joined or at storage reservoirs, a flow-weighted average concentration (Males et. al., 1985) is computed. The model also allowed decay of non-conservative constituents to be modeled. The main decision required for applying this method was the appropriate time increment, $\Delta t$. Shorter time increments provided greater computational accuracy, but necessitated increased computational time. Specific details on the computation of the number and length of sublinks and
the concentrations at nodes and sub-nodes was provided in Grayman et. al. (1988).

Liou and Kroon (1987) developed a constituent tracking algorithm that divides each link into volume elements such that the concentration of each element will reflect the concentration gradient in the pipe. Thus, if no constituent is present, each link will be represented with a single volume element. This algorithm was designed to be linked to a sequential steady-state hydraulic model using a time increment, designated \( \Delta T \), that was sufficient for hydraulic modeling. The time increments for constituent transport calculations, designated \( \Delta t \), are calculated separately from the increment used in the hydraulic model. Liou and Kroon (1987) showed that, in order to accurately represent the concentration of the outgoing stream from a junction after mixing has occurred, three time steps are required and the sum of these three increments is equal to the hydraulic time increment (that is, \( \Delta t_1 + \Delta t_2 + \Delta t_3 = \Delta T \)). The complexity of the calculations and the storage requirements were kept to a minimum by using a scheme for consolidating small volume elements with the nearest element of similar concentration. The maximum number of volume elements (plugs) per pipe can be prespecified. This algorithm was initially developed and linked to the hydraulic model LIQVARS(1983) by Liou and Kroon (1987) and was demonstrated on the Carlisle, PA distribution system. As discussed in the next chapter, the algorithm was linked to the hydraulic model WATER (1990) by Jones (1992) and used to study the propagation of a contaminant in a hypothetical distribution system.
An aspect shared by both algorithms was the assumption of no longitudinal mixing. Liou and Kroon (1987) pointed out that this assumption as well as the complete mixing assumption at junctions were matters that need further investigation before their validity was assured. Both of the algorithms discussed allowed the user to model the decay or growth of a constituent using a first-order decay function of the form:

\[ C_{t+1} = C_t e^{-k \Delta t} \]  

(4)

Using this function, the decay or growth of the substance can easily be applied to each volume element within the transport algorithm (Grayman et. al., 1988; Liou and Kroon, 1987) and the concentration of that element computed for the next time step.

c) Applications of constituent transport models Dynamic distribution water quality models have been used to model the propagation of waterborne substances for a variety of purposes. Steady-state and dynamic models were used to investigate the outbreak of disease related to *E. coli* 0157:H7 in Cabool, MO. Hydraulic and transport models showed that the pattern of occurrence of illness was closely related to the flow patterns of the water in the distribution system (Geldrich, 1991).

Grayman et. al. (1988) modeled the propagation of total trihalomethanes (TTHMs), chloroform, and hardness in the Cheshire distribution system. The model was calibrated to match the conditions present during a 34 hour pilot sampling study.
in an effort to assess the impact of dynamic hydraulic conditions on TTHM concentrations throughout the system. This study noted several variations between the predicted values obtained by the model and the observations obtained from field sampling. In an attempt to more thoroughly understand the effect of temporal variables on the spatial propagation of contamination, an extensive field study using fluoride tracers was conducted in the Cheshire system (Clark et. al., 1991). The concentration of the fluoride tracer at monitoring points showed a temporal variation that was closely correlated with the discharge from storage tanks.

Jones (1992) developed a constituent tracking model to investigate the relative performance of sampling strategies under a variety of hydraulic conditions and assumptions concerning the nature of contamination. Twenty year simulations were performed using two layouts of a hypothetical distribution system. In one layout, the storage reservoir was located near the source pump and the other layout located the storage tank away from the source pump. Simulations were performed for source node contamination events, transient node contamination events, tank contamination, and contamination resulting from biofilm sloughing. Several basic observations were made by Jones (1992) regarding the effect of tank operation and location on system contamination. Storage had the effect of diluting the concentration of contamination entering the tanks, but the tanks could reintroduce contamination into the distribution system well after the initial contamination event had ceased. In addition, water released from the storage tank could displace contaminated water in the distribution
system and, in effect, push the contamination farther out in the system. When the tank was located far away from the source node, the effects of tank behavior on pipe hydraulics and on the distribution of contamination in the system were found to be greater. Jones' model also allowed the comparison of monitoring plan performance. Several plans were compared based on their ability to detect system non-compliance.

In general, plans that were based on traditional "engineering judgement" were found to be inferior to plans that took advantage of the models predictions regarding the effect of tank operation on contamination patterns.

Both the study by Jones (1992) and the Cheshire study (Clark et. al., 1991) demonstrated the effect that changes in hydraulic conditions have on the temporal and spatial distribution of constituent. In particular, the behavior of the storage reservoirs was closely related to constituent travel and concentration.

4. Model Calibration

Distribution water quality models require calibration of the model for accurate hydraulic simulation as well as calibration for constituent transport. Walski (1985) addressed the problem of hydraulic calibration given limited information on C-factors and the spatial distribution of water use. He presented several methods for assuring accurate model calibration by the use of flow test data. Two methods, the "analytical approach" and the "trial and error approach", gave methods for back-calculating C-factors and water use. A third approach was based on conducting flow tests during.
low-flow periods. The accuracy of hydraulic modeling was formally addressed by Bargiela and Hainsworth (1989). Confidence intervals about flow and pressure estimates were derived using several mathematical techniques. Two methods, an optimization method and a sensitivity matrix method, were based on linearized models. Both of these methods compared favorably to confidence interval estimation based on Monte Carlo studies.

Calibration of a constituent transport model has been accomplished using conservative fluoride tracers (Clark et. al., 1991; Deininger et. al., 1992; Goodrich et. al., 1991; Kennedy et. al., 1991). In calibrating a water quality model for the Cheshire system, the concentration of a fluoride tracer was measured at several sampling points during a two month period (Clark et. al., 1991; Goodrich et. al., 1991). The calibration of the model to the observed field data was highly dependent on the mixing assumptions for the storage reservoirs. A two compartment model was developed to simulate partial stratification in the storage reservoirs and was found to agree well with the field data (Clark et. al., 1991; Grayman et. al., 1991).
C. Mathematical Optimization

1. Unconstrained and Constrained Optimization

The mathematical approach to systems analysis entails the formulation of a mathematical model that describes the goals and constraints of the system. Ossenbruggen (1984) described the formulation of an objective function that gives a quantitative measure of the goals of the system in terms of control variables. Optimization methods determine the level of the control variables that achieve the best possible value of the objective function (e.g., maximum value or minimum value).

For unconstrained problems, the classical approach is to locate critical points of a function and then determine optimality from second order conditions. This method has been described in numerous texts (Ossenbruggen, 1984; Taha, 1987; Skwokowski, 1984) and is based on theorems from differential calculus. When an objective function is particularly complicated, numerical methods such as the Newton-Raphson method may be employed (Press et. al., 1989; Taha, 1987). The Newton-Raphson method is a type of gradient search method. Other numerical routines have been developed for determining the minimum or maximum of an objective function (Press et. al., 1989). Some of the alternative methods are appropriate when local extrema exist and the desired result is a globally optimal value.

In many applications, there are numerous constraints on the control variables that prevent the optimal value of an unconstrained objective function from being
feasible. Ossenbruggen (1984) describes a large sub-set of these types of problems under the classification of resource allocation problems. The typical resource allocation problem consists of an objective function that is to be maximized or minimized and a set of resource constraints. These constraints represent financial constraints (due to limited resources) and institutional constraints (e.g., design requirements, regulatory requirements, etc.). Resource constraints are expressed as equalities or inequalities. A solution to the objective function that satisfies these constraints is said to be feasible. The best possible value of the objective function such that the control variables satisfy the resource constraints is said to be feasible and optimal (Taha, 1987). The classical approach to constrained optimization is based on theorems in calculus; the Jacobian method employs constrained derivatives while the Lagrangean method computes a bordered matrix of second order terms (Taha, 1987). These methods are appropriate when the resource constraints are expressed as equalities. When inequality constraints are present, the classical approach relies on the solution of the Kuhn-Tucker conditions (Taha, 1987). The classical approach is often not a feasible means of determining the constrained optimum for realistic problems. Numerous numerical routines have been developed for this problem. As discussed in the next section, the most important and widely used of these methods have been developed for linear optimization problems and problems where the control variables assume only integer values.
2. Linear and Integer Optimization

a) Linear formulations  Linear optimization models have a linear objective function and linear constraints. The linearity of a system may be due to the nature of the system or may be the result of linear approximations. The most common approach to solving a linear optimization problem is the simplex method developed by Danzig (Ossenbruggen, 1984; Press et. al., 1989; Taha, 1987). Provided that the problem is properly formulated as a resource allocation problem, this method guarantees the optimal feasible solution. The texts cited discuss the problems with obtaining a solution when improper formulations are used.

Linear optimization models have been widely used in hydraulic and hydrologic modeling. Bargiela and Hainsworth (1989) formulated a linear optimization model for assessing the uncertainty in hydraulic models. This formulation, while solvable by the simplex method, was solved by an alternative algorithm that took advantage of the structure of the particular linear system. Revelle et. al. (1969) used a linear model to analyze reservoir management and determine an optimal policy for reservoir release.

b) Integer formulations  In many applications, the control variables are integer variables. In this case, the solution space is limited to integer values of the control variables. The use of zero-one integer variables allows the incorporation of two-state decision variables in the model. Several algorithms have been developed to find the optimal integer solution of a linear problem. The traditional methods, such
as the cutting-plane algorithm and the branch and bound method are extensions of the simplex method for linear optimization (Taha, 1987). Both of these methods repeatedly impose additional constraints on the optimal tableau until the solution obtained is an integer solution. Alternative methods such as simulated annealing (Press et. al., 1989), allow nonlinear integer problems to be solved and offer the potential of faster solutions to linear integer problems. However, an optimal solution is not guaranteed by most alternative solution methods.

Integer formulations have been commonly used to analyze problems related to networks. An example of a network problem is the maximal coverage location problem (MCLP) formulated by Church and Revelle (1974, 1976) for determining optimal locations on a network for distribution facilities given that demand can only be covered within a maximal service distance of a node on the network and that a limited number of distribution facilities can be built. The algorithm chooses a set of nodes for the location of distribution facilities that maximizes the demand served. This formulation was adapted for locating groundwater monitoring wells by Meyer and Brill (1988). Their formulation treated groundwater contamination episodes as "demands" on the system and monitoring wells as "distribution facilities." A "demand" was served by the "facility" if a monitoring well was located in a position to detect the contamination event.
3. Optimal Sampling Design

Parameters that determine the number and location of sample points have been determined using mathematical optimization. Gilbert (1987) reviewed the main approaches to sample design and demonstrated the optimization of sample design based on specific objective criteria and constraints. This approach is particularly applicable to more complicated sample designs such as stratified random sampling. For example, Gilbert (1987) presented Cochran's results (Cochran, 1977) for minimizing the variance of the sample mean subject to a cost constraint when stratified random sampling is used. Given the cost per unit sampled in each stratum, the result provides the optimum number of samples to be collected in each stratum. Similarly, the problem was set up to provide the least cost sample allocation for a prespecified minimum variance. These problems illustrated the optimization approach to sample design using classical statistical theory in the context of a resource allocation problem.

Myer and Brill (1988) used an integer program based on the MCLP to determine optimal well locations for sampling groundwater near a landfill. This formulation used the number of water quality violations detected as the objective. The objective was maximized subject to resource constraints (represented by a maximum possible number of wells) and constraints that defined detection of an event by each potential well site. This formulation provided optimal locations for sampling given a fixed number of samples. The objective of maximizing detection, as opposed
to minimizing the variance of some observed response, reflected the purpose of the sample design as being primarily compliance monitoring. The formulation presented by Myer and Brill (1988) differed from Church and Revelle (1976) in the definitions of the variables but not in the formulation itself. Myer and Brill (1988) proposed a grid that represented points where monitoring wells could be located. A set of simulated ground water contamination events were used to obtain information on the effectiveness of each location for groundwater monitoring.

A similar optimization approach to distribution water quality monitoring was developed using an objective function that measured monitoring plan performance in terms of coverage of the system (Deininger, 1991). This formulation used the concept of coverage as defined by Lee, Deininger, and Clark (1991). Given a fixed number of samples to be collected, the solution to the integer optimization problem provided the location of sample points such that there would be maximum coverage of demand. This approach demonstrated the spatial allocation of sample points on a network given an objective function based on hydraulic characteristics. Thus, the objective was not directly linked to the performance of the sample design in detecting contamination, but was based on a measure that was deemed to be a good proxy for the actual performance of the sample design.
4. Combined Simulation-Optimization

Combined simulation-optimization is the process of using Monte Carlo simulation to generate data for the formulation of constraints in the optimization problem. Burn (1989) developed a combined simulation-optimization method for determining the optimal waste load for a series of discharge points on a body of water. Monte Carlo simulation was used to generate a set of potential steady-state water quality responses. The stochastic nature of the water quality parameters was modeled by the set of Monte Carlo simulations. Using the simulation results, Burn (1989) developed the constraint set for a cost optimization model that selected the optimal treatment levels at various discharge points such that the water quality standards were not violated. A similar approach was used by Meyer and Brill (1988) to analyze the previously discussed problem of locating ground-water monitoring wells. Monte Carlo simulation of constituent transport through an aquifer was used to identify which potential well locations would identify simulated ground water contamination events. The set of responses included the list of events detected at each potential well location. These responses were used to construct the detection constraints in the MCLP formulation used to locate monitoring wells such that the maximum possible number of violations of the water quality standard would be detected.

The combined simulation-optimization method seems appropriate when sufficient information is available for simulation of a system, but there is not enough
empirical data to describe the probability distribution of water quality responses. There are, however, two limitations that must be kept in mind. The first limitation, alluded to by Burn (1989) and Meyer and Brill (1988), is the necessity of having sufficient information and computational resources to run a large number of simulations that will provide a reasonable representation of the system. The other limitation, pointed out by Meyer and Brill (1989), was the limitation of the optimization formulation as truly representing the goals and constraints of the problem. Their intent was to use the well location model within the context of a cost-benefit framework as described by Massmann and Freeze (1987a,b). Any solution obtained using a simulation-optimization approach must be considered within the context of these limitations.
III. METHODS AND MATERIALS

A. Overview

A simulation-optimization methodology was used to choose a set of monitoring points that would maximize the detection of contamination in a water distribution system. The research was conducted in two phases. In the first phase, data on the layout and operation of the Blacksburg distribution system was used to construct a network model that served as input for a contaminant transport model. This model simulated possible contamination events and tracked the movement of residual contamination through the distribution network. Multiple trials, each trial representing a distinct contamination event, were performed so that the results would reflect the variability of possible contamination events. The output from the simulation trials served as input to a formal mathematical optimization formulation. This mathematical problem was solved in the second phase. The solution provided a set of monitoring points in time and space that detected the maximum possible number of contamination events. The simulation-optimization methodology was applied separately to source node contamination events and random node contamination events. Source node events resulted from the input of contamination at the node where water entered the Blacksburg distribution network. Random node events resulted from the input of contamination at a random location within the Blacksburg network. The performance
of optimal monitoring plans was compared with alternative monitoring strategies using independent sets of simulation trials. A flow-diagram illustrating the process followed during this study is presented in Figure 1.
Figure 1. A simple diagram showing the flow of data between the major steps in the research.
B. The Contaminant Transport Model - TRAK

1. Model Description

The computer program TRAK (Jones and Gallagher, 1991) is a set of subroutines for simulating the travel of a constituent through a water distribution network. The model is linked to the hydraulic model WATER (Municipal Hydraulics, 1990) which was adapted for extended period simulation (Jones, 1992). Additional subroutines provide stochastic inputs for demand and contamination events. The model allows simulation of source node contamination, random node contamination, and biofilm related contamination. The algorithm for tracking constituents in the system is based on the plug flow algorithm developed by Liou and Kroon (1987). The hydraulic solution is based on the Epp and Fowler algorithm (Epp and Fowler, 1970) for solving the loop equations. Source code for both TRAK and WATER is in Fortran 77. Both of these algorithms have been discussed in greater detail in section B of the literature review.

2. Stochastic Data Generation

The constituent transport model TRAK included subroutines for the generation of stochastic variables during the course of a simulation trial. Jones (1992) documented the method of generating uniform random variables and transforming
these variables to represent stochastic responses from appropriate distributions. As discussed below, stochastic data generation was used to simulate variability in water demand and to simulate variability in the parameters defining a contamination event. The types of probability distribution used to represent various random variables were the same as those used by Jones (1992). Contaminant concentrations were modeled as exponential random variables. The begin time and location (random node events only) were modeled as uniform random variables. The duration of contaminant input was held constant at one hour. Estimation and selection of mean values is discussed in greater detail in sections C and D of this chapter. The random number generator used a recursive formula that required a seed value to begin a unique string of random numbers on the interval (0,1). In order to ensure the independence of simulation trials, the input for each trial contained a unique integer seed value.

3. Input Requirements

The input data file consisted of a listing of all pipes with the appropriate length and roughness coefficient, a list of all nodes with elevation and average demand, a list of all pumps with pump curves, and a list of all storage reservoirs with dimensions and initial water levels. In addition, the maximum number of plugs per pipe was specified at 20 plugs per pipe. Plugs were consolidated by the program in order to prevent this number from being exceeded. The input file for each trial contained an exclusive seed value to insure that the sequences of random numbers varied from trial
to trial. Stochastic inputs for total demand and the parameters for random contamination events were specified in a subroutine. The model contained a random number routine that generated stochastic variables according to the appropriate probability distribution. The specification of parameters defining the random variables is described in sections C and D.

4. Model Validation

The model TRAK consists of two portions: the steady-state hydraulic solver and the program code for constituent tracking and updating information for quasi-dynamic modeling. It was assumed that the hydraulic portion, which was based on code from a commercially available package (Municipal Hydraulics, 1990), had been widely used and was reliable. Jones (1992) checked the capability of the constituent tracking algorithm by comparing the results of a simple simulation with travel times and concentrations computed by hand.

As discussed in the literature review, validation of the model requires calibrating the results to empirical data. This process requires reliable field data for both hydraulic analysis and the analysis of constituent travel. No reliable field data was available for validation and the performance of fluoride tracer studies was beyond the resources available for this research. Given that an exact representation of the Blacksburg system was not a primary goal of the research, it was decided not to attempt to formally validate the results.
5. Model Output

The output of each simulation consisted of information about the hydraulic performance of the system and the identification of contaminant location and concentration. The pressure at each head, the flow in each pipe, and the demand at each node was written to a file each time a hydraulic solution was obtained (approximately once per simulated hour). This file was overwritten at the start of each simulated day in order to preserve storage capacity. Therefore, the detailed hydraulic solution was preserved for the last simulated day for each multi-day simulation. Reservoir levels and the concentration of constituent in each reservoir was recorded for each hour of the simulation.

Specific information on contaminant transport was recorded in two files. One file recorded the begin time, end time, concentration, and location of each contamination event. The other file consisted of an hourly record of all nodes with a contaminant concentration in excess of the MCL and the corresponding concentration. This file, therefore, was the contamination record used to formulate the optimization problem for the design of monitoring strategies.
C. The Blacksburg, VA Water Distribution System

1. Blacksburg, VA Water Supply

The town of Blacksburg purchased water from the Blacksburg, Christiansburg, VPI Water Authority. The water authority was responsible for pumping raw water from the New River, treating the raw water, and distributing the drinking water to the local systems. The water treatment process included a flash mixing chamber, flocculation basins, high rate filter units, clearwells with 0.426 mg of capacity, and additional storage in the authority's distribution system (Virginia State Water Control Board, 1987). Maintenance and operation of the distribution network and water quality monitoring inside the Blacksburg town limits was the responsibility of the Town of Blacksburg. A schematic diagram showing the major service areas of the water authority is presented in Figure 2.
Figure 2: Schematic of the Blacksburg, Christiansburg, VPI & SU Water Authority service areas. (Not to scale)
2. The Distribution Network

Information on the layout of the Blacksburg water distribution system was obtained directly from the town's blue-prints of the pipe network (1 in = 200 ft) and from a published engineering survey (Anderson and Associates, 1986). Blacksburg (Shaver, 1993) also provided output from their own steady-state hydraulic analysis which used the University of Kentucky Pipe Network Analysis Program (KPIPE) to solve the linearized flow equations (Wood and Rayes, 1981). The Blacksburg hydraulic analysis divided the Blacksburg system into three individual networks (labeled as "expansions") for steady-state hydraulic analysis with the storage tanks serving as the sole source of water. The three expansions of the network (expansion A, expansion B, and the Tank model) consisted of 290 links with 2 storage tanks, 204 links with 2 storage tanks, and 213 links with 1 storage tank, respectively. There was some overlap in the regions of the system modeled by each expansion and only a portion of the area served by the Blacksburg distribution system was modeled. Certain regions of each expansion were modeled using all pipes with a diameter greater than 2 inches. The connection of these regions with the reservoirs was represented with only a few larger mains, however. Thus, the degree of skeletonization was not consistent over the entire model. This steady-state analysis was performed in 1990.

The combination of these sources was used to construct a network model that included all pipes with a diameter of at least 4 inches. The resulting model consisted
of 844 pipes and 712 nodes. The set of nodes included the source node and 4 storage reservoirs. A greater level of skeletonization was not employed because research by Hunt (1986) and Ferreira (1991) indicated that removal of smaller pipes may affect the computation of constituent travel times. Pipes of less than a 2 inch diameter were not included because of the need to keep the model small enough to perform the simulation trials on a personal computer.

Figure 3 shows a schematic of the distribution network model. Specific information on the components of the network model are discussed in the remainder of this section.
Figure 3. Schematic diagram of the Blacksburg water distribution system (approximate scale: 1 in = 4000 ft). The source node represents the point at which water enters the Blacksburg distribution network from the Blacksburg, Christiansburg, VPI Water Authority system. Storage tanks are located between the source node and the water treatment plant. The system was skeletonized to include pipes with diameters of 4 inches or greater.
a) Pipes A list of all pipes over 4 inches in diameter was compiled and the length of each pipe was determined from the blue-prints. When possible, pipe definitions and lengths were matched to the Blacksburg model. Since the level of skeletonization in the Blacksburg model was not the same as the level desired for this model, such matching was not always practical. No information was available on roughness coefficients for individual pipes, so a value of 100 was assumed for all pipes. A total of 844 pipes with a capacity of approximately 1.91 MG were included in the model.

b) Nodes A node was assumed to exist at the intersection of two or more pipes and at the location of fixtures such as pumps, valves, and reservoirs. Elevations were available for the nodes included in Blacksburg’s steady-state hydraulic model. The remaining node elevations were read to the nearest 10 feet from contours on the Anderson and associates survey (Anderson and Associates, 1986). This survey showed a skeletonized pipe network overlaying U.S. Geological Survey maps of the region. Elevation contours were at 20 foot intervals on these maps.

c) Source Pump The Blacksburg distribution system is connected at a single point to the Blacksburg, Christiansburg, VPI Water Authority system. Flows into the Blacksburg network were available on a monthly basis. Therefore, it was necessary to make certain simplifying assumptions concerning the source node. Specifically, it was assumed that water entered the Blacksburg system at a flow equal to the average daily demand. Determination of this demand is discussed in the next section. Due to sparse
information on tank and pump operation in the Blacksburg system, the pressure at the source node was set constant at 200 psi in order maintain pressure heads in the 35 to 120 psi range at the majority of nodes in the system. This range was determined according to reasonable operating pressures as defined in Culp, Wesner, and Culp (1986).

d) Storage Reservoirs Four storage reservoirs with a maximum capacity of 5.5 MG were included in the model. Specific information on the control and operation of these reservoirs was not available, so it was assumed that they were free to fill and empty according to hydraulic conditions. In other words, during periods of high demand they were free to empty in order to meet demand. During low demand periods they were free to fill. In this manner, the mass balance of the system was maintained without adjustments to the flow at the source node. Floating reservoir operation was seen as consistent with typical reservoir operation as described in the literature (Culp, Wesner, and Culp, 1986). Reservoirs were assumed to fill and empty through a single pipe with the outlet at the bottom of the tank. Table II lists the storage reservoirs with dimensions.
Table II. Dimensions of Storage Reservoirs modeled as part of the Blacksburg distribution network. Free-floating operation was assumed for all reservoirs.

<table>
<thead>
<tr>
<th>Reservoir</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Capacity (gal. *1000)</td>
<td>558</td>
<td>1,584</td>
<td>1,584</td>
<td>1,706</td>
</tr>
<tr>
<td>Height (ft)</td>
<td>38</td>
<td>24</td>
<td>24</td>
<td>24</td>
</tr>
<tr>
<td>Diameter (ft)</td>
<td>50</td>
<td>106</td>
<td>106</td>
<td>110</td>
</tr>
<tr>
<td>Elevation at Base (ft above sea level)</td>
<td>2,376</td>
<td>2,260</td>
<td>2,346</td>
<td>2,260</td>
</tr>
</tbody>
</table>

Source: Output of Blacksburg’s hydraulic simulation (Shaver, 1993)
3. Water Demands

a) System Demand  Data on water use from July 1992 through June 1993 was obtained from the Blacksburg, Christiansburg, VPI\&SU Water Authority (Higgins, 1993). This data included monthly meter readings that recorded the amount of water consumed by Blacksburg and VPI\&SU. Also available were quarterly meter readings that gave the quantity of water consumed by VPI\&SU alone. Water use for both Blacksburg and VPI\&SU was included in the model since nodal demands in Blacksburg’s own hydraulic model reflected use by VPI\&SU. This information was used to calculate an average daily demand of approximately 4.3 MGD for the system modeled. Seasonal effects were not included in the simulation since a single year of data did not provide sufficient replication for meaningful estimation of the seasonal effects. More significantly, the event-based simulation methodology did not lend itself to seasonal modeling, at least not with a reasonable number of simulation runs.

Hourly variations in demand were not directly available from the water authority. Therefore, a typical diurnal demand curve was assumed to exist. This curve was constructed with an average daily demand derived from the one year of data obtained from the water authority and followed the diurnal cycle typical of many systems (AWWA, 1981; Jones, 1992). The diurnal demand curve provided the mean water use for each hour of the day. During simulation, demand factors were randomly generated for each hour with an hourly mean designated by the demand curve. A beta distribution with upper and lower bounds and a coefficient of variation
that provided a slightly skewed distribution that is typical of demand variations was used to generate stochastic demands. A lagging flow adjustment was used to smooth large variations in demand between consecutive hours. Details on the development of the stochastic generation of demand factors may be found in Jones (1992). Figure 3 gives the diurnal demand curve showing the mean demand factor and the upper and lower limits on the demand factor for each hour of the day.

**b) Spatial Demand Allocation** The spatial allocation of demand was available from Blacksburg’s steady-state model output. However, this allocation was assigned to a smaller set of nodes than used in the TRAK model and represented information that was several years old. To obtain a reasonable allocation of demand, two steps were performed. First, the nodal demands from Blacksburg’s steady-state model were allocated equally to nearby nodes. Second, the total demand represented by this allocation was subtracted from more recent total demand data obtained from the Blacksburg, Christiansburg, VPI Water Authority. The remaining demand was allocated proportionately to sections of the network not included in Blacksburg’s steady-state model. Figure 4 shows the spatial allocation of demand used to model the Blacksburg system.
Figure 4. Mean hourly demand factors with upper and lower limits. System demand was modeled as a Beta random variable with upper and lower limits of $130\%$ and $80\%$, respectively, and a coefficient of variation of $0.0594$. 

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Figure 5. Average daily demand at nodes in cubic feet per second. Total system demand averaged approximately 4.3 mgd or about 6.6 cfs.
D. Simulations Performed

1. Objectives of Simulation

Event-based simulation was used to model the transport of contaminant through the distribution system as the result of individual contamination events. The event-based simulation methodology limited the simulation period to the duration of a single event with no concurrent events. The simulation was performed with the goal of identifying the temporal and spatial location of points that would be in violation of the MCL as a result of specific contamination events. Each simulation trial consisted of a two day period during which no contamination was present in the system. This "warm-up" period was intended to dilute the effects of initial hydraulic conditions that may not have been representative of the long-run hydraulic performance of the system. A single contamination event was then simulated to occur on the third simulated day of operation. This consisted of the simulation of a contaminant of fixed concentration entering the system at a single point for a fixed duration of time. The remainder of the simulation trials modeled the propagation of the contaminant within the distribution system.
Two types of contamination events were modeled: source node contamination events and random node contamination events. Both types of event were modeled using individual event-based simulation trials with the contamination entering a clean system at a random time on the third simulated day of the trial. Information on the parameters for simulating contamination events is presented in the next two sections.
2. Source Node Contamination

The pump station at the entrance of the Blacksburg system was considered the source node. Contamination at this node represented breakthrough of treatment barriers at the water treatment facility or contamination arising in that portion of the system upstream from the Blacksburg system. There were four parameters defining a contamination event:

1. the concentration of the contaminant;
2. the beginning time of the event;
3. the beginning day;
4. the duration of the event.

The constituent was assumed to be conservative, so no growth or decay of the substance was modeled. The concentration was treated as an exponential random variable with a mean of 5 units. No specific information was available to determine a mean concentration for contamination, so a level was chosen based on preliminary observations. A level of contamination was chosen such that meaningful patterns of system contamination could be observed. The simulated event began at a random minute on the third day of the simulation and lasted for a fixed duration of sixty minutes.

Each trial allowed 10 simulated days for the contamination to leave the system. The 10 day limit was determined from the early simulation runs. Figure 10 in the Results indicates that this was an adequate total simulation time. A total of
112 trials were performed. The results of the first 56 trials provided data for the optimization of the sample design based on stabilization of the optimal solution (see Figures 32 and 33 in the results). The remaining 56 were performed while the analysis of results was taking place and were therefore used only for independent analyses of sample plan performance. Table III summarizes the parameters of the simulated source node contamination events.
Table III. Parameters defining each simulated contamination event. Each event was an independent realization of these parameters.

<table>
<thead>
<tr>
<th>Event Parameter</th>
<th>Source Node</th>
<th>Random Node</th>
</tr>
</thead>
<tbody>
<tr>
<td>Begin Time</td>
<td>Uniform random minute on the 3rd simulated day</td>
<td>Uniform random minute on the 3rd simulated day</td>
</tr>
<tr>
<td>Concentration of Inflow</td>
<td>Exponential random variable with a mean of 5 units</td>
<td>Exponential random variable with a mean of 5 units</td>
</tr>
<tr>
<td>Duration of Inflow</td>
<td>60 minutes</td>
<td>60 minutes</td>
</tr>
<tr>
<td>Volume of Contaminated Water</td>
<td>Approximately 179 thousand gallons over 60 minutes</td>
<td>Varies according to flow at the specific node</td>
</tr>
<tr>
<td>Location of Inflow</td>
<td>Contaminant input at the single source node</td>
<td>Contaminant input at a random node selected uniformly from the set of nodes excluding the source node and the storage reservoirs</td>
</tr>
<tr>
<td>Number of Simulation Trials</td>
<td>Number of trials (56) determined from stability of optimal monitoring plan design. An equal number used for independent evaluation of monitoring plan performance.</td>
<td>Number of trials (56) determined from stability of optimal monitoring plan design. An equal number used for independent evaluation of monitoring plan performance.</td>
</tr>
</tbody>
</table>
3. Random Node Contamination

The simulation of random (or transient) node contamination represented the introduction of contamination as a result of a breach of system integrity due to cross-connection, back-siphon, and other external sources. These simulations required the specification of the same parameters as source contamination event simulations with the addition of a random node in the system where the contamination was introduced. The location of each random node contamination event was treated as a discrete uniform random variable. Each node, with the exception of the source node and reservoirs, had an equal chance of being the location of a contamination event. The concentration increment, beginning time of the event, and the duration of the event were treated the same as in the source node simulations. No decay of the constituent was modeled for random node simulations.

Each trial allowed three simulated days for contamination to leave the system. Figure 23 in the Results indicated that this was an adequate simulation time. A total of 112 random node simulations were performed. Data from the first 56 simulations were used for optimal sample design. The remaining simulations provided data for an independent analysis of monitoring plan performance. A summary of the parameters of the simulated random node contamination events appears in Table III.
E. Optimization of Fixed-Point Monitoring Strategy

1. Definition of the Problem

Mathematical optimization was used to select a set of monitoring points, designated by node and time, that would maximize the number of simulated events detected by the monitoring plan. A formulation based on the maximal covering location problem (MCLP) was used. The MCLP and its application to compliance monitoring was discussed in the literature review. Appendix I provides simple examples of this problem in terms of a hypothetical location problem, a monitoring well location problem, and develops the logic for applying the formulation to distribution system monitoring.

The event-based Monte Carlo simulations of distribution system contamination provided a list of the time and location of each violation of the water quality standard resulting from the contamination event. This information was used to formulate the constraints for three optimization problems that differed in terms of certain basic assumptions about monitoring point selection. Specifically, two formulations assumed that monitoring was performed to identify the possible existence of contamination when a contamination event is suspected to have occurred. The time coordinate of these monitoring points was measured from the beginning of the simulation to the end of the simulation; a period of approximately 264 hours for source node events and 96 hours for random node events. The first formulation allows monitoring to begin the
day on which contamination has been introduced in the system while the second formulation restricts monitoring to a time period beginning at some time after contamination was introduced. This second formulation was used to reflect the possibility that immediate monitoring may not be feasible and a delay in monitoring may occur. An additional constraint that restricted the time of day during which samples could be collected was added to the first two formulations to assess the relative performance of morning monitoring, afternoon monitoring, and full day monitoring. The third formulation was designed to choose an optimal set of daily monitoring points, so the time coordinate of the monitoring point was based on the 24 hour day. The three formulations are summarized in table IV.

Each of these optimization formulations were applied separately to source node contamination events and random node contamination events.
Table IV. Three formulations used to define optimal monitoring plans. Monitoring points were chosen to be optimal with respect to the objectives and constraints defined in a formulation.

<table>
<thead>
<tr>
<th>Attribute of Formulation</th>
<th>Optimization Formulation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>No-Delay Formulation</td>
</tr>
<tr>
<td>Objective</td>
<td>Maximize Number of Events Detected</td>
</tr>
<tr>
<td>Frequency of Monitoring</td>
<td>Once at each monitoring point during the simulation period.</td>
</tr>
<tr>
<td>Feasible set of nodes that can be monitored</td>
<td>All nodes can be monitored</td>
</tr>
<tr>
<td>Time that monitoring can take place</td>
<td>Monitoring may start at hour 0 on the begin day of the contamination event.</td>
</tr>
<tr>
<td>Maximum number of monitoring points</td>
<td>Varied to assess the effect of monitoring plan size on detection</td>
</tr>
<tr>
<td>Additional Restrictions</td>
<td>No Restriction Hours 6-11 Only Hours 12-17 Only</td>
</tr>
</tbody>
</table>
2. Definition of Variables

The following variables were used in defining the optimization formulation for selecting monitoring points during the time period following a contamination event. These variable definitions are applicable to the formulations that allow monitoring at specific times and locations during the contamination episode.

- **I** set of contamination events - indexed by \(i (1, \ldots, 56)\) for this research;
- **J** set of distinct nodes on the distribution network - indexed by \(j\);
- **T** set of hours of the simulation during which a sample may be taken - indexed by \(t\);
- \((J,T)\) set of potential sample points defined by location and time \((J \times T)\) points;
- **M** maximum contaminant level (MCL) defining a violation;
- **\(c_{ijt}\)** contaminant concentration at node \(j\) and time \(t\) resulting from contamination event \(i\);
- **\(v_{ijt}\)** = 1 if \(c_{ijt} \geq M\);
- **\(v_{ijt}\)** = 0, otherwise;
- **\(x_{jt}\)** = 1 if a sample is collected at time \(t\) and node \(j\);
- **\(x_{jt}\)** = 0, otherwise;
- **\(y_i\)** = 1 if event \(i\) is detected by a sample;
- **\(y_i\)** = 0, otherwise;
- \(N_i = \{(j,t) \in (J,T) | v_{ijt} = 1\}\) the set of points that would result in the detection of event \(i\) if sampled - can be restricted to reflect other constraints on allowable monitoring points;
- **S** number of samples to be collected during the prescribed period of time.
In addition to the variables defined above, the following variables are required for formulation of an optimization of a daily monitoring plan:

\[ H \text{ hour of the day corresponding to } t \text{ - indexed by } h = 1, \ldots, 24; \]

\( \langle J, H \rangle \) set of potential daily monitoring points;

\[ d_{ijh} = 1 \text{ if } c_{ij} \geq M \text{ for any } t \text{ corresponding to } h; \]

\[ d_{ijh} = 0, \text{ otherwise}; \]

\[ D_i = \{(j, h) \in \langle J, H \rangle \mid d_{ijh} = 1\} \text{ the set of points that would result in the detection of event } i \text{ if sampled every day;} \]

\[ n_{jh} = 1 \text{ if a sample is collected daily at node } j \text{ and hour } h; \]

\[ n_{jh} = 0, \text{ otherwise.} \]
3. Constraints

Two types of constraints are required: the detection constraints allow detection of an event only if a point capable of detecting that event is in the set of monitoring points and a resource constraint specifying the maximum number of points that can be monitored. As discussed above, these constraints were formulated with two basic types of monitoring in mind. The first formulation of the constraints, given by (1) and (2), assume that monitoring will take place during the time immediately following the introduction of contamination while residual contamination is propagated through the system. The two formulations of this type differ only in the assumption of when monitoring may begin (ie., immediately versus one or more days after contamination was introduced). The other type of formulation was for determining optimal daily monitoring points and the constraints for this formulation are given by (3) and (4).

For the optimization of sample locations during the duration of residual system contamination, the detection constraints are formulated as:

\[ y_i - \sum_{(j,t) \in N_i} x_{jt} \geq 0 \]  \hspace{1cm} (1)

for \( i = 1, \ldots, I \)

This set of equations, one for each contamination event, prevents the 0/1 integer variable \( y_i \) that indicates detection of an event from being non-zero unless at least one potential monitoring point capable of detecting the event is included in the set of
points to be sampled. The set of available monitoring points defined by $N_i$ can be defined to allow monitoring only during designated time periods. This method was used to incorporate restrictions on monitoring to morning or afternoon periods and was also used to enforce delays in monitoring after the begin day of contamination.

The resource constraint defines the maximum number of points that may be sampled during the sampling period and is given by:

$$\sum_{j=1}^{J} \sum_{t=1}^{T} x_{jt} \leq S$$
For the optimization of daily monitoring points, the constraints are slightly different. The detection constraints for optimal daily monitoring are given by:

\[ y_i - \sum_{(j,k) \in D_i} n_{jk} \leq 0 \]  \hspace{1cm} (3)

for \( i = 1, \ldots, I \).

Here, the variable \( n_{jk} \) references monitoring point locations by node and hour of the day. The set of sample points defined by \( D_i \) are capable of detecting event \( i \) if sampled on a daily basis. Otherwise, this set of constraints perform the same function for the optimal daily monitoring formulation as constraint (1) does for the optimal fixed-period monitoring formulations. The resource constraint for optimal daily monitoring, defined in terms of the number of samples collected at a fixed set of locations per day, is given by:

\[ \sum_{j=1}^{J} \sum_{k=1}^{24} n_{jk} \geq S \]  \hspace{1cm} (4)
4. Objective Function

The objective of distribution system monitoring was considered to be the detection of individual contamination events. The use of event-based simulation precluded problems arising from coincidental contamination from two or more sources and allowed the identification of the detection of specific events. Thus, many of the issues discussed in the literature review (Beckers et. al., 1972; Casey et. al., 1983) concerning the specification of a measure of monitoring effectiveness are not an issue here. A reasonable objective is, therefore, to maximize the expected fraction of contamination events that can be detected by a monitoring plan. In terms of the results from a fixed number of simulation trials, this becomes the maximization of the number of events detected. This was expressed as:

\[
\text{Maximize: } z = \sum_{i=1}^{I} y_i \quad (5)
\]

The fraction of events detected is easily computed as the number of detections \((z)\) divided by the number of event-based simulation trials used to formulate the problem. If the number of simulation trials is sufficient to represent the range of potential contamination event parameters, then this may be used as an estimate of the expected fraction of contamination events that can be detected by the optimal monitoring plan.
5. Solution Method

Optimization problems were initially solved as continuous variable problems using the simplex method. A Fortran program based on algorithms and code from Taha (1987) and Press et al. (1989) was employed. The size of the problems was reduced by eliminating redundant points in the input data. While this would eliminate many alternative but equivalent optima, the solution of the initial problem would not be affected.

Most problems were anticipated to terminate in integer solutions when the simplex method was employed. For those problems that did not terminate in integer solutions, a branch and bound technique was to be used as time and computer resources allowed. In the event that a branch and bound was not practical, an approximation of the optimal solution was found by a combination of judgement and trial and error. It was anticipated that the optimal value of the objective function could be placed between two bounds. An upper bound was provided by the integer portion of the non-integer solution. A lower bound could be obtained by examining the optimal integer solutions of problems with more severe constraints. With the use of a spreadsheet, trial and error could be used to find solutions that evaluated as close to the upper bound as possible. In this way, "near optimal" solutions could be obtained for certain problems.
F. Alternative Monitoring Strategies

In order to assess the relative performance of the monitoring plans designed using the formulations described above, several alternative sampling plans were devised. These alternative plans were based on criteria that have been commonly used in practice and are similar to plans evaluated by Jones (1992). The first two plans were simple random samples from the set of possible monitoring points and so represented a design that did not incorporate any prior information on system hydraulics or constituent transport. The other plans were devised using various heuristic rules and represent common practice among water utilities. Table V provides a description of each alternative sampling plan.
Table V. Monitoring plans designed as possible alternatives to optimally designed monitoring strategies.

<table>
<thead>
<tr>
<th>Plan</th>
<th>Description</th>
<th>Used to detect this type of event</th>
</tr>
</thead>
<tbody>
<tr>
<td>A-1, A-2.</td>
<td>Simple Random Sample - 10 points chosen at random from the set of 712 nodes and the time of sampling chosen at random from 264 hours corresponding to the simulation period for source node contamination event simulation.</td>
<td>Source Node</td>
</tr>
<tr>
<td>A-3.</td>
<td>Source node sampled at a random time each day.</td>
<td>Source Node</td>
</tr>
<tr>
<td>A-4.</td>
<td>Source node sampled at 9:00 am each day.</td>
<td>Source Node</td>
</tr>
<tr>
<td>A-5.</td>
<td>Random node sampled at a random time each day for first 10 days.</td>
<td>Source Node</td>
</tr>
<tr>
<td>A-6.</td>
<td>Random node sampled at 9:00 am each day for first 10 days.</td>
<td>Source Node</td>
</tr>
<tr>
<td>A-7.</td>
<td>10 random nodes sampled at random times over the first two days of a contamination event.</td>
<td>Source Node</td>
</tr>
<tr>
<td>A-8.</td>
<td>10 random nodes sampled over the first three days of a contamination event.</td>
<td>Source Node</td>
</tr>
<tr>
<td>A-9.</td>
<td>10 random nodes sampled over the first five days of a contamination event.</td>
<td>Source Node</td>
</tr>
</tbody>
</table>
G. Analysis of Simulated Contamination and Monitoring Plans

1. Patterns of System Contamination

The distribution of system contamination resulting from simulated contamination events was hypothesized to vary spatially and temporally. The results of the simulation trials were used to assess the existence of clearly defined spatial and temporal patterns in system contamination. In the temporal domain, the extent of the contamination as measured by the average number of nodes in violation during each hour of the day was expected to show some correlation with the diurnal cycle. This hypothesis was examined graphically for both source node and transient node contamination simulations. The spatial patterns of contamination were assessed by locating nodes that were in violation of the MCL during a high proportion of simulation trials and by identifying nodes that were infrequently violated. In addition, contour plots providing estimates of the mean concentration at points throughout the system were prepared in order to isolate regions where contamination tended to concentrate. Contour plots showing the estimated standard error of these means were also prepared.
2. Optimal Selection of Monitoring Points

The adequacy of the number of simulation trials was assessed by looking for stability in the solution of the optimization formulation. The number of trials used to calculate the optimal sample plan was increased until the fraction of events detected by the optimal plan stabilized near a single value. A clear way of seeing this was to plot the change in the fraction detected due to an increase in the number of trials (i.e., Δdetection fraction/Δ# of trials) versus the number of trials. If this derivative was approximately zero after a particular number of trials, then the solution was considered stable. Since stochastic variables were involved in the simulation, it was not expected that the change in the optimal detection fraction stabilize exactly at zero. Judgement was used to determine when the value was close enough to zero.

3. Analysis of Monitoring Plan Performance

An independent set of simulation trials was used in assessing the performance of the optimal sampling plans and comparing this performance with alternative monitoring strategies. Plans were compared with respect to the fraction of events detected by the plan. This independent assessment was a means of checking the stability of optimal plans as well as measuring the relative effectiveness of optimization in choosing superior monitoring points.
IV. RESULTS

A. System Hydraulics

The first set of simulation trials, 56 source node events and 56 random node events, were used for an analysis of system performance and the design of monitoring plans. A second set of simulation trials were performed concurrent with this analysis. Simulation of free-floating reservoirs allowed for hourly fluctuations in system demand. Figures 6 and 7 show the mean hourly reservoir levels and the top water level for each of the four storage reservoirs. All four reservoirs show a general pattern of filling during the late evening and early morning periods when system demand is low and emptying during the late morning/early afternoon and late afternoon periods of high demand. Reservoirs 2 and 4 attained their maximum mean levels at hour 6 and a minimum at hour 21. Reservoir 1 and reservoir 3 operated at very low levels throughout the simulation (see Figure 7) and tended to lag the other two reservoirs’ operation by one hour and two hours, respectively.

The effect of free-floating reservoir behavior is illustrated by looking at the percentage of total storage capacity that was filled during each hour of the day. Figure 8 shows the mean percentage of system storage capacity filled increased during low demand periods (hours 22 through 6 and at hour 15) and decreased during high demand periods (hours 7 through 14 and hours 16 through 21). The mean quantity of
water in storage peaked at 73.75 percent of capacity at hour 6. During the late evening and early morning hours, the mean quantity of water in storage increased. The level of storage decreased during the high demand hours. The mean utilization of storage was at a minimum of 58.75 percent of capacity at hour 21.
Figure 6. Mean reservoir levels as a fraction of the top water level. Mean computed from 56 simulation trials of 13 days each. These two reservoirs operated at relatively high levels throughout the simulation period. Reservoir number corresponds to identification on the network schematic. Top water level was 24 feet for both reservoirs.
Figure 7. Mean reservoir levels as a fraction of the top water level. Mean computed from 56 simulation trials of 13 days each. These two reservoirs operated at very low levels throughout the simulation period. Reservoir number corresponds to identification on the network schematic. Top water levels were 38 feet and 24 feet for reservoirs 1 and 3, respectively.
Figure 8. The mean percent storage capacity filled during each hour of the day. Mean was computed from 56 trials with 13 simulated days each.
B. Simulated Source Node Contamination

1. Source Node Contamination Events

Fifty-six event-based simulation trials were used to assess the temporal and spatial characteristics of contaminant propagation in the distribution system as a result of the introduction of contamination at the source node. Each trial represented a unique contamination event during which a quantity of contaminant was introduced into the system at the source node for 60 minutes and the propagation of the contaminant was tracked throughout the distribution system. Simulated contamination events were distinguished by the realization of two stochastic variables: the begin time of the event and the concentration of the contaminant. Only trials that resulted in at least one violation of the MCL of 1 unit were included. Therefore, simulation trials that resulted in contaminant concentrations below the MCL at all locations throughout the simulation period were not included.

Contamination was introduced into a clean system at a random minute on the third simulated day of system operation. This was the begin time of the contamination event. Figure 9 shows the distribution of begin times for 56 simulated source node contamination events. The figure shows the number of trials with begin times during each hour of the day. The distribution of begin times was fairly uniform over the 24 hours of the day. Only hour 6 was not represented in the distribution of begin times.
Figure 10 shows the frequency distribution of the concentration of each simulated event. The minimum concentration that resulted in a violation of the MCL was 1 unit. The distribution of event concentrations is skewed left with the majority of responses between 1 unit and 8 units. Other concentrations occurred at higher levels with a maximum concentration of about 24 units.

Figure 11 shows the concentration and corresponding begin time for each simulation trial. The figure is a scatter plot with a fairly random pattern of points. The pattern is somewhat denser at lower concentrations; a reflection of the skewed distribution of contaminant concentrations. There does not appear to be any clear correlation between the two variables, however.
Figure 9. Distribution of begin times for 56 simulated source node contamination events. Begin times represented the minute at which contamination was introduced at the source node for a period of 1 hour and were modeled as uniform random variables.
Figure 10. Distribution of event concentrations for 56 simulated source node contamination events. Contaminant of the given concentration entered the system at the source node for a period of 1 hour. Concentration was modeled as an exponential random variable.
Figure 11. Scatter plot of begin times versus concentrations for 56 simulated source node contamination events. The two variables were modeled as independent random variables.
2. Temporal Distribution of System Contamination

The third simulated day of system operation was the begin day for each contamination event. Contaminant propagation in the distribution system was recorded from the time contamination was introduced into the system (the begin time) on the third day through the subsequent days during which residual contamination was present in the distribution system. During this time, a record of all nodes with a contaminant concentration in excess of the 1 unit MCL was compiled on an hourly basis. This record of violations facilitated the assessment of temporal patterns of system contamination during the simulation period and during the 24 hour demand cycle.

The duration of residual contamination was a measure of the time required for the system to "flush out" all contamination. This should not be confused with the duration of the initial contamination event which was the period of time during which new contamination was input to the system. As discussed in the Methods and Materials section, the first set of simulation trials indicated that a period of 10 days following the begin day was adequate for the system to flush out all residual contamination. This is illustrated by Figure 12 which shows the number of simulated days required for flushing out. The majority of the simulation trials required less than 10 simulated days for the level of system contamination to fall below the detection level. Three of the trials required 10 days for contamination to flush out.

The relationship between the duration of system contamination and selected
parameters are plotted in Figures 13 and 14. Figure 13 shows a plot of the number of hours from the begin time to the hour when the system had flushed out all residual contamination versus the begin time of each trial. Eight trials resulted in more than 200 hours of system operation before the contaminant was flushed out. Seven of these trials had begin times in the evening and one trial had a begin time in the early morning. These low demand periods also produced events of shorter duration, however. The duration of residual contamination appeared to be in two groups, one group was below 100 hours and the other group was greater than 150 hours. Few events had durations in between these levels. Figure 14 shows the relationship between the initial event concentration and the duration of residual contamination. Longer periods of residual contamination appear to correspond to higher initial concentrations, but there is considerable variation.
Figure 12. Duration of system non-compliance including the day contamination was introduced into the system. This time represents the number of simulated days required for the system to "flush out" contamination based on 56 simulated source node contamination events.
Figure 13. Duration of system non-compliance versus the begin time of the event for 56 simulated source node contamination events.
Figure 14. Duration of system non-compliance versus the concentration of introduced contamination for 56 simulated source node contamination events.
The extent of system contamination was measured by the number of nodes in violation of the MCL during a given time interval. Figure 15 shows the mean number of nodes in violation of the MCL during each hour of the simulation beginning with hour 0 of the third day of system operation. Since contamination was introduced on the third day, the system was clean on day 1 and day 2. In Figure 15, the largest mean number of contaminated nodes (38.9) can be seen to occur at hour 27. The system appears to remain continually contaminated until about hour 122. At this time, the contamination begins to reappear at irregular intervals and with few nodes affected.

The data used to construct Figure 15 were consolidated to provide the mean number of violated nodes over the 24 hour demand cycle. This is shown in Figure 16. The horizontal bars indicate one standard deviation more and less than the overall mean number of violated nodes per hour. The maximum extent of contamination occurred at hour 3 with additional lesser peaks at hours 16 and 20. The minimum mean number of violated nodes occurred at hour 12.
Figure 15. Mean number of nodes in violation of the MCL for each hour of simulated source node contamination events beginning with hour 0 of the begin day of the events. The mean is based on observations from 56 trials.
Figure 16. Mean number of nodes in violation of the MCL for each hour of the day for simulated source node contamination events beginning with hour 0 of the begin day of the events. The mean is based on observations from 56 trials of 13 days each. Solid bars show plus and minus one standard deviation from the overall hourly mean.
3. Spatial Distribution of System Contamination

The purpose of spatial analysis was to identify individual nodes and regions of the system that were the most and least affected by contamination introduced at the source node. Some effort was also expended to identify nodes that were subject to contamination when the initial surge of contaminant had passed and the hydraulic regime resulting from reservoir behavior was hypothesized to exert greater influence over the spatial distribution of contaminant.

Each node was ranked according to the number of events that resulted in that node being in violation of the MCL for at least one (1) hour of the simulation trial. Figure 17 shows nodes that were in violation for at least one hour during all 56 simulated source node contamination events. Figure 18 shows the nodes in the estimated 90 percent quantile based on the ranking criteria. The nodes in Figure 18 correspond to those nodes in violation of the MCL during at least 53 of 56 simulation trials. These figures indicate that the most frequently violated nodes tend to occur on the main lines immediately down stream from the source node. Figure 19 shows nodes that were contaminated during at least one hour after the 5th day of system contamination. Nine nodes were in violation after the 5th day of system contamination during at least 1 trial. Of the 56 trials, there were 29 trials that resulted in a violation after the 5th day of contamination. The set of nodes displayed in Figure 18 do not coincide with the set of most frequently contaminated nodes. Only one node appears on both Figure 18 and Figure 19.
Figure 20 shows nodes that were never in violation of the MCL. Figure 21 shows the 10 percent quantile based on the ranking of nodes according to the number of events during which a node was in violation of the MCL. These nodes represent locations of infrequent violation. These nodes tended to be along the northeast periphery of the system, but the set does not include peripheral nodes to the northwest nor does it include all peripheral nodes in the northeast region. Most notably, many nodes at the end of branches were not part of the set of infrequently violated nodes.

Contours were estimated for the mean concentration of contaminant (Figure 22) and the associated standard error (Figure 23). The simulation record only provided concentrations that were in excess of the MCL (1 unit). Concentrations below this level were assumed to be zero. The estimated mean contours provided a pattern of contamination similar to that shown by the plots of most frequently contaminated nodes. The higher mean concentrations tended to be directly downstream from the source node, in the central regions of the system, and in the southwestern region of the system. Low concentrations were prevalent in the northeast periphery of the system where the majority of infrequently contaminated nodes appeared. The standard deviations tended to be proportional to the estimated means. Figure 23 shows that the contours for standard error followed a pattern that was similar to that of the means.
Figure 17. Nodes that were in violation for at least 1 hour during all 56 simulated source node contamination events.
Figure 18. Nodes that were in violation during 53 or more (estimated 90 % quantile) simulated source node contamination events.
Figure 19. Nodes that were in violation for at least 1 hour after hour 120 during at least 1 of 56 simulated source node contamination events. Twenty-nine simulations caused violations after hour 120.
Figure 20. Nodes that were never in violation during any of the 56 simulated source node contamination events.
Figure 21. Nodes that were in violation during fewer than 19 (estimated 10 percent quantile) simulated source node contamination events.
Figure 22. Contours of estimated mean concentration for 264 hourly observations from each of 56 simulated source node contamination events. Concentration is in generic units.
Figure 23. Contours of estimated standard error of the mean concentration for 264 hourly observations from each of 56 simulated source node contamination events. Concentration is in generic units.
C. Simulated Random Node Contamination

1. Random Node Contamination Events

The simulation of random node contamination events was carried out in a manner analogous to the simulation of source node contamination. The primary difference was that random node simulations included the realization of a random location in the distribution system where the contaminant was introduced. While the mean concentration of random node events was equal to the mean concentration of source node events, the flow at random nodes was generally lower than at the source node. This implies that the total volume of contaminated water resulting from a random node event was, on average, less than what resulted from source node contamination. As with the simulation of source node contamination, only trials that resulted in at least one violation of the MCL were included in the total set of 56 simulation trials.

Figure 24 shows the begin time of random node events. Event begin times were distributed over the 24 hours of day 3. Although the begin times were distributed fairly uniform over the day, no events began during hours 0 or 1. The location of random node contamination events are plotted on a system diagram in Figure 25. Contamination was introduced at locations throughout the system. The distribution of random node locations is not spatially uniform, but does appear to have been fairly uniform over the set of nodes.
The concentration of random node events is plotted in Figure 26. The maximum concentration is over 31 units. The minimum event concentration that resulted in a violation was 1 unit. The distribution is skewed to the left with the majority of concentrations between 1 unit and 7 units.

Figure 27 shows a scatter diagram of the event concentrations and the corresponding begin times. The higher concentration events tended to occur after hour 12, although there is no definite correlation present. Events with concentrations less than 10 units were distributed uniformly over the set of begin times.
Figure 24. Distribution of begin times for 56 simulated random node contamination events. Begin times represented the minute at which contamination was introduced at the source node for a period of 1 hour and were modeled as uniform random variables.
Figure 25. Locations of 56 simulated random node contamination events. Contamination entered at the node for a period of 1 hour.
Figure 26. Distribution of event concentrations for 56 simulated random node contamination events. Contaminant of the given concentration entered the system at the source node for a period of 1 hour. Concentration was modeled as an exponential random variable.
Figure 27. Scatter plot of begin times versus concentrations for 56 simulated random node contamination events. The two variables were modeled as independent random variables.
2. Temporal Distribution of Contamination

The assessment of temporal variations in system contamination followed the same procedure as used for source node simulations. The record of MCL violations was used to look at the patterns of system contamination over the period of the simulation and over the 24 hour demand cycle.

The duration required for the system to flush out contamination resulting from random node events is plotted for 56 trials in Figure 28. As discussed previously, early trials indicated a simulation time of two days following the day that the event occurred would provide adequate time for the contamination to flush out of the system. Figure 28 indicates that, for the majority of trials, the contamination was flushed out on the day of the event. Only two trials required two days following the day of the event to flush out contamination.

The duration of system contamination, in hours, is plotted with the corresponding begin time of the event in Figure 29. No correlation appears to be present. One event of particularly long duration, began at hour 11.

The duration of system contamination and the corresponding event concentration are plotted in Figure 30. The higher density of points towards the bottom of the graph reflects the skewed distribution of event concentrations. The points are distributed randomly along the horizontal axis and provide no indication of correlation between the duration of system contamination and the event concentration.
Figure 28. Duration of system non-compliance including the day contamination was introduced into the system. This time represents the number of simulated days required for the system to "flush out" contamination based on 56 simulated random node contamination events.
Figure 29. Duration of system non-compliance versus the begin time of the event for 56 simulated random node contamination events.
Figure 30. Duration of system non-compliance versus the concentration of introduced contamination for 56 simulated random node contamination events.
The extent of system contamination, as measured by the mean number of nodes in violation of the MCL during a given hour, is plotted in Figure 31. The peak mean number of non-compliant nodes (1.2) occurred during hour 12 on the day of the event. System contamination quickly tapered off starting the day after the event started. No pattern of recurring contamination was apparent. Figure 32 shows the mean number of nodes in violation during each hour of the 24 hour day. The mean number of contaminated nodes peaked at hour 4 and was at a minimum at hour 14. Secondary peaks occurred at hour 11 and at hour 19. The shape of the curve is similar to that observed for the source node simulations though the two curves are not exactly in phase and the range of random node means appears to be less than the range of source node means.
Figure 31. Mean number of nodes in violation of the MCL for each hour of simulated random node contamination events beginning with hour 0 of the begin day of the events. The mean is based on observations from 56 trials.
Figure 32. Mean number of nodes in violation of the MCL for each hour of the day for simulated random node contamination events beginning with hour 0 of the begin day of the events. The mean is based on observations from 56 trials of 3 days each. Solid bars indicate the overall hourly mean plus or minus one standard deviation.
3. Spatial Distribution of System Contamination

Figure 33 shows the nodes that were most frequently contaminated during the simulation of random node contamination events. Nodes that were never in violation of the MCL during any of the simulated random node contamination events were plotted in Figure 34. In contrast to the plot derived from source node contamination events, unviolated nodes were prevalent throughout the system in the case of simulated random node contamination.

The estimated mean concentration contours and the associated standard errors are provided in Figure 35 and Figure 36, respectively. Means tended to be higher in the central region of the system where the density of nodes was higher. Also, several isolated spots showed higher mean concentrations. Standard deviations tended to follow the same pattern as the means with higher standard errors associated with higher means.

In general, there were no specific regions that demonstrated a propensity for frequent violations nor were there specific regions that were infrequently in violation. The pattern of frequently violated nodes appeared to be fairly random.
Figure 33. Nodes that were in violation of the MCL at least once during 4 or more simulated random node contamination events.
Figure 34. Nodes that were never in violation during any of the 56 simulated random node contamination events.
Figure 35. Contours of estimated mean concentration for 72 hourly observations from each of 56 simulated random node contamination events. Concentration is in generic units.
Figure 36. Contours of estimated standard error of the mean concentration for 72 hourly observations from each of 56 simulated random node contamination events. Concentration is in generic units.
D. Distribution System Monitoring

1. Optimal Monitoring Strategies - Overview

Integer optimization was used to obtain a set of monitoring points, defined by hour and location, that would maximize the detection of contamination events. This optimization was performed separately for source node contamination and random node contamination. Most optimization problems terminated with integer solutions when solved with the simplex method. As discussed in Methods and Materials section E, the use of an integer programming method that ensures an optimal integer solution was not feasible due to limitations on computer resources. In these cases, the methods described in section E of Methods and Materials were used to obtain solutions that were, at the very least, near optimal. The following sections provide the results for three sets of formulations. The first formulation optimized monitoring over the entire simulation period. For source node events, this corresponds to a period of 264 hours beginning at hour 0 on the day contamination was introduced. For random node events, this corresponds to a period of 72 hours beginning at hour 0 on the day the contamination event started. The second set of formulations (restricted monitoring) was used to assess the effect of beginning system monitoring at some point after the day of the contamination event and also to assess the effect of restricting the time of monitoring to specific times of day. The final formulation resulted in an optimal set of daily monitoring points. The time period for this
formulation was the 24 hour demand cycle; points were assumed to be monitored every 24 hours.
2. Optimal Monitoring

a) Source node events  The adequacy of the number of simulation trials in
representing distribution system monitoring under conditions of uncertainty was
assessed by looking for stability in the optimal value of the objective function. In
particular, the optimization was repeatedly solved using data from an increasing
number of trials. When the fraction of detections began to stabilize near a constant
value, the number of simulation trials was considered adequate for the purposes of
designing an optimal monitoring plan under uncertain conditions. This procedure was
used for several monitoring plan sizes. As discussed below, the solutions that were
obtained never reached a truly stable level. It was necessary, however, to proceed
with the analysis due to constraints on the available time to perform the research.

Figure 37a shows a plot of the fraction of events detected for four sizes of
monitoring plan: 1 point, 4 points, 7 points, and 10 points. The size indicates the
maximum number of points that can be monitored. Larger sample sizes tended to
perform better than the smaller ones. Stability began to occur after 50 trials. This is
particularly true for the 10 point monitoring plan. There was still a general
downward trend in the fraction detected for the smaller monitoring plans, but the rate
of decrease appeared to be lessening. Figure 37b shows the rate of change in the
fraction detected as the number of simulation trials increased. Subsequent points
reflect a decreasing reduction in the fraction detected. The zero line represented a
constant value for the objective function. All four plans began to converge towards
this value as the number of trials increased. Changes in the detection of events were less than 5 percent when the number of trials increased from 50 to 56 for all four plans. The 10 point plan suffered almost no change in the fraction detected when the number of trials was increased to 56.

A more detailed analysis of monitoring plan size was performed using 56 simulation trials for input to the formulation. Figure 38a shows the fraction detected by optimal plans beginning with 1 monitoring point and increasing by 1 point until all events were detected. The curve shows that 15 points were required to detect all 56 events. The increase in fraction detected was not a linear function of the number of monitoring points. The curve increased at a decreasing rate indicating a decreasing marginal value of additional monitoring points. This is more precisely illustrated in Figure 38b which shows the increase in the fraction detected if an additional point were added to a monitoring plan of a given size. This plot suggests a generally decreasing benefit from the addition of monitoring points. An additional 7 events were detected (an increase of 0.125 in the fraction detected) for each additional monitoring point up to a total of 35 detections with 5 points. Larger plans had a resulted in smaller increases in the fraction of events detected. The curve shows an increase in the fraction detected of approximately 0.02 (1 additional detection) for each additional monitoring point above the size of 11 points. Figure 37 and Figure 38 do not show smooth curves, but show linear segments that combine to provide a general trend. In particular, Figure 38 appears like a step function with narrow
ranges of monitoring plan sizes having the same marginal benefit from an additional monitoring point.

Table VI lists the points included in the optimal monitoring plans with the corresponding time of monitoring. The locations of these points are plotted on Figures 39, 40, and 41. Any point in the optimal 4-point plan is, by itself, an optimal 1-point plan. Indeed it is likely that alternative optima exist for many of the plans, but determining these alternative optima was beyond the scope of this research. The monitoring times tended to be early in the period of system contamination. All points were chosen to be monitored at hours within the first two days of system contamination. The locations of monitoring points were generally towards the southern part of the system near the source node. There was no restriction on monitoring a single node more than once. One node, noted in the figures, was chosen as the location for three monitoring points in the 10-point plan. Also, it is noteworthy that points in the smaller plans tended to be included in the larger optimal plans.
Figure 37. Fraction of source node events detected by optimal monitoring plans with 1, 4, 7, and 10 monitoring points for increasing number of simulation trials. Leveling-off indicates the stability of optimal solutions.

a. Fraction of events detected at each number of input trials
b. Change in fraction detected from previous number of input trials
Figure 38. Fraction of source node events detected for an increasing number of monitoring points. Optimal monitoring plans used 56 simulation trials for input.

a. Fraction of events detected at each number of input trials.

b. Change in fraction detected resulting from the addition of one monitoring point.
Table VI. Monitoring plans designed to detect source node contamination events. Monitoring times are measured from hour 0 of the beginning day of contamination.

<table>
<thead>
<tr>
<th>PLAN</th>
<th>POINT</th>
<th>HOUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-point plan: (see Figure 39)</td>
<td>1</td>
<td>13</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>11</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>23</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>27</td>
</tr>
<tr>
<td>7-point plan: (see Figure 40)</td>
<td>1</td>
<td>13</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>11</td>
</tr>
<tr>
<td></td>
<td>3</td>
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<td>5</td>
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<td></td>
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<td>17</td>
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<tr>
<td></td>
<td>7</td>
<td>30</td>
</tr>
<tr>
<td>10-point plan (see Figure 41)</td>
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<td>15</td>
</tr>
<tr>
<td></td>
<td>2</td>
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<td>15</td>
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<tr>
<td></td>
<td>10</td>
<td>28</td>
</tr>
</tbody>
</table>
Figure 39. Locations of optimal monitoring points for detecting source node contamination events. The corresponding times of monitoring are provided in Table VI. These points were the result of optimization over the entire simulation period of 264 hours with a maximum of 4 monitoring points allowed.
Figure 40. Locations of optimal monitoring points for detecting source node contamination events. The corresponding times of monitoring are provided in Table VI. These points were the result of optimization over the entire simulation period of 264 hours with a maximum of 7 monitoring points allowed.
Figure 41. Locations of optimal monitoring points for detecting source node contamination events. The corresponding times of monitoring are provided in Table VI. These points were the result of optimization over the entire simulation period of 264 hours with a maximum of 10 monitoring points allowed.
b) Random node events

The results of optimizing a monitoring plan for the detection of random node contamination events were analyzed in the same manner as the optimization of monitoring for source node events. Figure 42a shows the optimal detection obtained using various numbers of trials as input for the optimization. The optimal solutions began to stabilize after 40 trials. This is readily apparent in Figure 42b which shows the change in the optimal solution. A steady but slight decline in the fraction detected continued after 40 trials. The fraction detected was generally much lower than was found for monitoring source node events.

Figure 43 shows the effect of monitoring plan size on detection when 56 trials were used for input. Additional monitoring points increased the fraction detected by 0.36 (2 additional detections) up to a monitoring plan size of 10 points. After that, additional points resulted in a 0.18 increase (1 additional detection) in the fraction of events detected. Forty-six points were required to obtain 100 percent detection of random node contamination events. The fraction of random node events detected was substantially less than was observed for the case of source node contamination for all sizes of monitoring plan.

Optimal monitoring plans for random node contamination are described in Table VII. All plans consisted of points that detected 2 individual events, thus by listing the 10-point plan all smaller plans can be obtained. For example, any 4 points from the 10-point plan is an optimal 4-point plan. The locations of monitoring points
are shown on Figure 44. Optimal monitoring points do not appear to be located in a specific region of the network and monitoring times are primarily on the day of the contamination input.
Figure 42. Fraction of random node events detected by optimal monitoring plans with 1, 4, 7, and 10 monitoring points for increasing number of simulation trials. Leveling-off indicates the stability of optimal solutions.

a. Fraction of events detected at each number of input trials
b. Change in fraction detected from previous number of input trials
Figure 43. Fraction of random node events detected for an increasing number of monitoring points. Optimal monitoring plans used 56 simulation trials for input.

a. Fraction of events detected at each number of input trials
b. Change in fraction detected resulting from the addition of one monitoring point
Table VII. Optimal monitoring points derived from simulated random node contamination events. The optimal 1, 4, and 7 point plans can be selected from any of the points listed. Points are plotted on Figure 44.

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Figure 44. Locations of optimal monitoring points for detecting random node contamination events. The corresponding times of monitoring are provided in Table VII. These points were the result of optimization over the entire simulation period of 72 hours with a maximum of 10 monitoring points allowed. Each point detected 2 individual events. 1, 4, and 7 point plans can be chosen from the points in the 10 point plan.
3. Optimal Monitoring - Additional Restrictions on Monitoring

Using source node contamination event simulation, optimization of the detection of events was used to assess the effect of delayed monitoring. The set of feasible monitoring points was restricted to hours beginning at some point well after the day on which contamination was introduced. In addition, optimization of the monitoring plan was performed with restrictions on what hours of the day a sample could be collected. Two restrictions of this sort were used. In one optimization, sampling was restricted to the morning hours from hour 6 to hour 11. In another optimization, monitoring was restricted to the afternoon hours from hour 12 to hour 17. These restrictions were designated as AM monitoring and PM monitoring, respectively. They were incorporated into the analysis to demonstrate how a practical constraint such as the hours when utility employees are available to collect samples may be accounted for in the formulation of the optimization problem.

A comparison of the optimal monitoring plan performance under different restrictions was made using optimal 10-point monitoring plans. Figure 45 shows that delays in monitoring of up to 24 hours appear to have little effect on the optimal detection. Longer delays begin to have an increasingly negative effect. The restriction of monitoring to specific times of day appeared to have little effect when monitoring points were allowed to be chosen over the entire time span of the simulation. Both morning and afternoon monitoring were markedly inferior to full day monitoring when delays in the monitoring were imposed. Morning monitoring
was equivalent or superior to afternoon monitoring in all cases except the 72 hour delay optimization. For both the restricted and the unrestricted cases, the effectiveness of optimal monitoring plans diminished at an increasing rate as a longer delays in monitoring were imposed.
Figure 45. Optimal detection of 56 simulated source node contamination events under restrictions. Morning monitoring was restricted to hours 6-11, afternoon monitoring was restricted to hours 14-17, and full day monitoring had no restrictions on monitoring. Delayed monitoring was restricted to the time period beginning the designated hour after hour 0 on the first day of the contamination event. Plans with 10 points were used for comparison.
4. Optimal Monitoring - Daily Monitoring

a) Source node events

Optimal daily monitoring consisted of a set of points that would maximize detection when the points were sampled every day. Fifty-six (56) trials were used to provide data for the optimization. The number of monitoring points was varied from one point per day to the number of points required for 100 percent detection (see Figure 46a,b). All events were detected by 14 points. As can be seen in Figure 46b, the marginal benefit of additional monitoring points quickly diminished after 5 monitoring points were included. A constant marginal benefit of a 0.18 increase in the fraction detected was achieved after 11 points were included in the plan.

Table VIII lists the optimal daily monitoring plans for the detection of source node contamination. The locations are plotted in Figures 47, 48, and 49. The locations are similar to those obtained from the original formulation for optimal monitoring of source node contamination and, in fact, many of the points are essentially identical. Of course, the daily plan implies that the points are monitored every day instead of just on a particular day.
Figure 46. Fraction of source node events detected for an increasing number of points monitored once a day. Optimal monitoring plans used 56 simulation trials for input.

a. Fraction of events detected at each number of input trials
b. Change in fraction detected resulting from the addition of one monitoring point
Table VIII. Daily monitoring plans designed to detect source node contamination events. Monitoring points are sampled at the given time each day.

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Figure 47. Locations of optimal daily monitoring points for detecting source node contamination events. The corresponding times of monitoring are provided in Table VIII. Points are based on the 4-point plan. Optimal 1-point plans can be any one of these 4 points.
Figure 48. Locations of optimal daily monitoring points for detecting source node contamination events. The corresponding times of monitoring are provided in Table VIII. Points are based on the 7-point plan.
Figure 49. Locations of optimal daily monitoring points for detecting source node contamination events. The corresponding times of monitoring are provided in Table VIII. Points are based on the 10-point plan.
b) Random node events

The fifty-six simulated random node events were used to obtain an optimal set of points for daily monitoring. The number of points to be monitored each day was varied from one point per day up to a number sufficient for 100 percent detection of the 56 simulated random node events (see Figure 50a). Fifty monitoring points per day were required to detect all 56 random node contamination events. As can be seen in Figure 50, a constant marginal benefit of a 0.36 increase in the fraction detected occurred for monitoring plan sizes up to 13 points. Larger monitoring plans had a constant marginal benefit of additional points of 0.18.

Table IX lists the hour of each monitoring point and provides a reference number for each monitoring location shown on Figure 51. As with the original random node formulation, all plans are a set of points that detect 2 individual contamination events. The points selected for the 10-point plan are provided. Any smaller size plan can be obtained by selecting from these points.
Figure 50. Fraction of random node events detected for an increasing number of points monitored once a day. Optimal monitoring plans used 56 simulation trials for input.
   a. Fraction of events detected at each number of input trials
   b. Change in fraction detected resulting from the addition of one monitoring point
Table IX. Optimal monitoring points derived from simulated random node contamination events. The optimal 1, 4, and 7 point plans can be selected from any of the points listed. Points are plotted on Figure 44.

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Figure 51. Locations of optimal daily monitoring points for detecting random node contamination events. The corresponding times of monitoring are provided in Table IX. These points were the result of optimization of a daily monitoring plan with 10 monitoring points allowed. Each point detected 2 individual events. 1, 4, and 7 point plans can be chosen from the points in the 10 point plan.
E. Analysis of Monitoring Plan Performance

1. Performance of Optimal Monitoring Plans

In order to assess the value of the simulation-optimization methodology, two sets of independent simulations trials were performed - an independent set of simulated source node events and an independent set of simulated random node events. These independent sets of trials were not used in the design of monitoring plans. The optimal plans obtained from the initial sets of simulation trials were evaluated in terms of their ability to detect contamination events simulated for the set of independent trials.

Figure 52 shows the performance of optimal plans derived from simulated source node contamination events. The unrestricted optimal plans detected a lower fraction of the independent trials than the optimal detection fraction would have predicted. The unrestricted optimal 10-point monitoring plan achieved a detection fraction of only 0.52 compared to the predicted fraction of 0.875 from the optimization. The performance of the optimal daily monitoring plan (17 percent detection) was similar to the predicted performance (12.5 percent detection) for the 1-point per day plan. Optimal monitoring plans based on simulated random node contamination events failed to detect any of the independent set of random node events.

It is likely that the 56 simulation trials used to design optimal monitoring plans
was not a sufficient number to ensure a reliable solution to the optimization problem.

In particular, the predicted fraction of events detected appears to be too high, especially in the case of random node events where no independent events were detected by the optimal plans.
Figure 52. Performance of optimal plans for detecting source node contamination when assessed using an independent set of simulation trials. The unrestricted 10-point monitoring plan and the 1-point daily monitoring plan are shown here.
2. Comparative Performance of Monitoring Plans

The alternative monitoring plans described in section F of Chapter III were compared with optimal plans in their ability to detect contamination events from the sets of independent simulation trials. This set of independent trials were not used to analyze the behavior of contamination nor were they used to design monitoring plans. They were, therefore, a test of the reliability of the monitoring plans and the optimization method. This analysis was performed separately for source node contamination events and random node contamination events. Figure 53 shows the performance of selected 10-point monitoring plans in detecting source node contamination events. Optimal daily monitoring was restricted to the first 10 days of the event in order to ensure that equivalently sized plans were being compared. In this particular case, this restriction had no effect on the resulting performance of the optimal daily plan.

Alternative monitoring plans that resulted in detections of source node events were: A-7 which sampled randomly over the first two days of the events, A-8 which sampled randomly over the first three days of the events, A-1 and A-2 which were random samples over the entire 11 days of the event, A-9 which sampled over the first five days of the event, and A-3 which sampled the source node at a random time each day. As seen in Figure 53 the unrestricted optimal monitoring plan performed best with a fraction detected of 0.52. Plan A-7 resulted in a detection fraction of 0.35. The other plans were noticeably inferior to these two. The alternative plans
not shown in Figure 53 did not detect any of the independent source node events.

Both optimal and alternative plans failed to detect any of the independent simulated random node contamination events. The predicted values from the solution to the optimization problems were apparently unreliable in the random node case. This is an indication that the solutions had not reached a stable level with 56 input trials.
**Figure 53.** Performance of selected optimal and alternative monitoring plans in terms of the fraction of independent source node contamination events detected. SN-DAY is the optimal daily monitoring plan with 1 point per day, SN-OPT is the optimal unrestricted monitoring plan with 10 points, the alternative 10-point plans were described in Table V. Alternative plans not shown on the graph resulted in zero detections.
V. DISCUSSION

A. Overview of Discussion

Simulations of source node and random node contamination were performed using a model of the Blacksburg, VA water distribution system and mathematical optimization was used to design monitoring plans based on the results of these simulations. Any conclusions derived from these results were necessarily influenced by a number of factors including the nature of the system being studied, simplifying assumptions used to create the network model, and the determination of parameters for the simulation of contamination. Jones (1992) used the same contaminant transport model, TRAK, to simulate contamination in a hypothetical distribution network. Included in Jones' research were simulations of source node contamination (called pump station events by Jones) and random node contamination. His study provided the primary source for a comparative analysis of the results of the Blacksburg simulation analysis.

The discussion of the Blacksburg simulation results and a comparison of these results with other studies (primarily Jones, 1992) follows in five sections. In section B, the Blacksburg distribution network and the modeling assumptions are discussed with an emphasis on how certain factors may affect the simulation results and how these factors compared with the network modeled by Jones. Section C discusses the
results of simulated source node and random node contamination events and discusses possible reasons for some variations from the patterns observed by Jones (1992). The results of monitoring plan optimization and a comparative analysis of optimal monitoring plans and alternative monitoring plans are presented in sections D and E. In particular, section E includes some discussion of the implications of the results for regulatory compliance monitoring. The final section, section F, is a discussion of some general observations concerning the simulation-optimization methodology as applied to the problem of monitoring drinking water distribution systems.

B. The Distribution System Model

1. Overview

Free-floating reservoir operation allowed the system to meet excess demands by releasing water from storage during high demand periods and to accommodate excess supply by increasing storage during low demand periods. In general, this assumption accomplished the goal of modeling dynamic system demand without specifying changes in the flow and pressure at the source node or modeling the behavior of pumps within the distribution system itself. The simplifying assumptions of constant flow at the source node and free-floating reservoir operation were necessary due to the limited information on distribution system operation that was available. While other assumptions could have been made that may have resulted in
more ideal hydraulic behavior, the assumptions used represented the simplest means of achieving reasonable hydraulic results without additional assumptions defining pump operation and reservoir operation. Likewise, the assumptions regarding the dynamic and spatial allocation of system demand represented the least presumptive means of obtaining a reasonable model of the system in the absence of empirical data.

Given that a precise representation of the Blacksburg system was neither possible nor a primary goal of this research, these assumptions allowed for a hydraulic model that satisfied the need for a realistic case study of contaminant transport. The results of the simulation trials were affected by these simplifying assumptions. In particular, the free-floating reservoir assumptions affected the hydraulic solutions and in some cases resulted in aborted trials due to an unsuccessful hydraulic solution. With regards to contaminant transport, the assumptions had a potential effect on the spatial dispersion of contaminant, on the mixing of contaminated water in the storage reservoirs, and on the reintroduction of contaminated water back into the distribution system from the storage reservoirs. The effect of assumptions about system operation and the nature of the distribution network on constituent transport modeling are discussed in greater detail in the following three sections and are compared to the system modeled by Jones (1992).
2. Storage Reservoirs and Hydraulic Results

The mean percentage of storage capacity filled during each hour of the day was presented in Figure 8 of the results. This figure is reproduced along with the mean system demand in Figure 54. A clear pattern of reservoir response to changing demand level can be seen. The system released water from storage during periods when the demand factor was above the mean and increased storage when the demand factor was below the mean. This regime of reservoir behavior was similar to that used by Jones (1992) in his hypothetical model.

The individual reservoirs showed diverse behavior. As indicated in Figure 6 of the results, reservoir 2 and reservoir 4 maintained fairly high levels that changed in response to system demand. Figure 7 in the results indicated that reservoir 1 and reservoir 3 maintained very low levels during the entire day. This was probably due to simplifying assumptions about the single input of pumped water at the source node. Also, seasonal demand fluctuations were not modeled. Therefore, the system may have storage capacity that is not utilized except during seasonally high demand periods. This low level of storage in two of the reservoirs may have been the primary cause of aborted simulation trials. During periods of high demand, the system relied on water from storage in order to meet the demand in excess of the flow at the source node. A particularly high value for the random demand could result in reservoirs 1 and 3 releasing water until they emptied. Without a means of adjusting the pressure at the other two reservoirs, the system would be unable to meet
the total system demand. In terms of the hydraulic model, this means that the balance of inflows and outflows could not be achieved and a solution could not be obtained.

Several possible solutions to the problem of "bad trials" were considered. Experimenting with the hydraulic configuration of the system was found to be an ineffective procedure. Fine tuning the pressure and flow conditions was an uncertain task with little empirical data for justification. Adjustments to the schedule of mean hourly demands seemed inappropriate since the system performed adequately when the demand levels were close to the mean levels. Adjusting the parameters of the probability distribution used in generating stochastic demand factors offered a means of limiting the number of extreme points. This approach would have entailed a degree of trial and error in finding suitable limits on the demand factor. The possibility of a run of high demands leading to a failure would not have been entirely removed. Given the small number of aborted trials (less than 5 percent of all trials), simply taking note of which trials aborted prematurely and continuing the Monte Carlo trials with the initial parameters was deemed the most expedient solution. As long as the set of successful trials did not show any significant bias in terms of the parameters of the simulation, this solution was not anticipated to have a large impact on the results. In fact, the results discussed in section C suggest that reservoir behavior was not an important factor in determining the results of this study. Given the limited availability of empirical data on the distribution system, it is unlikely that any of the other options would have been more representative of the actual system.
Figure 54. The relationship between mean hourly demand and the fraction of reservoir storage filled. The mean demand factor was a parameter of the simulation. The mean fraction of storage capacity filled was observed from 56 simulation trials.
3. System Demands

Demand in the Blacksburg system consisted of a few regions of high demand nodes with little variation in nodal demand in the remainder of the system (see Figure 5). The peripheral regions of the system tended to have lower demands due to a lower density of nodes and low demand per node. Jones (1992) noted that, in his hypothetical system, flow velocities were lower at the periphery of the system where water demand was low and that this may have accounted for a higher frequency of violations in these regions of the system. His hypothesis was that contamination moved slowly in the regions of low flow velocity and was therefore more likely to contaminate a node over a longer period of time. Additionally, low flow implies that there would be less dilution of contaminated water. Jones also observed that the frequency of node contamination was closely correlated with the 24-hour demand cycle; the number of violated nodes increased when the system demand increased.

Two explanations were proposed. First, if the reservoir had been contaminated then a release from the reservoir during a high demand period would introduce contaminated water back into the system. The other explanation suggested that a reservoir release, even a release of clean water, would displace water in the network by forcing contaminated water to the periphery where demand, and consequently flow velocities, were lower. The Blacksburg model used the same 24-hour demand cycle as Jones (1992) and the configuration of lower demand at the periphery is similar to his hypothetical network. However, as discussed in section C, the Blacksburg model
showed low contamination frequency at the peripheral nodes and a markedly different temporal cycle. It seems unlikely that these differences are due to the allocation of system demand given the similarities in the two systems in this regard.

4. The Distribution Network

Water was assumed to enter the system through a single source node at a constant flow rate. This assumption may provide the false impression that this water is pumped directly from the treatment plant. In actuality, the regional water authority maintains storage facilities in their distribution system. Therefore, although source node contamination is generally considered to be the result of breakthrough at the treatment plant, in this study source node contamination must be viewed as resulting from any possible contamination in the regional distribution system at points upstream from the Blacksburg system. This includes breakthrough contamination and contamination resulting from breaches of distribution system integrity at points upstream from the Blacksburg source node. Since the Town of Blacksburg had no authority or responsibility for water quality until it entered the Blacksburg system but was responsible for the quality of water delivered in town limits, it seemed reasonable to model the input of contaminated water at the point of entry to the Blacksburg system.

Constant flow at the source node has implications for modeling source node contamination. A constant flow at the source node means that, in the case of source
node events, the total quantity of contamination, or loading, is dependent only on the concentration of the contaminant input to the system and the duration of the input. Jones’ model allowed for some variation in the flow of water pumped into the system. Thus, in his study two source node events of equal concentration and duration could result in a different loading of contamination to the system if the events began at different times of the day. It is likely that his simulations may have encompassed a wider range of contaminant loading than is apparent from the probability density used to model the concentration of contamination input to the system. The effect of contaminant loading is discussed in greater detail in section C, when the simulation results are discussed.

The model of the Blacksburg network consisted of 844 pipes (approximately 524 thousand feet of pipe) with a capacity of 1.91 million gallons within the pipe network itself. The four reservoirs are located away from the source node along the eastern periphery of the system (see Figure 3). The system is considerably larger than the hypothetical system modeled by Jones (1992). Jones’ system contained a single storage reservoir and 58 pipes. In this smaller system, contamination was more likely to spread throughout the system and possibly enter the storage reservoir before dilution occurred. As mentioned in the discussion of system demands, Jones found that the peripheral nodes were the most frequently contaminated and that the number of contaminated nodes increased with the reservoir releases. As discussed in greater detail in section C, the pattern found by Jones did not completely agree with the
results of the Blacksburg simulation. The size of the Blacksburg system and the comparatively long pathway from the source node to any reservoir suggests that dilution of the contaminant in the network may be a primary factor in defining the dispersion of contamination in the Blacksburg network. Additional factors, including differences in contaminant loading, are discussed in more detail in section C.

5. The Contaminant Transport Algorithm

Some characteristics of the constituent transport algorithm deserve some consideration with regards to the interpretation of the simulation results. The algorithm used in TRAK (Jones, 1992; Liou and Kroon, 1987) models contaminant concentrations in discrete plugs of constant concentration. In addition, the program checks each node for contamination at discrete time intervals (on the hour). It is possible for a plug of high concentration to be trapped between two nodes at the time the system checks the nodes and so go unrecorded. At a later time, this plug may reach a node and cause that node to be recorded as being in violation. The impression that may be gained by looking at an hourly record of system contamination is that contamination mysteriously reappears after a period when the system is clean. In actuality, the system was not clean; the contamination was simply between nodes and was not recorded by the program as being a violation.

One final characteristic of the algorithm is the complete mixing assumption. At all junctions and reservoirs, the assumption is that the resulting concentration of
contamination is the flow-weighted average of contaminant concentrations entering the node or reservoir. Grayman et al. (1991) performed a calibration of a constituent transport model by comparing the results of a fluoride tracer study with the predictions of their model. Calibration of their model was achieved by adjusting the assumptions regarding mixing in the storage reservoirs. The assumption of stratification of the water in storage reservoirs resulted in higher concentrations of contaminant being released from storage. This minor adjustment to the mixing calculations is likely to have an impact on the predicted dispersion of contaminant when significant quantities of contamination enter the storage reservoirs. It seems likely that an assumption of stratified mixing would have increased the influence of reservoir releases on system wide contamination and would, therefore, not alter the general conclusions reached by Jones (1992). In fact, a stratified mixing assumption would probably have made the patterns observed by Jones (1992) even more prominent. As discussed in section C, reservoir contamination played virtually no role in defining patterns of contamination in the Blacksburg system. Since almost no contamination ever reached the reservoirs in the Blacksburg study, it is unlikely that altering the assumption of complete mixing in the reservoirs would have a significant impact on the results and any variation in the results of Jones (1992) and the results of the Blacksburg simulations are most likely the result of differences in the system modeled (as discussed in the previous sub-section) and differences in the parameters defining contamination events (as discussed in the following section).
C. Simulation of Distribution System Contamination

1. Event-Based Simulation Trials

Each event of system contamination was modeled as an independent trial. Each trial consisted of a warm-up period during which the system was clean, a begin day on which contamination was introduced, and a period of days during which contamination traveled through the system and was eventually flushed out. This approach differed from that used by Jones (1992). Jones (1992) performed 20 year simulations. The occurrence of contamination events was modeled using stochastic processes derived from reliability theory. In particular, Jones (1992) specified a mean time between events (MTBE) that described the expected time increment between contamination events. This approach allowed for a direct correspondence between a time during the simulation and a time during the regulatory compliance period. Therefore, it was possible to consider events that affected two or more monitoring periods and the possibility of two or more events affecting a single monitoring period. However, simulation of long periods of time requires that the assumptions governing system operation are suitable for that time span. If long term trends such as seasonal behavior and long term shifts in the system parameters exist, then these must be incorporated into the model in order for it to reflect long term system behavior. In addition, it is often necessary to limit the computer run time to a manageable period and may be necessary to use several computers running simultaneously to obtain results within given time frame. It should also be noted that
the system modeled by Jones was relatively small and therefore did not require the extensive computational resources that were necessary for the Blacksburg simulations. The need to limit computer run times and the lack of field data to account for seasonal and other long term system behavior were the primary factors that prevented a long-term simulation approach as used by Jones. By performing several simulation trials independent of one another, it was possible to use more than one computer to perform simulations and allowed the computer to be periodically freed for other uses. Such practical constraints as computer availability and time constraints are significant issues in determining the potential of simulation as a decision tool and are discussed further in section F.

In terms of modeling system contamination, the use of an event-based simulation dictated that only one contamination event took place at a time. There was never the possibility of an event beginning while residual contamination from a previous event was present in the system. Since the complete mixing assumption precludes the possibility of an increase in concentration resulting from the mixing of two contaminant plugs, it is unlikely that the event-based methodology would affect the resulting patterns of violations. Jones (1992) allowed for the possibility of concurrent contamination events. The primary effect of this was that contaminated nodes could appear in two or more distinct regions of the network at the same time. This would be apparent if the patterns of violated nodes were looked at during a limited time interval. However, when the frequencies of node violations are averaged
over all of the contamination events, there should be no apparent effect as a result of concurrent events. Thus the use of event-based simulation should have had no effect on the observed contamination patterns. However, there were implications for the design of optimal monitoring strategies and for interpreting the results in the framework of regulatory compliance monitoring. These issues are discussed in further detail in the discussion of distribution system monitoring in section E.

2. Simulated Source Node Contamination

a) Parameters Defining Contamination Events Constant flow at the source node dictated that the contaminant loading was dependent on the concentration of contamination input to the system. The contaminant concentration was modeled as an exponential random variable with a mean of 5 units and was introduced into the system for a duration of 1 hour. Jones (1992) simulated source node contamination with a higher mean concentration of 10 units and performed several simulation trials with the duration of contaminant input ranging from 1 hour to 16 hours. Therefore, the contaminant loading in Jones’ study was significantly higher than the loading in this study. Jones performed several simulations that incorporated the process of constituent decay and found that the process served to limit the spread of contamination in the distribution system. Decay was not modeled in the study of the Blacksburg system, so dilution in the distribution network and outflow from the system were the only means by which the concentration of contaminant could be
reduced below the MCL.

The differences in contaminant loading are particularly significant given the difference in the size and complexity of the two systems. The hypothetical system simulated by Jones (1992) was considerably smaller than the Blacksburg system and had a much lower volume of water in the distribution network. His simulations of source node contamination served to completely inundate the hypothetical system with contamination leading to frequent contamination of peripheral nodes and the storage reservoir. The lower contaminant loading coupled with a much higher volume of water in the Blacksburg distribution network allowed for a much greater degree of dilution in the pipe network. As discussed in the next sub-section, the contrasting results of this study and the study performed by Jones (1992) can be attributed primarily to the differences in the two distribution networks and the difference in the relative quantities of contamination simulated to enter the systems.

b) Patterns of Source Node Contamination  Source node contamination patterns suggested that the dilution of the contamination in the distribution network was the primary influence on the location of violated nodes in the Blacksburg system. The volume of water in the network and the length of the pathways to the reservoirs was sufficient for contamination to be diluted to concentrations below the MCL before storage reservoirs were contaminated and before contamination reached the nodes at the northern periphery of the system. These results provide a different scenario of system contamination than the one observed by Jones (1992). In his study, the
quantity of contamination was high enough such that concentrations above the MCL reached the peripheral nodes and frequently contaminated the storage reservoir. The differences in the results of these two simulation studies can be seen by looking at the duration of the residual contamination in the system, comparing the spatial location of frequently contaminated nodes, and noting the different relationships between the demand cycle and the extent of system contamination.

Figure 15 showed the mean number of nodes violated during each hour of the source node contamination simulations beginning at hour 0 on the begin day of the contamination events. The extent of contamination reached a maximum early on the second day of the contamination episode and rapidly diminished thereafter. Contamination in excess of the MCL was nonexistent by the end of the eleventh day of the simulated contamination episodes. The decline in the number of violated nodes appeared to be consistent with a steady decrease in the amount of contamination in the pipe network and not a downward trending cyclical pattern. There was no indication that contamination was introduced back into the system during reservoir releases.

The duration of residual contamination appeared to be independent of the begin time of the episode (see Figure 13) and showed some indication of being positively correlated with the concentration of the introduced contamination (see Figure 14). These observations, along with the smooth decline in the extent of contamination over the simulation period, support the conclusion that dilution of the contaminant in the distribution pipes was the factor that limited the spread of contamination. The
correlation of the duration of system contamination with the initial concentration suggests that higher concentration contamination took longer to be diluted and therefore traveled farther in the distribution network. The time at which contamination was introduced appeared to be uncorrelated with the duration of contamination. Thus, it appears that contaminant propagation was not significantly affected by reservoir releases of inflows at the time contamination was introduced to the system. This suggests that the reservoirs were not contaminated and that the constant flow from the source node was the main factor in determining the dispersion of contaminant in the network.

An additional observation concerning the duration of system contamination was the appearance of two distinct groups of data in Figures 13 and 14. System contamination tended to last less than 100 hours or longer than 150 hours with few durations observed between. There does not appear to be any definite reason for this phenomenon; it exists consistently over the entire span of begin times and there is no gap in the initial concentration levels. It seems reasonable to relate this pattern to some inconsistencies in Figure 15. In particular, after hour 120 the mean number of violated nodes seemed to fluctuate irregularly between zero and a small number of nodes. There does not appear to be any consistent cyclical pattern and the general pattern of a steady decline in the number of violated nodes is not contradicted. A possible explanation is that contamination tended to reach one of a handful of longer pipes during these hours. If this contamination was below the MCL, then no more
violations would occur and the event would be over. If the contamination was above the MCL, then it would emerge at a node at a later time and the event would not be over until that plug was diluted to a level below the MCL. Since contamination was only checked at nodes on an hourly basis, any plugs with concentrations above the MCL that were between nodes would not be recorded until they reached a node. As mentioned previously in section B.5, these discrete patterns are most likely the result of using an algorithm that models contamination as a discrete rather than a continuous phenomenon. This problem was not observed by Jones (1992), but his network consisted of shorter pipes so the discrete nature of the model may not have been as apparent.

The spatial locations of frequently violated nodes were plotted in Figures 17 and 18. The most frequently contaminated nodes were at the south end of the system near mains that led directly from the source node. It is apparent from Figure 18 that contamination rarely reached the storage reservoirs at concentrations in excess of the MCL. Figures 20 and 21 indicate that nodes at the northern periphery of the system, the greatest distance from the source node, were contaminated infrequently or not at all. These patterns tend to suggest that contamination spread away from the source node and was diluted below the MCL before reaching the reservoirs or the peripheral regions of the network. Jones (1992) observed high frequencies of contamination at peripheral nodes in his simulation study. The pattern observed by Jones (1992) was most likely the result of loading a small system with large quantities of contamination.
that reached all regions of his network. The main factor in determining which nodes were violated most frequently was hypothesized to be the velocity of flow. Jones (1992) hypothesized that in his system, low velocities in pipes at the periphery resulted in slower movement of contaminant plugs in this region. It was, therefore, more likely for the same plug to violate a node during consecutive hours and the process of dilution at the nodes would take place at a slower rate. In the simulation of the Blacksburg system, low velocities at the periphery did not have a significant effect since contamination was diluted below the MCL before it reached the periphery. Jones (1992) also noted a higher frequency of contamination in the vicinity downstream from the storage reservoirs. This pattern was particularly apparent when events of higher mean concentration were simulated. This was attributed to the release of contaminated water from storage. This process did not occur in the simulation of contamination in the Blacksburg system. As stated before, dilution in the distribution pipes prevented contamination of the storage reservoirs.

Some important distinctions between the study by Jones (1992) and the results of this simulation study can be seen by looking at the relationship between the hourly system demand and the 24-hour demand cycle. Figure 55 shows the mean number of violated nodes for each hour of the day along with the mean system demand factor. The mean number of violated nodes peaked at hour 2 when system demand was below the average daily demand. This result contradicts the observation by Jones (1992) which showed the number of violated nodes peaking during high demand periods.
when water was released from storage reservoirs. The result supports the contention that the behavior of storage reservoirs had little effect on the distribution of contamination in the Blacksburg system. The higher frequency of violations during low demand periods may be related to the flow velocity in the pipe network. As water is diverted to the reservoirs, the velocity of water moving through pipes away from the pathway between the source node and the reservoirs would be reduced. Thus, contamination would move through the network at a slower rate and could lead to more frequent hourly violations of individual nodes. This explanation is similar to the argument proposed by Jones to explain higher violation frequencies at peripheral nodes in his system.
Figure 55. The relationship between mean hourly demand and the mean number of violated nodes as a result of source node contamination. The mean demand factor was a parameter of the simulation. The mean number of violated nodes observed from 56 simulation trials.
A number of factors influenced the results of simulated source node contamination. The contrast between the results of Jones (1992) and the results of this study seems to illustrate the influence of contaminant loading and the relative size of the distribution system on the observed temporal and spatial patterns of system contamination. The hypothetical system modeled by Jones was small compared to the length and volume of the Blacksburg system. In addition, Jones loaded his system with a comparatively high quantity of contamination. This resulted in a system that was contaminated at high concentrations at virtually all nodes. The frequency of violations at a node was determined largely by the velocity of flow at the node and by the release of contaminated water from storage. The Blacksburg system was simulated with a comparatively low level of contamination. The lower contaminant loading and the larger size of the system resulted in contamination events that were controlled mainly by the dilution of the contaminant in the pipe network. Reservoir contamination was not a factor in the resulting patterns of violated nodes. The results of these two studies present distinctly different patterns of contamination and possess quite different implications for designing a strategy for monitoring the distribution system. The possible implications of these results, in so far as distribution system monitoring are concerned, are discussed in greater detail in sections D and E.
2. Simulated Random Node Contamination

a) Parameters Defining Contamination Events Random node events were simulated with the same parameters as simulated source node events with the exception of the location of the contaminant input. The location was applied at a random node on the distribution network. While the mean concentration of 5 units and the 1-hour duration of the input were the same as for source node events, the resulting quantity of contamination was generally less because flows at most nodes were less than the flow at the source node. Jones (1992) simulated random node contamination with mean concentrations ranging from 10 units to as high as 10,000 units. The duration of contaminant input was 1 hour in Jones' study with additional trials using 4 and 16 hour durations for the 100 unit mean concentration. The random node study performed for the Blacksburg study resulted in much lower loadings than either the source node simulations or the study performed by Jones (1992).

b) Patterns of Random Node Contamination Random node contamination was diluted or flushed from the system in less than three days for all simulation trials. The process of dilution was undoubtedly a significant factor in limiting the spread of contamination beyond the immediate vicinity of the node where the contaminant was introduced. There was no indication of reservoir contamination, even though some events began at locations near the reservoir inlets (see Figure 25). Random node contamination simulated by Jones (1992) resulted in occasional reservoir contamination, particularly for the simulations with higher mean concentrations. As
with source node contamination, but to a lesser degree, Jones (1992) found that the peripheral nodes were the most frequently contaminated nodes during random node contamination. The duration of system contamination, the spatial patterns of frequent violations, and the correlation of violations with the demand cycle are results that illustrate the difference in the outcomes of this random node simulation as opposed to Jones’ simulations of relatively high contaminant loading. As in the case of source node simulations, it is possible to look at differences in contaminant loading and at differences in the relative size of the systems as probable reasons for the results that differ from Jones (1992).

Figure 31 showed the mean number of nodes in violation of the MCL during each hour of simulated random node contamination. The highest frequency of contaminated nodes occurred on the begin day of the contamination event. A rapid decline in the number of contaminated nodes occurred after hour 24 and no violations appeared after the third day of the event. This observation is consistent with a rapid dilution of random node contamination. The duration of residual contamination was much less than that observed for source node events and the mean number of contaminated nodes was generally lower as well. The difference in the extent of system contamination between source node and random node events may have been due, in large part, to the difference in the contaminant loading. As discussed at the beginning of this section, the flow at random nodes was generally less than the flow at the source node, so a smaller total quantity of contamination entered the system for
a given concentration.

The spatial pattern of frequently violated nodes and infrequently violated nodes were depicted in Figures 33 and 34, respectively. No single region of the network appears to be prone to violation and no single region of the network appears devoid of any violation. Violations appear to have occurred in a pattern that is as random as the locations of initial contaminant input (see Figure 25). This suggests that contamination did not spread far beyond the immediate region of the initial contamination. At higher loadings, a system-wide pattern may have developed. This was observed by Jones (1992). In his study, random node contamination sometimes contaminated the reservoirs and was often of high enough concentration to spread over large areas of his small network. The result was a pattern of more frequent violations at the peripheral nodes and at nodes close to the reservoirs. In the case of the Blacksburg simulations, lower concentrations and a higher volume of water in the system served to keep the random node events spatially isolated.

The variation in the extent of system contamination over the 24-hour demand cycle followed a pattern similar to the one observed for source node contamination. The peak number of contaminated nodes occurred at hour 4 when demand was below the average for the day (see Figure 56). This suggests that more frequent violations occurred when the flow velocities were lower and the effect of dilution in the pipes was limited. In Jones (1992), the percentage of nodes in violation peaked at hour 9 during random node contamination events. This hour was during the high demand
period when the reservoir was releasing water. Thus, in Jones (1992), it appears that
the release of contaminated water from the reservoir was an important factor.
Additionally, Jones (1992) suggested that reservoir releases pushed contamination in
the network to the periphery where low flow velocities resulted in a higher frequency
of contamination among the peripheral nodes. While the pattern of violations
resulting from random node contamination showed some similarity to those observed
as a result of source node contamination in the study by Jones (1992), it should be
noted that the random node patterns were much less prominent than the source node
patterns. It is apparent that the effect of reservoir releases was not an important
factor in the patterns of random node contamination as simulated for the Blacksburg
system.
Figure 56. The relationship between mean hourly demand and the mean number of violated nodes as a result of random node contamination. The mean demand factor was a parameter of the simulation. The mean number of violated nodes observed from 56 simulation trials.
In summary, simulated random node contamination did not result in any clearly identifiable spatial patterns of violations. Rapid dilution of the contamination in the pipes served to limit the duration of residual contamination and prevented its spread beyond the region where contamination was introduced. This result was different than the observations of Jones (1992), but these differences are most likely the result of using different contaminant concentrations and are also due to differences in the size and complexity of the networks studied. The results of the simulated random node contamination events provide little help in identifying good monitoring points. In section D, the results of optimal monitoring design are discussed and implications of these results as applied to distribution system monitoring are discussed in section E.
D. Optimization of Distribution System Monitoring

1. Formulation of Optimization Problems

Mathematical optimization was used to choose a set of monitoring points that would result in the detection of the maximum number of contamination events. A number of details concerning the construction of the optimization problems are pertinent to the interpretation of the optimal solutions. It should be noted that a monitoring point was identified by two parameters: the location (node) and the hour. The same node monitored at two different hours constituted two individual monitoring points. Likewise, two different nodes monitored at the same hour constituted two distinct monitoring points. There was no attempt to restrict the replication of a particular hour or a particular node in the set of monitoring points. Therefore, it was perfectly feasible, for example, for the resulting solution to consist of a single node monitored at several different times. Conversely, it was perfectly feasible for the solution to be a set of different nodes all monitored at the same time. While it is reasonable to assume that regulatory authorities may reject either of these scenarios, it should be considered that the purpose of this study was to look at the results and implications of a simulation-optimization approach to designing a monitoring plan and not to design a single plan that encompasses every objective and constraint that may be implied by regulations or common practice.

As discussed in section D of the Methods and Materials chapter, delays in the
time between hour 0 of the begin day of contamination and the first hour that monitoring for source node contamination was allowed to begin were introduced to assess whether events were more likely to be detected shortly after contamination entered the system or after the contamination had opportunity to spread in the system. The analysis in section C suggested that a delays in monitoring after the peak hour of contamination (see Figure 15) would substantially reduce the number of violated nodes that are candidates for the detection of source node contamination. The results discussed later in this section provide an indication of how important the temporal aspect of monitoring may be.

The importance of the fluctuation in the number of violated nodes over the 24-hour demand cycle was assessed by using restrictions on the time of day during which monitoring could take place. Specifically, the restriction of monitoring to only the morning hours or only the afternoon hours was intended to represent the possibility that monitoring could only take place during certain parts of the work day and provided an indication of how important time of day was to the detection of contamination events.

The optimization of daily monitoring was used to assess the relative performance of monitoring the same location(s) at the same hour on a regular daily basis versus monitoring a cluster of points on a specific day or series of days. To a certain degree, the optimization of a daily monitoring point is more applicable to the general problem of regulatory monitoring than the less restricted formulation since
daily monitoring optimization does not depend on knowing the begin day of the contamination event. As discussed in section E.2, both formulations provide some information that is pertinent to the problem of regulatory compliance monitoring.

The following two sub-sections discuss the solutions of the optimization problems. Specifically, the stability of the solutions as a function of the number of simulation trials is examined to assess the reliability of the resulting monitoring plans. The characteristics of the different solutions are compared with the qualitative predictions that may be inferred from the discussion in section C. Finally, the sensitivity of the optimal solutions to the preset size of the plan and to the adjustment of other constraints on the time of monitoring is assessed. This part of the discussion focuses specifically on the results of the optimization in terms of the simulation trials from which the optimal monitoring plans were derived. Section E looks at the performance of these optimal plans given an independent set of simulation trials that were not used as data for the optimization.

2. Optimal Monitoring - Stability of Solutions

a) Measure of Stability Simulation trials were used to generate input for the optimization problem. As seen in Figures 37 and 40, the value of the optimal fraction of events detected varied with the number of simulation trials used as input for both the source node problem and the random node problem. As the number of simulation trials was increased, a greater number of possible contamination scenarios
were represented in the data set and it became more difficult to find a small set of points that are common to all events. The stability of the optimal solution was indicated by the change in the optimal fraction of detections as the number of trials was increased; when the value of the objective function becomes constant it may be inferred that the breadth of possible contamination scenarios was adequately represented in the input data. This direct measure of stability was presented in Figures 37b and 40b which showed the change in the optimal fraction detected from the previous level. When this change in values remains close to zero as more and more trials are used for input, then it can be inferred that the solution is stabilizing at a constant value. It is, of course, impossible to represent every possible combination of input parameters in the data set when many of the parameters are continuous values. It is therefore reasonable to expect that the optimal value of the objective function will not become constant, however the magnitude of any change may well be expected to eventually move within an acceptable tolerance. In this study, a maximum tolerance was not prespecified. The number of simulation trials used for the optimization was largely determined by the time constraints under which the research was performed. There was an attempt to insure that some stabilization of the solutions was beginning to occur. The results discussed in the remainder of this section and in section E suggest that the solutions were not sufficiently stable to predict the performance of the optimal plans, particularly in the case of optimal plans based on random node contamination events.
b) Stability - Monitoring for Source Node Events Figure 37 showed increasing stability of the solutions for optimal monitoring plans for different monitoring plan sizes (1, 4, 7, and 10 points). It is apparent that an increase in the number of events would most likely have resulted in some decline in the predicted fraction of detection, but it is equally apparent that a very large number of simulation trials would be required to achieve solutions that are significantly more stable than the ones obtained with 56 trials. Figure 37b showed that the fraction detected by optimal plans decreased by less than 0.05 for all plans when the number of trials was increased from 50 to 56. When compared to the decrease of over 0.10 in the fraction detected by the 7-point plan when the number of trials increased from 20 to 30, it appears that the relative stability of solutions with 56 trials has improved considerably. In section E, the performance of optimal plans is assessed by testing their performance on simulation trials that were not used to determine the optimal plans. As discussed in that section, independent analysis suggests that more simulations are needed to achieve a reliable solution to the optimization problem.

c) Stability - Monitoring for Random Node Events Optimal solutions based on random node simulations showed much less stability than the corresponding source node solutions when the number of trials was less than 30 (see Figure 42). However, as the number of trials was increased above 30, the solutions stabilized at a rate similar to that found in the problem solved using source node data. As with the
solutions obtained using source node data, the random node solutions never achieved a constant value and showed signs of decreasing at a fairly slow rate if more simulations were used as input to the formulation. Section E provides an independent assessment of optimal plans based on random node simulation. As discussed in that section, the solution of the random node formulation may be less stable than Figure 42 indicates. In fact, the nature of random node contamination, as simulated in this study, may preclude the determination of a plan that is superior to simple random sampling.

3. Optimal Plans for Detecting Source Node Contamination

a) Effect of Monitoring Plan Size The fraction of events detected increased as the allowable number of monitoring points was increased. While this was certainly to be expected, it may be significant to note that the rate of increase was not constant but showed a pattern that suggested that after 5 points were included in the plan, additional monitoring points provided a decreasing return in terms of the increase in the fraction of events detected. This characteristic was apparent for the original formulation (see Figure 38) and the formulation of daily monitoring (see Figure 46).

b) Effect of Additional Constraints The effect of restricting the time during which monitoring could take place was assessed using 10-point plans. Two types of restrictions on the time of monitoring were evaluated: a restriction on the time of day and the enforcement of a delay from the begin day of contamination. A delay of 24
hours from hour 0 on the begin day appeared to have no effect on the fraction of

detections. Further delays reduced the fraction of detections in a pattern similar to
the decline in the mean number of contaminated nodes. It should be noted, however,
that almost 50 percent of the events can be detected by a 10-point plan that is
restricted to begin monitoring 120 hours after the first day. Thus, even though a
small number of nodes are violated during this time, the time and location of the few
violations is common to a number of events. Figure 19 showed that there were only
nine nodes that were contaminated after hour 120. Twenty-nine events lasted long
enough to cause violations at these nodes. This implies that a limited number of
pathways are available through which contamination can spread.

When monitoring was restricted to either the morning hours or the afternoon
hours, the fraction of detections decreased for the general formulation. This became
more apparent when delays in the start of monitoring were also enforced. As fewer
points were available for detection, the restriction on the time of day became more
important. Morning monitoring was slightly superior to afternoon monitoring for all
situations except the 72 hour delay. The superiority of morning monitoring is
consistent with the observation of a higher number of violated nodes during the early
morning low demand period. The case of afternoon monitoring performing better
than morning monitoring when a 72-hour delay is enforced does not appear have a
simple explanation and may be an atypical result that would not be observed if a
greater number of simulations were used.
Morning and afternoon monitoring restrictions were also assessed for optimal daily monitoring. In the case of a single point to be monitored each day, there was no decrease in the detection of events when monitoring was restricted to the morning or the afternoon. The affect of restrictions was not assessed for larger daily monitoring plans.

c) **Optimal Monitoring Points**  Monitoring points were identified by location and time. Monitoring locations were primarily in the regions where the highest frequency of violations occurred. That is, the southern end of the system near the source node. The time of monitoring was primarily during the first 48 hours of event simulation. The 10-point plan had only two points monitored after hour 48. The location of monitoring points in the optimal plan for daily-monitoring were also in the region of the network with a high number of frequently contaminated nodes. Effective times for daily monitoring were not isolated to one part of the day. This contradicts the 24-hour pattern in the number of node violations that was observed previously. It is possible that the high mean number of nodes observed at during the early morning hours was due to a small number of contamination events and that the cyclical pattern was not predominant for all events.
4. Optimal Plans for Detecting Random Node Contamination

a) Effect of Monitoring Plan Size  A limited number of points were capable of detecting more than one random node event. Two detections per point was possible with nine or fewer points. Points added after nine points contributed one detection apiece. This indicates that there were few patterns of contamination that were common to groups of random node contamination events.

b) Optimal Monitoring Points  Optimal monitoring points were in close correspondence with the time and location of the initial contamination. Few were points were capable of detecting multiple events. The points that detected more than one event tended to be in the central section of the network where the density of nodes was higher and the pipe lengths were shorter. This was probably a result of contamination events taking place in closer proximity to one another in this region and not the result of some system-wide pattern of contaminant transport. The points in the optimal plan that detected a single event were somewhat arbitrary since a violated point from another contamination event could be substituted with no change in the fraction detected. The times of multiple detection monitoring points were primarily distributed throughout the first day, with only one point early on the second day. Daily monitoring points for random node contamination were located similarly to the plan for monitoring over the entire simulation period. The distribution of
monitoring times was relatively uniform over the day. This suggests that the 24-hour cycle in the extent of system contamination was not a significant factor in choosing monitoring points.
E. Comparative Analysis of Monitoring Plans

1. Monitoring Plan Performance

Optimal 10-point monitoring plans were compared with alternative monitoring plans using a set of independent simulations. This set of simulations was independent in that they were not used as input to the optimization process that yielded the optimal monitoring plans. The alternative monitoring plans were described in Table V. Some of these plans were only relevant to the period of time corresponding to the simulation of source node data.

Figure 53 showed the comparison of plans in terms of the detection of independent source node contamination events. The optimal plan performed best, although it detected a smaller fraction of events than was predicted by the solution of the optimization problem. The solution of the optimization problem predicted that 87.5 percent of the events would be detected, but the plan only detected approximately 52 percent of the independent contamination events. This is a strong indication that more simulation trials were needed for input to the optimization formulation in order to achieve a stable solution. The optimal daily monitoring plan with 1-point per day over the first 10 days of the event detected approximately 17 percent of the events compared to a predicted 12.5 percent. This closer correspondence indicates that the number of simulation trials may have been adequate for selecting a single point to be monitored each day.
In general, the plans that were best at detecting source node contamination were those that monitored at times within the first two days of contamination. The second best plan, for example, consisted of random points selected from the first 48 hours of the simulation period. As a general rule, a plan’s effectiveness was inversely related to the number of monitoring points that were sampled late in the simulation period. Monitoring the source node was a relatively ineffective plan. When the source node was monitored at the same time each day, there were no detections. Monitoring the source node at a random time each day resulted in less than 5 percent of the events detected. Since contamination was introduced at the source node for only 1 hour, detection at the source node was dependent on sampling at the exact hour that contamination was introduced. High flow at the source node prevented contamination from lingering.

There were no detections of independent random node contamination events by either the optimal monitoring plan or by alternative monitoring plans. This indicates that the 56 simulation trials used to design the optimal plans were not an adequate number to represent the possible contamination patterns of random node contamination. In view of the fact that no events were detected, it seems reasonable to conclude that random node contamination may defy attempts to design a successful monitoring plan that does not have an unreasonably large number of monitoring points. Similar results were reported by Jones (1992). In his study, there was no single monitoring plan that performed well in the detection of random node
contamination events. Successful detection of random node events in Jones (1992) was generally the result of high concentration events that contaminated the storage reservoirs and so produced a more predictable pattern of contamination.

The methods used in the design and the assessment of these monitoring plans were the result of using the event-based method of simulating individual contamination events over periods of time that were significantly less than the regulatory monitoring period. As discussed in section C.1, it was not possible to design and test plans for monitoring the system over numerous compliance periods using event-based simulation. The results of this study do have implications for the more general problem of monitoring a distribution system for source node and random node contamination. These implications may, in turn, suggest some criteria for selecting monitoring points to fulfill regulatory requirements. This subject is discussed in more detail in the next sub-section.

2. Implications for Distribution System Monitoring

Two types of optimal plan were derived from simulated source node contamination events and from simulated random node contamination events. The first type of plan assumed knowledge of the begin day of the event and so was able to select points on specific days in order to maximize detection of events. The second type of plan assumed monitoring on a daily basis and was more within the framework of an actual monitoring situation; no information concerning the begin time of an
event was used in determining the plan. Each formulation and the resulting solutions provided information useful to analyzing the general problem of compliance monitoring.

The performance plans that were designed with knowledge of the beginning of a source node contamination event indicated that monitoring within two days of the start of contamination dramatically improved the chance of detecting the contamination. The longer the delay, the less likely that a source node event could be detected. Optimization results reinforced the observations of the spatial distribution of violations by demonstrating that nodes in the region near the source node were the best locations for monitoring. The optimal monitoring locations were consistent with Figure 18 which showed the most frequently violated nodes.

Optimal daily monitoring for source node contamination represented a more realistic scenario in that no knowledge of the begin time of the events were assumed. Optimal monitoring of one point per day appeared to be superior to alternative plans that selected points over the entire simulation period without regard to the begin day of contamination. The locations of optimal daily monitoring points were similar to the locations of optimal points discussed in the previous paragraph. The superiority of optimal daily monitoring to the equivalent alternatives suggests that optimization methods are useful for improving monitoring plans for the detection of source node contamination.

The results of the comparative analysis of monitoring random node
contamination suggests that it may not be possible to design a truly effective monitoring strategy for the detection of random node contamination of low concentration and short duration. Jones (1992) observed that the monitoring plans that he evaluated were generally poor at detecting random node contamination. In his study, detection of random node events usually occurred when the event was of high concentration so that the storage reservoirs were contaminated.

In summary, while the design of an optimal plan for monthly compliance monitoring was not feasible in this study, optimization was of value in determining the characteristics of a monitoring plan that would be beneficial in the detection of source node contamination as simulated for the Blacksburg distribution system. It was also shown that random node contamination may defy attempts to design an effective monitoring scheme.
F. The Simulation-Optimization Methodology

1. Simulation Modeling

Simulation modeling provided a means of assessing the contamination of a distribution system under conditions of uncertainty. However, the results of this study as compared to previous work suggest that the specification of mean values and the physical size of the distribution system heavily influence the resulting patterns of contamination. The parameters that define contamination events must be chosen to reflect the type of contamination that is expected to occur in the system under investigation. In the case of coliform contamination, this may be difficult since the possible sources and causes of contamination are numerous.

2. Optimization Based on Monte Carlo Studies

The monitoring plans derived from the formulation of optimization problems were dependent on two factors: the design and results of the simulation model and the formulation of the optimization problem. These factors are not independent of one another however. The formulation of the optimization problem was dependent on the nature of the simulation trial. The simulation model employed for this study used event-based simulation to generate data for the optimization problem. The use of event-based simulations precluded the design of a monitoring plan based on the regulatory compliance period. The optimal daily monitoring plans were the only
plans that may be fit directly into a scheme for regulatory compliance monitoring. For this reason, the optimization process was used primarily as a tool for assessing the characteristics of a monitoring plan that would provide the best opportunity for detecting a contamination event. The design of an optimal monthly monitoring protocol was not feasible with the simulation model used in this study.

The independent assessment of optimal monitoring plans suggested that more simulation trials were needed to achieve stable solutions to the optimization problem. This was particularly true for the optimal monitoring plans based on random node contamination events. However, an increase in the number of trials may result in a more realistic prediction of the fraction detected without yielding a better monitoring plan. The results of Jones (1992) suggested that random node contamination of moderate concentration is difficult to detect. Given this result, it would be quite reasonable to expect the fraction of random node events detected by an optimal plan to continue to decrease as more simulation trials are employed until it reaches a very low level. The plans based on source node contamination appeared to incorporate some commonalities that existed among the source node contamination events. While it is reasonable to assume that the actual fraction of events detected by an optimal plan may be lower than the prediction based on 56 trials, the performance of the plans in detecting independent events suggests that the solution was approaching a reasonably stable level. More importantly, the optimal plans appeared to be superior to plans that did not incorporate the information provided by the simulation results.
The above average performance of the 1-point daily monitoring plan was particularly promising since this formulation did not use the begin day of contamination as a reference time. This provides some indication that optimization may be useful in the design of monitoring plans for the detection of source node contamination.

3. Future Work and Concluding Comments

This study served as an exploratory look at the application of the simulation-optimization methodology to the design of monitoring strategies for detecting contamination in a realistic water distribution network. Practical constraints and limited field data did not prevent the main goals of the study from being achieved, but they did limit the scope of the investigation to a certain degree. It is important to note that the obstacles that necessitated certain compromises in the performance of this research are indeed the subjects that require further investigation if the simulation-optimization methodology is to become a useful decision tool for managers of water utilities.

Several aspects of this study warrant further investigation. It would be beneficial to apply the optimization techniques using data from a long-term simulation that allows the definition of compliance periods. This may have to be done using a smaller system at first. Related to this area of research is the formulation of the optimization. Numerous objectives and constraints are present in the design of a program for compliance monitoring. Further research is necessary to incorporate
these multiple objectives and constraints into the framework of formal optimization. In order for this methodology to be of practical use, it is desirable to research methods of improving the efficiency of the computer code used to perform the simulation model and also to assess numerical methods of solving the optimization that are less calculation-intensive. Finally, it is desirable to achieve some calibration of the model. This would involve calibrating the model parameters to match the results of a tracer study and determining the range of contamination parameters that are most appropriate for a given system.

Before the simulation-optimization methodology can be used as a practical decision tool, advances need to be made in all of these areas. It is possible that improvements in computer hardware will assist to a certain degree, but the solution of most of the problems encountered in performing this research require further investigation of actual distribution system contamination and a realistic assessment of what is expected and what can be achieved through distribution system monitoring.
CONCLUSIONS

Six specific objectives were described in the Introduction of this thesis. With reference to these specific goals, the following conclusions were derived from the results of this study:

1. A model based on the Blacksburg distribution network was used to model contaminant propagation under conditions of uncertainty. Calibration of the model would be required before the results could be attributed to the actual Blacksburg system. Contamination simulated to enter at the source node was diluted in the system before it reached reservoirs, so the regions directly downstream of the source node exhibited more frequent violations of the MCL than peripheral regions. Simulations of random node contamination were of short duration and only resulted in violations in the vicinity of the contamination event. These observations were found to be different than what was observed in a similar study. This suggests that the specific system layout and the loading of contamination may have a significant impact on the resulting pattern of violations in a distribution system.
2. An optimization formulation was designed to choose monitoring points that provided maximal detection of contamination events. The formulation was based on the use of event-based simulations and was, therefore, incapable of providing monitoring plans that were in accordance with the monthly compliance monitoring as prescribed by regulations. The solution of the optimization problem on a 486-based personal computer proved to be difficult given the size of the input data set. Alternatives to traditional integer programming methods may be required in order to incorporate this type of analysis into the regular decision process of utility managers.

3. Monte Carlo simulation provided data that allowed the design of optimal monitoring plans with any required number of monitoring points. Optimization demonstrated a discrete pattern of decreasing returns on additional monitoring points as measured by the fraction of contamination events detected.

4. The number of simulation trials used in the design of optimal monitoring plans was not sufficient to represent the full range of possible contamination scenarios. The optimal solutions did not reach a truly stable level with the number of input trials used.
5. Independent simulation trials were used to assess the performance of monitoring plans. Optimal plans detected fewer contamination events than predicted by the optimal solutions. In particular, optimal plans based on simulated random node contamination proved to be completely ineffective when tested with independent simulation trials. Optimal plans based on source node simulations tended to perform as well or better than alternative monitoring plans.

6. The use of the combined simulation-optimization showed promise as a tool for the design of distribution system monitoring plans when used to isolate points that were prone to violation as a result of contamination entering at the source node. The method failed to provide an effective monitoring plan for the detection of random node contamination events. The sensitivity of the simulation results to the mean level of contaminant loading and to the size of the system suggested that the selection of an appropriate level of contamination would be critical to obtaining results that were relevant to a particular situation.
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VITA

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