A thesis submitted to the Faculty and the Board of Trustees of the Colorado School of Mines in partial fulfillment of the requirements for the degree of Doctorate of Philosophy (Operations Research with Engineering).

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ABSTRACT

This dissertation consists of three papers; the first is published in *Annals of Operations Research*, the second is nearing submission to *INFORMS Journal on Computing*, and the third is the predecessor of a paper nearing submission to *Progress in Nuclear Energy*. We apply operations research techniques to nuclear waste disposal and nuclear safeguards. Although these fields are different, they allow us to showcase some benefits of using operations research techniques to enhance nuclear energy applications. The first paper, “Optimizing High-Level Nuclear Waste Disposal within a Deep Geologic Repository,” presents a mixed-integer programming model that determines where to place high-level nuclear waste packages in a deep geologic repository to minimize heat load concentration. We develop a heuristic that increases the size of solvable model instances. The second paper, “Optimally Configuring a Measurement System to Detect Diversions from a Nuclear Fuel Cycle,” introduces a simulation-optimization algorithm and an integer-programming model to find the best, or near-best, resource-limited nuclear fuel cycle measurement system with a high degree of confidence. Given location-dependent measurement method precisions, we (i) optimize the configuration of $n$ methods at $n$ locations of a hypothetical nuclear fuel cycle facility, (ii) find the most important location at which to improve method precision, and (iii) determine the effect of measurement frequency on near-optimal configurations and objective values. Our results correspond to existing outcomes but we obtain them at least an order of magnitude faster. The third paper, “Optimizing Nuclear Material Control and Accountability Measurement Systems,” extends the integer program from the second paper to locate measurement methods in a larger, hypothetical nuclear fuel cycle scenario given fixed purchase and utilization budgets. This paper also presents two mixed-integer quadratic programming models to increase the precision of existing methods given a fixed improvement budget and to reduce the measurement uncertainty in the system while limiting improvement costs. We quickly obtain similar or better solutions compared to several intuitive analyses that take much longer to perform.
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Operations research is a field that uses various analytical techniques to make better, more informed decisions by combining methods such as statistical analysis and mathematical modeling to arrive at optimal or near-optimal solutions to complex problems. We apply operations research techniques to two distinct fields within the nuclear energy industry: nuclear waste disposal and nuclear safeguards. Although these fields are very different, they allow us to showcase some benefits of using operations research techniques to enhance nuclear energy applications; these benefits include reducing solution times, increasing the size of solvable model instances, and providing higher quality solutions.

Mathematical programming models require input parameters, decision variables, an objective function, and problem-specific constraints. Input parameters are fixed values that depict physical aspects of reality. Parameters can also include physical or desired limits on system variable values. Decision variables represent continuous or discrete outputs of the problem that are initially unknown and are determined by finding the optimal or near-optimal solution to the problem. The objective function is a combination of parameters and decision variables that describes the goal of the problem. Constraints are needed to ensure that limitations imposed by the nature of the problem are upheld.

The civilian nuclear fuel cycle is a set of industrial processes that utilize naturally occurring uranium from the time it is mined as ore, converted into an energy source, and permanently disposed underground after its energy value is depleted. Nuclear waste disposal consists of permanently disposing of nuclear materials and other materials that have been contaminated with radioactivity, and requires careful planning and proper implementation. However, little work has been documented on methods to find the best way to fill a nuclear waste repository while achieving desired objectives and meeting operational constraints. We develop a mixed-integer programming model that deter-
mines where to place nuclear waste packages in a given time period with the goal of minimizing heat load concentration within a repository. The result is an optimal, reproducible schedule for nuclear waste placement.

We use Yucca Mountain as a case study because it was planned to be the United States’ permanent repository for high-level waste and spent nuclear fuel; however, due to political opposition, construction stopped in 2010 after an estimated $15 billion was spent on research and development (McCullough Jr., 2014). Many other countries are also generating large quantities of nuclear waste which will have to be permanently disposed of. Our mathematical model can be easily applied to any other deep-geologic repository constructed around the world for nuclear waste disposal.

The dangerous ability to create nuclear weapons from enriched uranium and plutonium makes it imperative to account closely for these materials as they progress through a nuclear fuel cycle because of their possible loss or diversion (i.e., theft). The International Atomic Energy Agency implements a group of activities, called nuclear safeguards, which try to ensure its 140 member states are not using their civilian nuclear fuel cycles to produce nuclear weapons (International Atomic Energy Agency, 2016). One type of nuclear safeguard, material control and accountability, attempts to prevent the illicit acquisition of nuclear materials, such as enriched uranium, and the subsequent development of weapons, by detecting and deterring the loss of these materials from within a nuclear fuel cycle (U.S. Department of Energy, 2011). A material control and accountability measurement system establishes the material and inventory balance of nuclear material at one or more nuclear fuel cycle facilities (International Atomic Energy Agency, 2002).

We develop a simulation-optimization algorithm and an integer-programming model to find the best, or near-best, resource-limited measurement system with a high degree of confidence. The simulation-optimization algorithm minimizes a weighted sum of false positive and false negative diversion-detection probabilities while accounting for material flows, inventory levels, and measurement errors across a finite, discrete time horizon in hypothetical non-diversion and diversion contexts. In each time period, the estimated cumulative material-unaccounted-for (MUF) is compared to a fixed or optimized threshold value to assess if a “significant amount of material” is
lost from the system. The integer-programming model minimizes the population variance of the estimated MUF in a measurement system. We also develop mixed-integer quadratic programming models to increase the precision of existing measurement methods in a system given a fixed improvement budget and to reduce the measurement uncertainty in the system while limiting improvement costs.

This dissertation contributes to the operations research, nuclear engineering, and statistics literature. We add to the operations research literature by introducing unique models that are flexible and extensible, and by utilizing various techniques to increase the size of solvable instances and to reduce solution times. We use these models to extend the nuclear engineering literature by providing better solutions to nuclear waste disposal and nuclear safeguards problems more quickly than existing or intuitive methods. This dissertation also examines the relationship between false positive and false negative diversion-detection probabilities and the population variance of the estimated MUF in a measurement system to expand the statistics literature.

The primary contributions of this dissertation are organized as follows: in Chapter 2, we develop a mixed-integer programming model to optimize nuclear waste disposal scheduling, which can feature various possible objectives (e.g., minimize heat load, minimize radiation exposure, minimize cost) and can be tailored to other repositories around the world. We implement multiple performance enhancements to reduce solution times and increase the size of solvable model instances. Chapter 3 introduces a simulation-optimization algorithm and an integer-programming model to optimally configure nuclear fuel cycle measurement systems, which (i) feature different objectives (e.g., minimize the weighted sum of false positive and false negative diversion-detection probabilities, minimize the population variance of the estimated MUF), (ii) easily solve different nuclear fuel cycle scenarios, and (iii) greatly reduce solution times compared to a Monte Carlo simulation. In Chapter 4, we formulate mixed-integer quadratic programming models to optimize nuclear fuel cycle measurement system improvements, which can (i) utilize different variance-based parameter improvements (e.g., bounds, mean), (ii) consider larger nuclear fuel cycle scenarios, and (iii) solve almost instantaneously. Chapter 5 concludes the dissertation with a summary of results.
CHAPTER 2
OPTIMIZING HIGH-LEVEL NUCLEAR WASTE DISPOSAL WITHIN A DEEP GEOLOGIC REPOSITORY

A paper published in *Annals of Operations Research*¹
Benjamin Johnson², Alexandra Newman³, Jeffrey King⁴

2.1 Abstract

Many countries produce significant quantities of nuclear waste which will have to be permanently and safely placed in a repository. We develop a mixed integer program that determines where to place each waste package of a specific waste type in a given time period with the goal of minimizing heat load concentration within a repository. Operational constraints include: (i) heat load limitations, (ii) location and time at which waste packages can be placed, and (iii) the number of waste packages that must be placed based on type and time period.

Although applicable to other settings, we use the Yucca Mountain repository in Nevada as a case study. Each of the three objectives used for minimizing heat load concentration improves upon existing greedy and sequential filling methods. Existing filling methods give at least a 17% to an 873% higher, i.e., worse, heat load concentration in the repository with respect to these objectives than do optimal methods. Enhancements, i.e., symmetry reduction constraints, perturbations, and heuristics, increase the size of solvable problem instances. This research can be applied to any deep geologic repository planned for operation around the world with slight modifications to incorporate site-specific objectives and constraints.

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2.2 Introduction

Nuclear waste disposal requires careful planning and proper implementation; however, little work has been documented on methods to find the best way to fill a repository while achieving desired objectives and meeting operational constraints. We develop a mixed integer program that determines where to place each waste package of a specific waste type in a given time period with the goal of minimizing heat load concentration within a repository. The result is an optimal, reproducible schedule for nuclear waste placement, using Yucca Mountain in Nevada as a case study.

The United States must currently dispose of over 70,000 metric tons of nuclear waste in a permanent nuclear waste repository (Nuclear Energy Institute, 2014). This waste is being stored at interim sites in either spent fuel pools or dry cask storage, meant only as short-term solutions with a much higher risk of radiation leakage than permanent placement underground. Yucca Mountain was planned to be the United States’ permanent repository for high-level waste and spent nuclear fuel; however, due to political opposition, construction stopped in 2010 after an estimated $15 billion was spent on research and development. In addition to the R&D cost, taxpayers have had to pay for interim storage at a current total sum of $20 billion dollars; this cost is projected to grow by $500 million per year (McCullough Jr., 2014). Questions exist about the suitability of Yucca Mountain to withstand all possible environmental impacts over the required 10,000 year compliance period (Ewing & Macfarlane, 2002). However, Yucca Mountain is specified by the Nuclear Waste Policy Act Amendment as the only site in the United States for spent nuclear fuel and high-level waste disposal. This means that although there is opposition to Yucca Mountain being reopened, an alternative site is not a viable option for nuclear waste disposal unless the Amendment is rescinded.

Many other countries are also producing large quantities of nuclear waste which will have to be permanently disposed of. Table 2.1 shows current and future worldwide high-level nuclear waste repository efforts (modified from World Nuclear Association (2014)). Figure 2.1 depicts the layout of high-level waste repositories in Sweden (SKB, 2014) and Finland (Posiva, 2015),
Table 2.1: Worldwide high-level nuclear waste repository efforts

<table>
<thead>
<tr>
<th>Country</th>
<th>Existing facilities and progress towards final repositories</th>
</tr>
</thead>
<tbody>
<tr>
<td>Belgium</td>
<td>Repository construction to begin in 2035</td>
</tr>
<tr>
<td>Canada</td>
<td>Repository site search in 2009, start filling in 2025</td>
</tr>
<tr>
<td>China</td>
<td>Site selected by 2020, disposal beginning in 2050</td>
</tr>
<tr>
<td>Finland</td>
<td>Repository open in 2020 (shown in Figure 2.1)</td>
</tr>
<tr>
<td>France</td>
<td>Repository site licensed in 2015, operations beginning in 2025</td>
</tr>
<tr>
<td>Germany</td>
<td>Repository operational in 2025</td>
</tr>
<tr>
<td>India</td>
<td>Research being conducted for a deep geological repository</td>
</tr>
<tr>
<td>Japan</td>
<td>Repository site selection completed by 2025, operations beginning in 2035</td>
</tr>
<tr>
<td>Russia</td>
<td></td>
</tr>
<tr>
<td>South Korea</td>
<td>Interim storage facilities currently being used</td>
</tr>
<tr>
<td>Spain</td>
<td></td>
</tr>
<tr>
<td>Sweden</td>
<td>Site selected for waste disposal (shown in Figure 2.1)</td>
</tr>
<tr>
<td>Switzerland</td>
<td>Repository operational by 2020</td>
</tr>
<tr>
<td>United Kingdom</td>
<td>Plans to make better progress soon on geological disposal</td>
</tr>
</tbody>
</table>

which are very similar to the layout of Yucca Mountain (Figure 2.3). This similarity enables the mathematical model we develop to be easily applied to other deep geologic repositories for any type of nuclear waste.

Figure 2.1: Proposed repository layouts in Forsmark, Sweden (left) and Olkiluoto, Finland (right)

2.2.1 Nuclear Fuel Cycle

A nuclear fuel cycle is composed of eight primary steps: mining and milling, conversion, enrichment, fuel fabrication, reactor power production, spent fuel management, reprocessing, and final disposal (Tsoulfanidis, 2013). Natural uranium is mined from the ground and then sent to a
conversion facility where the milled uranium is converted into uranium hexafluoride which is necessary for the enrichment process. The 0.72 atomic percent (at.%) uranium-235 in natural uranium is separated from the rest of the uranium (0.0055 at.% uranium-234 and 99.2745 at.% uranium-238) and then enriched to around 5 at.% for material used in power reactors and over 90 at.% for material used for weapons development (Lewis, 2008).

After the uranium-235 is enriched, it is converted to an oxide and formed into pellets which are packed into metal enclosures that compose the fuel rods in a reactor. Power is produced in a reactor when nuclear fission heats up the water surrounding the fuel rods into steam, which is used to produce electricity via a turbine. Reactor waste material is stored in cooling pools to reduce the high heat content from radioactive decay. After the waste is cooled, it is put into dry casks and stored above ground. Depending on the type of fuel cycle, the waste is then either reprocessed into reusable reactor fuel or is sent for permanent disposal in an underground repository (Tsoulfanidis, 2013). Figure 2.2 shows the nuclear fuel cycle (Nuclear Regulatory Commission, 2014).

Figure 2.2: The nuclear fuel cycle
2.2.2 Nuclear Waste

There are four primary types of nuclear waste: high-level waste, spent nuclear fuel, transuranic waste, and low-level waste. Although the primary concern for deep geologic disposal around the world includes all waste types except low-level, only high-level waste and spent nuclear fuel are planned for placement in Yucca Mountain. These two waste types include fission products and transuranic elements (contained in spent nuclear fuel) generated in the reactor core, which are highly radioactive and give the waste a high heat output.

High-level waste and spent nuclear fuel are put into waste packages that are placed into drifts, which are long tunnels mined into Yucca Mountain. Yucca Mountain has five panels (outlined in Figure 2.3, modified from Yucca Mountain Project (2009)) that are each comprised of up to 30 drifts. Each drift (shown in Figure 2.4, modified from Lawrence Livermore National Laboratory (2005)) contains up to 170 slots where waste packages can be placed horizontally. The drifts in Figure 2.4 are depicted by the horizontal lines within the panels in Figure 2.3.

Figure 2.3: Yucca Mountain drift layout

2.2.3 Yucca Mountain Operations

The total operational horizon for Yucca Mountain was planned to be 100 years, which included construction of the repository, placement of the waste, and evaluation procedures. Placement activities were scheduled to occur over a span of 54 years with concurrent construction activities. Figure 2.5 shows the proposed timeline for the placement of waste packages in Yucca Mountain.
based on the current supply of waste packages at interim storage facilities and the projected future supply.

2.2.4 Waste Disposal Techniques

There are two simple methods that can be used to sequence waste disposal in a repository - sequential filling and greedy filling. Greedy filling should theoretically reduce high heat load or radiation concentration areas in the repository relative to sequential filling.

The sequential filling method places an available waste package in the closest unfilled slot without considering the waste package’s characteristics. This is the most straight-forward disposal method but does not necessarily provide a low heat load or radiation concentration in the repository.
In terms of heat load, Figure 2.6 shows that the next waste package (4.0 kW) that arrives will be placed in Slot 5 in Drift 1 (filling top-to-bottom and left-to-right).

The greedy filling method places an available waste package in the next unfilled slot in the drift that currently has the lowest total heat load or radiation. In terms of heat load, Figure 2.7 shows that the next waste package (4.0 kW) that arrives will be placed in Slot 6 in Drift 2 (filling top-to-bottom and left-to-right).

However, the optimization model we present determines a sequence of waste placements that will significantly reduce heat load concentration relative to either the sequential or greedy filling methods. The remainder of the paper is organized as follows: Section 2.3 provides a literature review of previous efforts to improve nuclear waste disposal; Section 2.4 contains the mathematical model and Section 2.5 describes how we improve model tractability. Section 2.6 provides the data we use for the model; Section 2.7 includes an analysis of the results from solving the model and Section 4.8 details the importance of our findings.

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<th>Slots</th>
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<tbody>
<tr>
<td>1-4</td>
<td>5-8</td>
<td>9-12</td>
</tr>
<tr>
<td>Drift 1</td>
<td>4.0</td>
<td></td>
</tr>
<tr>
<td>Drift 2</td>
<td>0.6</td>
<td></td>
</tr>
<tr>
<td>Drift 3</td>
<td>1.0</td>
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<tr>
<td>Drift 4</td>
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Figure 2.6: Sequential filling method (heat load in kW)

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<th>Slots</th>
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<tr>
<td>1-4</td>
<td>5-8</td>
<td>9-12</td>
</tr>
<tr>
<td>Drift 1</td>
<td>4.0</td>
<td></td>
</tr>
<tr>
<td>Drift 2</td>
<td>0.6</td>
<td>4.0</td>
</tr>
<tr>
<td>Drift 3</td>
<td>1.0</td>
<td></td>
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<tr>
<td>Drift 4</td>
<td>1.0</td>
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</table>

Figure 2.7: Greedy filling method (heat load in kW)
2.3 Literature Review

Much of the research to improve waste disposal efforts focuses on routing and locating waste materials that are not specifically nuclear. Ghose et al. (2006) use a geographic information system (GIS) optimal routing model to obtain a solution that minimizes the cost and distance of transporting solid wastes to a landfill. The Asansol Municipality Corporation in India can save 16.6 million rupees or about $300,000 in annual operating costs. Tung & Pinnoi (2000) create a mixed-integer program to optimize vehicle routing and scheduling for waste collection in Hanoi, Vietnam. They show improvements in total cost and the number of vehicles utilized compared to previous routing and scheduling techniques.

A related study by Leao et al. (2001) uses Monte Carlo simulation to model the effects of population growth, urban sprawl, and waste generation on land supply. The study gives decision makers a better idea of the relationship between waste management and urban development to help decide where to dispose of solid waste material. Erkut & Neuman (1992) develop a multiobjective, mixed-integer program that minimizes the total cost of undesirable waste facilities and the total opposition to the facilities while maximizing the disutility imposed on an individual. They provide a realistic example that examines the tradeoffs between the objectives. Angilella et al. (2015) apply the Non Additive Robust Ordinal Regression method to determine the best urban landfill location based on population presence, hydrogeological risk, possible transport infrastructure interferences, and economic cost.

Multiple objectives can increase the flexibility of waste material location and routing optimization models. Alumur & Kara (2007) develop a multiobjective location-routing mixed integer programming model that determines where to open treatment and disposal centers for hazardous waste, as well as how to route the waste to those centers. They successfully apply their model to the Central Anatolian Region of Turkey. Giannikos (1998) develops a multiobjective model to locate hazardous waste disposal or treatment facilities and to transport the waste, considering four objectives: (i) minimize total operating cost; (ii) minimize total perceived risk; (iii) distribute risk equally among population centers; and (iv) distribute the negative utility incurred by operating
treatment facilities equally.

Some nuclear waste disposal research focuses on where to place a potential repository. Tají et al. (2005) use multiple criteria decision analysis to determine potential repositories for nuclear waste disposal. Weighted preferences evaluate safety and environmental concerns, relative cost, and robustness; the combination of associated solutions yield an overall score for each repository.

Additional research focuses on the best type of disposal option for nuclear waste. Filbert et al. (2008) outline a new nuclear waste disposal technique which places canisters into deep vertical boreholes instead of placing them horizontally into a repository. Their goal is to optimize transport, handling, and disposal efforts relative to horizontal waste placement. Jin (1994) explores the optimal strategy for multimedia waste disposal. The primary decision is whether to dispose of waste in the ocean or on land, the latter of which is more financially burdensome. He finds that the optimal strategy based on moderate risk aversion is to use land-based facilities for waste disposal.

Mohr & O’Brien (1973) develop a generalized economic model to optimize a multi-source, variably distributed system for waste disposal. A decision map shows an optimal plan for different methods of deep-well disposal of liquid wastes. Similarly, Crowe et al. (2002) improve the accuracy and amount of information collected for maintenance of facilities where low-level radioactive waste is disposed, specifically, at the Nevada Test Site (NTS). A probabilistic extension of the NTS maintenance model allows the authors to incorporate uncertainty in input parameters such as inventory, transportation, and exposure to radioactive material.

There is limited research regarding optimizing nuclear waste disposal processes using operations research techniques, and none specifically on how to optimize placement of nuclear waste within a repository once the location of repository has been selected. Hutchinson (1983) develops a linear programming model for the United Kingdom that optimizes at-sea disposal of radioactive waste from all supply streams, subject to operational and political constraints. Rautman et al. (1993) also use a linear programming model to minimize the total land area required to absorb and dissipate the heat from the nuclear waste planned for disposal in Yucca Mountain. They find that the size of Yucca Mountain is 17% too small to achieve optimal heat absorption and dissipation.
based on the amount of waste planned for placement. Our research addresses an important segment of nuclear industry operations, that of waste disposal placement.

2.4 Mathematical Model (P)

There are several important objectives in nuclear waste disposal operations: (i) minimize the radiation dose received by the workers; (ii) minimize the absolute deviation from the average worker exposure; (iii) minimize the maximum worker exposure; (iv) minimize cost; and (v) minimize placement time. Although our model has the ability to incorporate each of these objectives, placement operations at Yucca Mountain were to be completely automated, limiting the applicability of minimizing radiation exposure to workers. Therefore, we minimize heat load concentration throughout the repository by implementing three different objective functions independently.

Three objectives provide different methods to minimize heat load concentration in the repository based on the six different classifications of waste packages, each of which has a different heat load. Objective (2.1) minimizes the total weighted heat load of all 3-waste-package×3-waste-package segments, which reduces hot spots in the repository by limiting the amount of high-heat-load waste packages placed in close proximity to other high-heat-load waste packages. Objective (2.2) minimizes the total difference from the average drift heat load, reducing the number of drifts that have either an extremely high or extremely low heat load compared to the other drifts. Objective (2.3) minimizes the total difference from the overall average 3-waste-package×3-waste-package segment weighted target heat load, which represents a slightly more complex method to reduce hot spots in the repository. Other objective functions can also be implemented to reduce heat load concentration, which, in some cases, might provide a more desirable solution (e.g., minimizing the maximum drift heat load).

The purpose of these three objective functions is to reduce heat load hot spots within the repository. The total heat load of the waste packages is constant regardless of their placement location so we analyze segments within the repository to depict the local effect of neighboring waste packages’ heat load concentrations. A 3-waste-package×3-waste-package segment is a 3×3 section of
the repository that consists of nine slots across three drifts with a target slot located at its center. We also implement the deviation from the average heat load in Objectives (2.2) and (2.3) to reduce local heat load concentrations across the entire repository, which ensures that each segment is not evaluated independently, but rather, in conjunction with all of the other local heat load concentrations.

Figure 2.8 shows an example of how 3-waste-package × 3-waste-package segments are represented in the repository. The first term determines the number of segments that are needed based on the total number of drifts (|D|). The second term determines the number of segments that are needed based on the number of slots per drift (|S|/|D|). A value of two is subtracted from each of these terms because of boundary effects. If there are 10 drifts and 100 slots, the total number of 3-waste-package × 3-waste-package segments is \((10 - 2) \cdot (100/10 - 2) = 64\).

Figures 2.9-2.11 show how each objective function is calculated for waste packages placed using the sequential filling method; this figure does not represent an optimal solution. For simplicity, the following heat load values are unweighted; the weighting scheme used in Objectives (2.1) and (2.3) is discussed in Section 2.6. The first 3-waste-package × 3-waste-package segment in Objectives (2.1) and (2.3) is shaded gray and the second 3-waste-package × 3-waste-package segment is depicted by the thick black border. The four drifts for Objective (2.2) are represented by the gray shading and thick black borders. The heat load values of the target slots for Objectives (2.1) and (2.3) are depicted in boldface font.
The heat load of the first 3-waste-package \( \times \) 3-waste-package segment in Figure 2.9 is 16.8 kW and the heat load for the second segment is 10.4 kW. The total heat load of all 3-waste-package \( \times \) 3-waste-package segments is \( 27.2 \text{ kW} \) (16.8 + 10.4). The average drift heat load in Figure 2.10 is 4.75 kW. The difference from the average heat load in a drift is 3.85 kW for Drift 1, 2.15 kW for Drift 2, 0.850 kW for Drift 3, and 2.55 kW for Drift 4. The total difference from the average drift heat load is \( 9.40 \text{ kW} \) (3.85 + 2.15 + 0.850 + 2.55). The total heat load of all waste packages in Figure 2.11 is 19.0 kW and the heat load for each of the 3-waste-package \( \times \) 3-waste-package segments is the same as in Figure 2.9. The average 3-waste-package \( \times \) 3-waste-package segment target heat load is 9.50 kW. The difference from the average 3-waste-package \( \times \) 3-waste-package segment target heat load is 7.30 kW for the first segment and 0.900 kW for the second segment. The total difference from the overall average 3-waste-package \( \times \) 3-waste-package segment target heat load is \( 8.20 \text{ kW} \) (7.30 + 0.900).

<table>
<thead>
<tr>
<th></th>
<th>Slots 1-4</th>
<th>Slots 5-8</th>
<th>Slots 9-12</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drift 1</td>
<td>4.0</td>
<td>4.0</td>
<td>0.6</td>
</tr>
<tr>
<td>Drift 2</td>
<td>0.6</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Drift 3</td>
<td>1.0</td>
<td>0.6</td>
<td>4.0</td>
</tr>
<tr>
<td>Drift 4</td>
<td>1.0</td>
<td>0.6</td>
<td>0.6</td>
</tr>
</tbody>
</table>

**Figure 2.9: Example of Objective (2.1) (heat load in kW)**

<table>
<thead>
<tr>
<th></th>
<th>Slots 1-4</th>
<th>Slots 5-8</th>
<th>Slots 9-12</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drift 1</td>
<td>4.0</td>
<td>4.0</td>
<td>0.6</td>
</tr>
<tr>
<td>Drift 2</td>
<td>0.6</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Drift 3</td>
<td>1.0</td>
<td>0.6</td>
<td>4.0</td>
</tr>
<tr>
<td>Drift 4</td>
<td>1.0</td>
<td>0.6</td>
<td>0.6</td>
</tr>
</tbody>
</table>

**Figure 2.10: Example of Objective (2.2) (heat load in kW)**

The model incorporates various constraints imposed by the design and functionality of the repository: (i) heat load limitations for the repository, (ii) location and time at which waste packages can be placed in the repository, and (iii) the number of waste packages that must be placed based on type and time period.
Figure 2.11: Example of Objective (2.3) (heat load in kW)

<table>
<thead>
<tr>
<th>Drift</th>
<th>Slots 1-4</th>
<th>Slots 5-8</th>
<th>Slots 9-12</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drift 1</td>
<td>4.0</td>
<td>4.0</td>
<td>0.6</td>
</tr>
<tr>
<td>Drift 2</td>
<td>0.6</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Drift 3</td>
<td>1.0</td>
<td>0.6</td>
<td>4.0</td>
</tr>
<tr>
<td>Drift 4</td>
<td>1.0</td>
<td>0.6</td>
<td>0.6</td>
</tr>
</tbody>
</table>

**Sets**
- $w \in W$: Waste package $w$
- $c \in C$: Waste package classification $c$
- $w \in W_c$: Waste package $w$ within waste package classification $c$
- $s \in S$: Drift slot $s$
- $s' \in S'$: Slot $s'$ within the 3-waste-package $\times$ 3-waste-package segment of target slot $s$
- $d \in D$: Repository drift $d$
- $s \in S_d$: Slot $s$ within repository drift $d$
- $t \in T$: Time period $t$

**Parameters**

**Heat Load**
- $Q_{cw}$: Heat load of waste package $w$ within waste package classification $c$ (watts)
- $\bar{Q}^2$: Average heat load for all drifts (Objective 2) (watts)
- $\bar{Q}^3$: Target heat load for all 3-waste-package $\times$ 3-waste-package segments (Objective 3) (watts)
- $\delta_s$: Heat load weighting factor on drift slot $s$ (unitless)

**Demand**
- $N_{cT}$: Number of waste packages of classification $c$ that must be disposed of in the repository, invariant by time period
- $N_{tC}$: Number of waste packages that must be disposed of in the repository in time period $t$, invariant by waste package classification

**Length**
- $L_c$: Length of waste package of classification $c$ (meters)
- $\bar{L}_d$: Maximum length of each drift $d$ (meters)
Average and Target Heat Load Values

\[
\bar{Q}^2 = \frac{\sum_{c \in C} \sum_{w \in \hat{W}_c} Q_{cw}}{|D|} \\
\bar{Q}^3 = \frac{\sum_{c \in C} \sum_{w \in \hat{W}_c} Q_{cw}}{(|D| - 2) \cdot ((|\mathcal{Y}|/|D|) - 2)}
\]

Variables

Difference Variables

\(Z^2_+\) Positive difference from the average drift heat load for target drift \(d\) (Objective 2) (watts)
\(Z^2_-\) Negative difference from the average drift heat load for target drift \(d\) (Objective 2) (watts)
\(Z^3_+\) Positive difference from the average 3-waste-package × 3-waste-package segment weighted target heat load for target slot \(s\) (Objective 3) (watts)
\(Z^3_-\) Negative difference from the average 3-waste-package × 3-waste-package segment weighted target heat load for target slot \(s\) (Objective 3) (watts)

Binary Variables

\[
y_{wst} = \begin{cases} 
1 & \text{if waste package } w \text{ is disposed of in drift slot } s \text{ during time period } t \\
0 & \text{otherwise}
\end{cases}
\]

Objectives

Objective 1: Minimize the total weighted heat load of all 3-waste-package × 3-waste-package segments (watts)

\[
\min \sum_{c \in C} \sum_{w \in \hat{W}_c} \sum_{s \in \mathcal{Y}} \sum_{s' \in \mathcal{Y}'} \sum_{t \in \mathcal{T}} [\delta_{s'} \cdot Q_{cw} \cdot y_{wst}]
\]  

(2.1)

Objective 2: Minimize the total difference from the average drift heat load (watts)

\[
\min \sum_{d \in \mathcal{D}} [Z^2_+ + Z^2_-]
\]  

(2.2)

Objective 3: Minimize the total difference from the average 3-waste-package × 3-waste-package segment weighted target heat load (watts)

\[
\min \sum_{s \in \mathcal{Y}} [Z^3_+ + Z^3_-]
\]  

(2.3)
Constraints

Variables within the model are subject to:

**Difference from Average Heat Load**

\[
\sum_{c \in C} \sum_{w \in \hat{W}} \sum_{s \in \hat{S}_d} \sum_{t \in T} \left[ Q_{cw} \cdot y_{wst} \right] = Z_d^2 + Z_d^2 - \hat{Q}^2 \\
\forall d \in D
\]  

(2.4)

\[
\sum_{c \in C} \sum_{w \in \hat{W}} \sum_{s \in \hat{S}_d} \sum_{t \in T} \left[ \delta_s \cdot Q_{cw} \cdot y_{wst} \right] = Z_s^3 + Z_s^3 - \hat{Q}^3 \\
\forall s \in \mathcal{S}
\]  

(2.5)

**Placement**

\[
\sum_{w \in W} \sum_{t \in T} y_{wst} \geq 1 \\
\forall d \in D, s \in \hat{S}_d, t \in \mathcal{T}
\]  

(2.6)

\[
\sum_{c \in C} \sum_{w \in \hat{W}} \sum_{s \in \hat{S}_d} \sum_{t \in T} L_c \cdot y_{wst} \leq L_d \\
\forall d \in D
\]  

(2.7)

\[
\sum_{w \in W} \sum_{t \in T} y_{wst} \leq 1 \\
\forall s \in \mathcal{S}
\]  

(2.8)

\[
\sum_{s \in \hat{S}_d} \sum_{t \in T} y_{wst} \leq 1 \\
\forall w \in W
\]  

(2.9)

**Demand**

\[
\sum_{w \in \hat{W}} \sum_{s \in \hat{S}_d} \sum_{t \in T} y_{wst} \geq N_c^2 \\
\forall c \in C
\]  

(2.10)

\[
\sum_{w \in \hat{W}} \sum_{s \in \hat{S}_d} \sum_{t \in T} y_{wst} \geq N_t^2 \\
\forall t \in \mathcal{T}
\]  

(2.11)

**Non-Negativity and Binary**

\[
y_{wst} \text{ binary} \\
\forall w \in W, s \in \mathcal{S}, t \in T
\]  

(2.12)

\[
Z_d^{2+}, Z_d^{2-}, Z_s^{3+}, Z_s^{3-} \geq 0 \\
\forall d \in D, s \in \mathcal{S}
\]  

(2.13)

**Description**

Objective (2.1) minimizes the total weighted heat load of all 3-waste-package × 3-waste-package segments in the repository. Objectives (2.2) and (2.3) minimize the absolute difference from an average heat load. This construct is nonlinear because of the absolute value term in the objective function. To linearize the model, the absolute difference is split into positive and negative terms to incorporate values above and below the average heat load, respectively.
Parameter $\bar{Q}^2$ accounts for the average drift heat load. The total difference from the average drift heat load, determined in Constraints (2.4), equals the difference between the average heat load and the actual heat load for each drift. Parameter $\bar{Q}^3$ accounts for the average 3-waste-package $\times$ 3-waste-package segment target heat load. The target heat load is calculated in a manner similar to that of $\bar{Q}^2$ because overlapping segments are not used in the calculations. The target heat load is the quotient of the total heat load of the waste packages and the total number of segments, as opposed to the quotient of the heat load of all the segments summed individually (including overlap) and the total number of segments. The target heat load is not dependent on the arrangement of the waste packages, which is beneficial because it provides a constant value against which to compare each segment’s heat load. Using the target heat load is valid because, although it does not directly depict the average 3-waste-package $\times$ 3-waste-package segment heat load, it does indicate the local average heat load of the waste packages without double-counting heat loads within the segments.

The total difference from the average 3-waste-package $\times$ 3-waste-package segment weighted target heat load, determined in Constraints (2.5), equals the difference between the target heat load and the actual heat load for each segment.

Constraints are necessary to force the waste packages to be placed in a logical manner. Constraints (2.6) ensure that a waste package can only be placed in a drift slot if the previous slot within the drift is already filled. Constraints (2.7) ensure that the total length of waste packages placed in a drift does not exceed the maximum length of the drift. Constraints (2.8) enforce a drift slot to be filled only once and Constraints (2.9) enforce a waste package to be placed only once.

Two different sets of demand constraints enforce placement quantity requirements which are determined by government or repository management criteria. Constraints (2.10) ensure that the demand for each waste package classification is met to prevent all of the waste packages in a particular classification from being placed in the same time period. Constraints (2.11) ensure that the demand for each time period is met to prevent time periods that have little or no waste placement.
2.5 Solution Methodology

Using the base model (Model \((\mathbb{P})\) with no performance enhancements), we only can solve problem instances with fewer than 100 waste packages in 10 drifts, which is a fraction of a realistic problem instance. We implement various performance enhancements to solve larger problem instances more quickly. In particular, we employ existing symmetry reduction techniques, described in Section 2.6.1, and utilize a high-quality initial solution, provided by a heuristic tailored specifically for our application, to solve larger problem instances.

2.5.1 Mathematical Model \((\mathbb{P}^0)\)

A modified mixed integer program constitutes part of the time-independent placement heuristic discussed in Section 2.5.2. The primary difference between this model, Model \((\mathbb{P}^0)\), and Model \((\mathbb{P})\) is the removal of the time period index on the variables. Model \((\mathbb{P}^0)\) requires all of the parameters from Model \((\mathbb{P})\), in addition to the new parameters given below. Objective (2.14) is modified from Objective (2.1) to reflect this new paradigm; Objectives (2.2) and (2.3) are changed in the same manner but, for the sake of brevity, are not shown.

Sets (Additional)
\[ t' \in \mathcal{T}' \quad \text{Time period } t' \]

Parameters (Additional)
\begin{align*}
\bar{s}_d & \quad \text{First slot within drift } d \\
\bar{s}'_d & \quad \text{Last slot within drift } d \\
T'_w & \quad \text{Earliest time period for the placement of waste package } w \\
T''_d & \quad \text{Earliest time period for the placement of the waste package in the previous slot of drift } d \\
N_c & \quad \text{Number of waste packages of classification } c \text{ that must be disposed of in the repository} \\
N^C & \quad \text{Number of waste packages that must be disposed of in the repository, invariant by waste package classification} \\
\end{align*}

Variables
\[ y_{ws} = \begin{cases} 
1 & \text{if waste package } w \text{ is disposed of in drift slot } s \\
0 & \text{otherwise} 
\end{cases} \]
Objectives

Objective 1: Minimize the total weighted heat load of all 3-waste-package×3-waste-package segments (watts)

\[
\min \sum_{c \in C} \sum_{w \in \hat{W}} \sum_{s \in \hat{S}'} y_{ws} \sum_{s' \in S} \left[ \delta_{s'} \cdot Q_{cw} \cdot y_{ws} \right] \quad (2.14)
\]

Constraints

Variables within the model are subject to:

\[
\sum_{d \in D} \sum_{s \in \hat{S}_d} \sum_{w \in \hat{W} | T_w = t'} y_{ws} \geq 1 \quad \forall \ t' \in \mathcal{T}' \quad (2.15)
\]

\[
\sum_{w \in \hat{W} | T_w = t'} y_{ws} \geq \sum_{w \in \hat{W} | T_w = t'} y_{w,s-1} \quad \forall \ t' \in \mathcal{T}', d \in D, \ s \in \hat{S}_d \ | \ S_d + 1 \leq s \leq S_d + N^{\mathcal{C}'}_t - 1 \quad (2.16)
\]

\[
\sum_{w \in \hat{W}} y_{w,s-1} \geq \sum_{w \in \hat{W}} y_{ws} \quad \forall \ d \in D, s \in \hat{S}_d \quad (2.17)
\]

\[
\sum_{c \in C} \sum_{w \in \hat{W}} \sum_{s \in \hat{S}_d} L_c \cdot y_{ws} \leq \bar{L}_d \quad \forall \ d \in D \quad (2.18)
\]

\[
\sum_{w \in \hat{W}} y_{ws} \leq 1 \quad \forall \ s \in \mathcal{S} \quad (2.19)
\]

\[
\sum_{s \in \mathcal{S}} y_{ws} \leq 1 \quad \forall \ w \in \hat{W} \quad (2.20)
\]

\[
\sum_{w \in \hat{W}} \sum_{s \in \mathcal{S}} y_{ws} \geq N_c \quad \forall \ c \in C \quad (2.21)
\]

\[
\sum_{w \in \hat{W}} \sum_{s \in \mathcal{S}} y_{ws} \geq N_c^{\hat{C}} \quad \forall \ w \in \hat{W}, s \in \mathcal{S} \quad (2.22)
\]

\[
y_{ws} \text{ binary} \quad \forall \ w \in \hat{W}, s \in \mathcal{S} \quad (2.23)
\]

Description

Two new constraint sets ensure precedence is maintained in Model (P), even though there are no placement time periods in Model (P0). We use space as a proxy for the temporal precedence that needs to be enforced in Model (P). Constraints (2.15) force each time period to be represented at least once by the earliest placement time of a waste package in the first slot of a drift, and ensure that placement demand for each time period can be met when time periods are later assigned to the solution from Model (P0). Constraints (2.16) force the next \( N^{\mathcal{C}'}_t - 1 \) number of slots within each...
drift to contain waste packages that have an earliest placement time no later than that of the waste package in the slot before it. These constraints ensure that precedence is enforced for the number of slots within a drift equal to the waste package placement demand for that time period and assume that the placement demand for each time period is less than the number of slots in a drift. If these two constraint sets are not present, the waste package placement schedule might not be possible when time periods are assigned because the first slots in a drift might contain waste packages that have late earliest placement times, which precludes the assignment of early time periods to slots in that drift due to temporal precedence. Constraints (2.17) enforce spatial precedence and are the same as Constraints (2.6) in Model \((P)\) with the time index dropped. Constraints (2.18)-(2.23) correspond to Constraints (2.7)-(2.12) in Model \((P)\).

2.5.2 Time-Independent Placement Heuristic

The time-independent placement heuristic provides an initial solution to Model \((P)\) for all objectives (Algorithm 1). Solving Model \((P^0)\) provides an assignment of waste packages to specific slots. Time periods are then assigned to each waste package-slot placement in any valid arrangement that is subject to precedence, waste package placement demand, and waste package availability. As long as the time is greater than or equal to the earliest placement time of the waste package in the slot before it, we assign each slot the earliest placement time of the waste package in the slot. Otherwise, a slot is assigned the earliest placement time corresponding to that of the waste package placed in the previous slot. Then, Model \((P)\) is solved with the result from Model \((P^0)\) used as an initial solution; this dramatically reduces the solution time of the model, which includes the time required to obtain the initial solution and to solve the model. A similar technique is used in the mining industry in which the ultimate pit limit, analogous to Model \((P^0)\), is used as a preprocessing tool for the open-pit mine production scheduling model, analogous to Model \((P)\) (Chicoisne et al., 2012; Espinoza et al., 2013; Lambert & Newman, 2014; Lerchs & Grossmann, 1965).
Algorithm 1 Time-Independent Placement Heuristic Pseudocode

Note: \( y^0_{ws} \) is an initial solution for Model (P)

1: procedure RUN FILE(Model)
2:   if Model (P) then
3:     if Scenario 1 then
4:       Drop Constraints (2.15) and (2.16)
5:       Solve Model (P) \( \rightarrow y^*_{ws} \)
6:     else if Model (P) then
7:       Let \( y_{ws} = y^0_{ws} \) \( \forall w \in W, s \in S, t \in T \)
8:       Solve Model (P) \( \rightarrow y^*_{ws} \)
9:   procedure JOB FILE
10:     RUN FILE(Model (P))
11:     if Scenario 1 then
12:       for \( t \in T \) do
13:         while \( \sum_{w \in W} \sum_{s \in S} y^0_{ws} < N^T_{ct} \) do
14:           for \( w \in W, s \in S \) do
15:             if \( y^0_{ws} = 1 \) then
16:               Fix \( y^0_{ws} = y^*_{ws} \)
17:           for \( w \in W, s \in S, t \in T \) do
18:             if \( y^*_{ws} = 1 \) and \( \sum_{t' \in T} y^0_{ws} = 0 \) then
19:               Fix \( y^0_{ws} = y^*_{ws} \)
20:     else if Scenario 2 then
21:       for \( w \in W, d \in D, s \in S_d \mid s = S_d, t \in T \mid t = T_{wy}^{ws} \) do
22:         if \( y^0_{ws} = 1 \) then
23:           Fix \( y^0_{ws} = y^*_{ws} \)
24:           Let \( T_{wy}^{ws} = T_{wy}^{ws} \)
25:       for \( d \in D, s \in S_d \mid S_d + 1 \leq s \leq S_d, w \in W \) do
26:         if \( y^0_{ws} = 1 \) then
27:           if \( T_{wy}^{ws} \leq T_{wy}^{ws} \) then
28:             Fix \( y^0_{ws,T_{wy}^{ws}} = y^*_{ws} \)
29:           else
30:             Fix \( y^0_{ws,T_{wy}^{ws}} = y^*_{ws} \)
31:           Let \( T_{wy}^{ws} = T_{wy}^{ws} \)
32:     RUN FILE(Model (P))

Two primary scenarios depict waste package availability. Scenario 1: there are enough waste packages initially available for placement over the five-year time horizon; this allows the model to be solved with no time restrictions on which waste packages can be placed in a specific slot during the time horizon. Constraints (2.15) and (2.16) are dropped for Scenario 1 because temporal precedence does not matter. Scenario 2: there are time restrictions on when waste packages are available for placement, which makes the model harder to solve because even though the number of variables is reduced, precedence constraints must still be satisfied in the presence of limited placement opportunities over the time horizon. Operations at Yucca Mountain are more likely to resemble those represented in Scenario 2 because waste packages would probably arrive on a yearly basis with limitations on the earliest and latest time periods for waste package placement.
Section 2.7 contains results for each objective-scenario combination.

2.5.3 Sliding Time Horizon Heuristic

The size of the repository is too large to obtain an operational lifetime placement scheme in a single solve. Therefore, we segment the repository into sizes reasonable for operational implementation; for Yucca Mountain, we use ten drifts with 85 slots per drift, and five time periods. After one segment is solved, the placement schedule can be fixed and the model can be resolved to obtain another five-year placement schedule. An alternative is to utilize a sliding time horizon heuristic that yields a placement scheme with “look-ahead,” e.g., solve for ten years, fix the placement schedule for the first five years, solve for the next ten years, fix the schedule for the second five years, etc. (Brown et al., 2001; Pochet & Wolsey, 2006).

2.5.4 Hardware and Software

We use the modeling language AMPL, Version 20130109 (AMPL Optimization LLC, 2013; Fourer et al., 2003) and solver CPLEX Version 12.6.0.1 with default settings (IBM, 2014; IBM ILOG AMPL, 2010) on a Dell PowerEdge R410 workstation under the Ubuntu 14.04 operating system with four Quad core CPUs running at 2.72 GHz with 28 GB RAM and a 160 GB HDD.

2.6 Data

Yucca Mountain was planned to have a total of 18,360 slots, 108 drifts, and 54 time periods with a fidelity of one year. We present results for a repository segment of ten drifts over a time horizon of five years, which reflects the concurrent development and placement plan for Yucca Mountain operations. The number of waste packages varies from 50 to 850. The largest model instance presented in this paper, 850 slots and 10 drifts, which corresponds to 85 slots per drift, includes half of the maximum available 170 slots per drift; we assume a drift is only filled with the shortest-length waste packages because there are no predetermined slots within the drifts.
2.6.1 Symmetry Reduction

There are six waste package classifications in Yucca Mountain: transportation, aging, and disposal (TAD), Department of Energy (DOE) short (DOE_S), DOE long (DOE_L), high-level waste (HLW), Naval short (Naval_S), and Naval long (Naval_L). The number of waste packages of each classification represents the expected number of waste packages arriving at Yucca Mountain. Table 2.2 shows the average heat load, length and placement demand values for each waste package classification.

In its original version, the model possesses significant symmetry. In the absence of actual heat load values, we use average heat loads, which yield identical values for each waste package classification. In addition, waste packages can be placed in different time period-slot combinations that are mirror images of each other. Symmetry reduction, introduced via perturbations and symmetry breaking constraints, creates distinctions between parameter values within the objective functions and constraints, which allows the solver to avoid alternative symmetric solutions.

Table 2.2: Waste package average heat load, length, and quantity data

<table>
<thead>
<tr>
<th>Classification</th>
<th>TAD</th>
<th>DOE_S</th>
<th>DOE_L</th>
<th>HLW</th>
<th>Naval_S</th>
<th>Naval_L</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat Load (W)</td>
<td>601</td>
<td>2,640</td>
<td>4,010</td>
<td>1,440</td>
<td>11,800</td>
<td>11,800</td>
</tr>
<tr>
<td>Length (m)</td>
<td>5.85</td>
<td>3.7</td>
<td>5.3</td>
<td>5.28</td>
<td>5.22</td>
<td>5.85</td>
</tr>
<tr>
<td>Demand (packages)</td>
<td>7,500</td>
<td>1,750</td>
<td>1,750</td>
<td>2,823</td>
<td>90</td>
<td>310</td>
</tr>
</tbody>
</table>

Individual heat loads are not known because no waste has been scheduled to be shipped to Yucca Mountain, so average heat load values for each of the waste package classifications are used (Nuclear Regulatory Commission, 2008). In addition, waste packages can be placed in different time period-slot combinations that are mirror images of each other. These attributes cause significant symmetry. Symmetry reduction, introduced via perturbations and symmetry breaking constraints, creates distinctions between parameter values within the objective functions and constraints, which allows the solver to avoid alternative symmetric solutions.

Specifically, heat load perturbations make every waste package’s heat load unique; this provides useful distinctions between parameter values without changing the optimal solution. We follow the
guidelines presented in Geoffrion & Nauss (1977) to ensure that the perturbations do not change the optimal solution. Perturbations are added to the heat load in the difference constraints for Objective (2.2) to further distinguish individual heat loads within drifts.

Symmetry breaking constraints can be implemented based on waste package, slot, or time period. The added constraints place an artificial precedence on a particular variable index. We implement waste package symmetry reduction constraints, i.e., $y_{1st} \geq y_{2st} \geq y_{3st}$, which give priority to variables $y_{1st}$ over variables $y_{2st}$ and $y_{2st}$ over $y_{3st}$ (Sherali & Smith, 2001). This is important because all waste packages within a specific classification have the same characteristics, such as length and heat load. Placing artificial precedence on waste packages for a given slot-time period combination helps the solver identify a difference between the waste packages, which reduces the solution time when used with Objective (2.1). Solution times are not decreased by symmetry reduction constraints for the models containing Objectives (2.2) and (2.3), which have an absolute difference construct. Alternate symmetry breaking constraints based on slot and/or time period did not yield solution time improvements.

2.6.2 Heat Load Weighting Factors

Figure 2.12 shows the heat load weighting factor $\delta_{s'}$ based on the position of slot $s'$ relative to the target slot $s$. The slots adjacent to the target slot (in the same drift) are weighted as 1 to reflect that there is almost no change in heat load concentration because of the close proximity and lack of barriers between the slots. The slots directly horizontal to the target slot (in different drifts) are weighted as 0.5 to reflect the decrease in heat transferred from the target slot to the slots in the neighboring drifts because of the added distance and the drift wall barrier. The corner slots of the 3-waste-package $\times$ 3-waste-package segment are weighted as 0.25 to reflect the decrease in heat transfer because of the drift wall barrier and even further distance from the target slot. If desired, the heat load weighting scheme can instead reflect a more advanced heat transfer analysis.
2.7 Numerical Results

Heat load and solution speed results for each objective are presented for both scenarios discussed in Section 2.5.2, incorporated independently for each objective. The model also has the capability to add restrictions on the earliest and latest time periods that slots are available to receive waste packages and to limit certain waste packages to be placed only in certain slots. The earliest placement times indicate when waste packages will arrive on-site. The DOE also has concerns about how long high-heat-load waste packages remain on-site without being disposed of; this is addressed by the latest placement time period capability of the model. All of the waste packages that arrive during the time horizon are known at the beginning of the horizon. The solution times from the model with performance enhancements for each objective are compared with solution times from the base model (no performance enhancements) to show the improvements from the added enhancements.

2.7.1 Heat Load Results

Objective function values are the same for both scenarios discussed in Section 2.5.2 because the optimal waste package placement is not heavily dependent on arrival times. The greedy and sequential filling methods give an 18.34% and a 17.57% higher total weighted heat load of all 3-waste-package×3-waste-package segments (Objective (2.1)), an 873% and a 701% higher total difference from the average drift heat load (Objective (2.2)), and a 28.44% and 27.27% higher total difference from the overall average 3-waste-package×3-waste-package segment weighted target heat load (Objective (2.3)) compared to the optimal filling method, respectively.
Figure 2.13: Graphical results of each filling method for Objective (2.1). Cell data represents disposal time period.

Unexpectedly, the greedy filling method provides a worse objective value than the sequential filling method for all three objectives. Intuitively, the former method appears to be a better option to reduce heat load concentration in the repository than the latter method because it places waste
packages in the lowest total heat load drift. However, the greedy method does not consider heat load impacts on neighboring drifts, i.e., cross-drifts, which might inadvertently be addressed better by the sequential method.

Greedy Method
- Total difference from the average drift heat load = \textbf{0.09 MW}
- \textbf{873\%} higher than the optimal method

Sequential Method
- Total difference from the average drift heat load = \textbf{0.07 MW}
- \textbf{701\%} higher than the optimal method

Optimal Method
- Total difference from the average drift heat load = \textbf{0.01 MW}

Figure 2.14: Graphical results of each filling method for Objective (2.2). Cell data represents disposal time period.
The highest-heat-load waste packages are placed on the edges in the optimal result for Objectives (2.1) and (2.3). (Figure 2.13 presents the results for Objective (2.1); a figure is not presented for Objective (2.3) because the results for each non-optimal filling method are exactly the same as those for Objective (2.1), and the results for the optimal filling method are visually similar. This result occurs because both Objectives (2.1) and (2.3) minimize some form of weighted heat load, which drives the solution behavior; it also indicates that the solution is robust because although the structures of the objective functions are very different, they give a similar waste package placement scheme.) This is expected due to the lower heat load weighting factors on the edges of each 3-waste-package × 3-waste-package segment and the reduced number of times that those waste packages are counted toward the objective. Placing higher heat load waste packages along the edge of the repository is desired in actual applications because the effect of high heat load on other waste packages is reduced on the edges where there are fewer waste packages. Also, there is more natural shielding along the edges of the repository, which helps negate high heat load effects outside of the drifts. Constraints can be added to force high heat load waste packages further from the boundary.

Even though there is no visible reduction in heat load between the filling methods seen in Figure 2.14 for Objective (2.2), the optimal filling method is better at ensuring that each drift has approximately the same total heat load. This objective is very applicable when there is adequate shielding between drifts that will mostly negate cross-drift heat load effects. Constraints can be added to increase the distance between high heat load waste packages within a drift. Overall, each of these methods for minimizing heat load concentration improves upon the sequential and greedy filling methods.

### 2.7.2 Solution Speed Results

The base model for all objectives does not incorporate symmetry reduction constraints, perturbations, or the time-independent placement heuristic. The best (most efficient) model for all objectives incorporates perturbations on the waste package heat loads, perturbations in the dif-
ference constraints for Objective (2.2), symmetry reduction constraints on the waste packages for Objective (2.1), and the *time-independent placement heuristic* for all objectives. The solution times for various model sizes, based on the number of waste packages, are shown in Table 2.3. If a problem instance cannot be solved within the time limit, its gap is shown in parenthesis. In some cases, the initial solution (obtained from Model (P₀)) cannot be identified within the time limit, and we report its gap and terminate the run.

**Table 2.3**: Solution times (in seconds) for each objective, scenario, and problem instance.

<table>
<thead>
<tr>
<th>Scenario 1: Shaded; Scenario 2: Unshaded</th>
<th>Number of waste packages</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>50</td>
</tr>
<tr>
<td>Base</td>
<td>6</td>
</tr>
<tr>
<td>Best</td>
<td>2</td>
</tr>
</tbody>
</table>

Objective (2.1)

| Base | 1  | 3  | 2  | 4  | 5  | 8   | 51  | 429  | 561  | 3789  | ~    | ~   | ~   |
| Best | 2  | 3  | 3  | 3  | 5  | 7   | 25  | 77   | 206  | 433   | 1621 | 2787 | 9267 |

Objective (2.2)

| Base | 861 | 287 | (25) | (100) | (100) | (100) | (100) | (100) | (100) | ~    | ~   | ~   | ~   | ~   |
| Best | (43.9) | (72.5) | (71.0) | (13.6)* | (40.0)* | (7.73)* | 205  | 130  | 274  | 534  | 860  | 1815 | 1983 | 3251 |

Objective (2.3)

| Base | 9  | 28 | 450 | (100) | (100) | (100) | (100) | (100) | (100) | ~    | ~   | ~   | ~   | ~   |
| Best | 3218 | (34.3) | (52.7)* | (18.2)* | (40.9)* | (23.3)* | 133  | 131  | 325  | 757  | 1169 | 1891 | 5469 | 4737 |

Greedy method

| Base | 8  | 7  | 8  | 9  | 15 | 20 | 174 | 701  | 3055 | ~    | ~   | ~   | ~   | ~   |
| Best | 6  | 5  | 6  | 9  | 10 | 42 | 123 | 254  | 557  | 1255 | 1973 | 2570 | 4070 |

Sequential method

| Base | 8  | 4  | 5  | 6  | 7  | 9  | 44  | 134  | 345  | 682  | 1340 | 2196 | 4245 | 6154 |
| Best | 1  | 1  | 1  | 2  | 3  | 4  | 22  | 91   | 142  | 346  | 587  | 863  | 1237 | 1584 |

| Best | 0  | 0  | 0  | 1  | 0  | 0  | 2   | 5    | 9    | 12   | 19   | 23   | 30   | 40   |

| Time limit = 10,000 seconds; ~ : No integer solution within time limit |
| (%) : Model (P) gap; (%)* : Model (P₀) gap |

The performance enhancements incorporated in the model increase the solvable model size and decrease the solution time for all problem instances with the exception of a few smaller instances associated with Objective (2.2). Restrictions on the availability of waste packages increase the solution time because, although the number of variables decreases, precedence constraints must still be satisfied in the presence of limited placement opportunities over the time horizon, which
increases the difficulty of the problem. For Objective (2.2), the solvable model size increases by an order of magnitude.

Small problem instances for both scenarios in Objective (2) have long solution times because the relative difference between the magnitude of the perturbations and the other values in the constraints does not provide enough symmetry reduction to obtain solution speed improvements. We can combat this by increasing the magnitude of the perturbations; however, to maintain uniformity, we use a constant perturbation magnitude that is ideal for the larger sized models. The \textit{time-independent placement heuristic} is the greatest contributor to increased performance.

2.8 Conclusion

We develop a mixed integer program that creates an optimal, reproducible schedule for nuclear waste placement, using the Yucca Mountain repository in Nevada as a case study. The optimal solution determines where to place each waste package of a specific type in a given time period with the goal of minimizing heat load concentration within a repository. This research can be applied to any of the repositories planned for operation around the world with slight modifications to incorporate site-specific objectives and constraints.

Three different objectives minimize heat load concentration in the repository, which increases the flexibility and effectiveness of the model for use at other deep geologic repositories with the same goals. Existing filling methods give at least a 17% to an 873% higher, i.e., worse, heat load concentration in the repository with respect to these objectives than do optimal methods. The performance enhancements incorporated in the model increase the solvable model size and decrease the solution time for all problem instances with the exception of a few smaller instances associated with Objective (2.2). The \textit{time-independent placement heuristic} is the greatest contributor to increased performance.

Our model is also able to incorporate other objectives that are important in nuclear waste disposal operations, such as: (i) minimize the radiation dose received by workers; (ii) minimize the absolute deviation from the average worker exposure; (iii) minimize the maximum worker expo-
sure; (iv) minimize cost; and (v) minimize placement time. Incorporating multiple objectives into the model allows a repository to obtain a solution that considers multiple goals.

A possible extension to this research is to optimize the entire process of nuclear waste transport from a reactor to permanent disposal in a repository. This includes transportation from a reactor location to interim storage, placement in the interim storage facility, and transportation from the interim storage facility to a permanent repository. The final piece is the optimization of waste placement within a permanent deep geologic repository, which is addressed in this research.

2.9 Acknowledgments

We acknowledge the insights provided by Eduardo Moreno of Universidad Adolfo Ibañez and Daniel Espinoza of Universidad de Chile regarding the time-independent placement heuristic. We also acknowledge helpful comments provided by the anonymous reviewers on a previous draft of this paper.
CHAPTER 3
OPTIMALLY CONFIGURING A MEASUREMENT SYSTEM TO DETECT DIVERSIONS FROM A NUCLEAR FUEL CYCLE

The predecessor of a paper to be submitted to *INFORMS Journal on Computing*

Benjamin Johnson\(^5\), Alexandra Newman\(^6\), Aaron Porter\(^7\), Jeffrey King\(^8\)

### 3.1 Abstract

The civilian nuclear fuel cycle is an industrial process that produces electrical power from nuclear fission of uranium. Using a measurement system to accurately account for nuclear material, such as uranium, in a fuel cycle is important because of the possible loss or diversion (i.e., theft) of this potentially dangerous material. A measurement system is defined by a set of measurement methods, or “devices,” used to account for material flows and inventory values at specific locations in the fuel cycle. We develop a simulation-optimization algorithm and an integer-programming model to find the best, or near-best, resource-limited measurement system with a high degree of confidence. The simulation-optimization algorithm minimizes a weighted sum of false positive and false negative diversion-detection probabilities while accounting for material quantities and measurement errors across a finite, discrete time horizon in hypothetical non-diversion and diversion contexts. In each time period, the estimated cumulative material unaccounted for is compared to a fixed or an optimized threshold value to assess if a “significant amount of material” is lost from a measurement system. The integer-programming model minimizes the population variance of the estimated material loss, i.e., material unaccounted for, in a measurement system. We analyze three potential problems in nuclear fuel cycle measurement systems: (i) given location-dependent device precisions, find the configuration of \( n \) devices at \( n \) locations (\( n=3 \)) that gives the lowest corresponding objective values using the simulation-optimization algorithm and integer-programming model,

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(ii) find the location at which improving device precision reduces objective values the most using the simulation-optimization algorithm, and (iii) determine the effect of measurement frequency on measurement system configurations and objective values using the simulation-optimization algorithm. We obtain comparable results for each problem at least an order of magnitude faster than existing methods. Using an optimized, rather than fixed, detection threshold in the simulation-optimization algorithm reduces the weighted sum of false positive and false negative probabilities.

3.2 Introduction

The civilian nuclear fuel cycle is a set of industrial processes that utilize naturally occurring uranium from the time it is mined as ore, converted into an energy source, and permanently disposed underground after its energy value is depleted. Naturally occurring uranium contains 0.7% uranium-235 by weight. The concentration of uranium-235 in nuclear fuel must be increased, or enriched, to 3-5% uranium-235 by weight before the fuel material can be used for electricity production. Enriched uranium is potentially dangerous because it could be used to produce nuclear weapons (International Atomic Energy Agency, 2002). It is imperative to closely monitor enriched uranium as it progresses through a fuel cycle because of its possible loss or diversion (i.e., theft).

This paper describes the development of the NUclear Measurement System Optimization (NUMSO) toolkit, which is composed of a simulation-optimization algorithm and an integer-programming model that identify an optimal measurement system configuration with high confidence. A measurement system is defined by a set of measurement methods, or “devices,” used to account for material quantities at input, output, and inventory locations of one or more fuel cycle facilities. A measurement system configuration is a unique, location-dependent arrangement of devices based on the detection threshold and corresponding parameter settings. NUMSO optimizes these configurations by identifying the one that yields the lowest weighted sum of false positive and false negative probabilities or the lowest population variance of estimated material loss.

We analyze and enhance nuclear fuel cycle measurement systems because the loss and theft of nuclear and other radioactive material is an international security concern (International Atomic
Energy Agency, 2015). Nuclear material can be used to produce nuclear weapons while “other radioactive material” emits ionizing radiation but is not capable of a nuclear explosion (International Atomic Energy Agency, 2002, 2007). From 1993-2014, there were 714 incidents of loss or theft of nuclear and other radioactive material from facilities or during transport reported to the Incident and Trafficking Database, most of which involved other radioactive materials from industrial or medical applications. However, several incidents included high-enriched uranium, which, if accumulated in sufficient quantities, can be made into a nuclear weapon. These incidents indicate that the loss of nuclear material is still a threat, which can be addressed by enhancing existing measurement systems (Williams, 2014).

Several software programs exist that account for simulated nuclear material at various stages in a fuel cycle (Cipiti & McDaniel, 2012; Cipiti & Zinaman, 2010a,b; Cipiti et al., 2011; Riley et al., 2016; Wilkey & Whitty, 1995). In particular, Shugart & King (2016) develop the SafeGuards Analysis (SGA) toolbox to evaluate a measurement system by simulating measurements at a single fuel cycle facility. SGA constructs a material balance equation from these measurements to identify if there is apparent material loss, i.e., material unaccounted for (MUF). The estimated cumulative material unaccounted for (CMUF) in a given time horizon is the estimated MUF accumulated over all previous time periods. SGA models statistical tests (e.g., cumulative sum, exponential weighted average) to determine if a single false positive or false negative error occurs in hypothetical diversion contexts. Shugart & King (2016) use a Monte Carlo approach to replicate this SGA process to estimate false positive and false negative error probabilities.

The software programs mentioned above only evaluate a single measurement system configuration per execution, which precludes the ability to quickly compare multiple configurations. NUMSO identifies the optimal measurement system configuration with high confidence provided a set of possible locations and devices in a single execution. Suzuki & Ihara (2008) introduce the only other similar tool. They use linear programming to compare the trade-off between cost and probability of detecting a hypothetical diversion of two specific measurement methods, destructive and non-destructive analysis.
In this paper, we develop the *Simulation Optimization Configuration Algorithm* (SOCA) to compare different measurement system configurations in simulated non-diversion and diversion contexts across a finite, discrete time horizon. SOCA identifies with high confidence the measurement system configuration that minimizes a weighted sum of false positive and negative error probabilities obtained from a cumulative material unaccounted for test (CUMUF test). A false positive error, i.e., Type I error, results from “falsely concluding that nuclear material has been lost when in fact no material has been lost.” A false negative error, i.e., Type II error, results from concluding that a material loss did not occur when it actually did occur (International Atomic Energy Agency, 2002). A CUMUF test compares the estimated CMUF to a detection threshold to decide if there is material loss. Beedgen (1988) also uses a CUMUF test in the Program for Statistical Analysis software program to identify potential uranium loss from the Allied General Nuclear Services Barnwell Nuclear Fuels Plant.

SOCA can implement either a pre-determined, fixed detection threshold or an optimized detection threshold, i.e., a threshold that results in the lowest weighted sum of Type I and Type II error probabilities. SOCA can also evaluate different statistical tests and hypothetical diversion contexts. We completely enumerate all measurement system configurations in SOCA because of the small scale of the system we analyze in this paper. However, to optimize a large system, we might need heuristics such as simulated annealing (Kirkpatrick *et al.*, 1983) or genetic algorithms (Srinivas & Patnaik, 1994) to identify a good configuration.

We also develop the *Minimum Variance Configuration Model* (MVCM) in this paper to identify the measurement system configuration that minimizes the population variance of the estimated MUF in a measurement system over a time horizon. Reducing measurement uncertainty enables us to more accurately estimate true material quantities. The purpose of MVCM is to find a configuration that produces a weighted sum of Type I and Type II error probabilities comparable to that from SOCA’s configuration. We show that MVCM obtains the same optimal configuration faster than SOCA using a different objective and simpler modeling framework; we provide mathematical justification of its properties in the appendix. Previously, Stewart (1970) finds how many measure-
ments to take at each location at a hypothetical fuel cycle facility by approximately minimizing the variance of the estimated MUF subject to a cost constraint. Bouchey et al. (1971) use a multi-stage dynamic program to solve the same problem but without using Stewart’s variance approximation. Rather than finding how many measurements to take at a location, we identify where to locate measurements.

For testing, we analyze three problems from Shugart & King (2016): given location-dependent device precisions, use SOCA and MVCM to optimize the configuration of $n$ devices at $n$ locations ($n=3$) (Problem 1), find the location at which improving device precision reduces objective values the most with SOCA (Problem 2), and determine the effect of measurement frequency on measurement system configurations and objective values with SOCA (Problem 3). Solving these problems produces representative answers to potential questions in nuclear safeguards and gives a basis for comparison to SGA (Shugart & King, 2016). To compare results, we use an example nuclear enrichment facility, which is detailed in Section 3.3.3 (Shugart & King, 2016; United States Nuclear Regulatory Commission, 2016).

We reduce the computation time to find solutions to Problems 1-3 compared to SGA by using simulation-optimization and integer-programming techniques. SOCA eliminates the overhead time SGA spends initializing each configuration. SGA uses “blocks,” i.e., independent groups of computer code, to input data, perform calculations, and produce results. This requires additional time to pass information between blocks and memory to store all of the required information the blocks generate. By contrast, SOCA executes calculations and evaluates results as necessary, and discards information as soon as possible to reduce computation time and memory requirements. SOCA replicates the CUMUF test in parallel to further reduce computation time and provides solutions with a pre-specified level of confidence. MVCM decreases the number of variables and constraints required to find the same measurement system configuration by utilizing the relationship between the population variance of the estimated MUF and the weighted sum of Type I and Type II error probabilities. In addition, MVCM exploits a branch-and-bound algorithm to avoid completely enumerating solutions (Land & Doig, 1960). Table 3.1 summarizes the models in
Table 3.1: **NUMSO** model summary

<table>
<thead>
<tr>
<th>Toolkit</th>
<th>Elements included</th>
<th>Element type</th>
<th>Objective</th>
<th>Statistical test</th>
<th>Detection threshold</th>
<th>Problems solved</th>
</tr>
</thead>
<tbody>
<tr>
<td>NUMSO</td>
<td></td>
<td>Simulation optimization</td>
<td>Minimize the weighted sum of Type I and Type II error probabilities</td>
<td>CUMUF</td>
<td>Fixed, optimized</td>
<td>1-3</td>
</tr>
<tr>
<td>MVCM</td>
<td>Integer program</td>
<td></td>
<td>Minimize the population variance of the estimated MUF</td>
<td>None</td>
<td>None</td>
<td>1</td>
</tr>
</tbody>
</table>

To the best of our knowledge, **NUMSO** is the first customizable toolkit that evaluates multiple, feasible measurement system configurations in a single execution and identifies the best one with high confidence. In addition, we are the first to employ an optimized detection threshold to reduce the weighted sum of Type I and Type II error probabilities and to provide a measurement system configuration heuristic based on minimizing the population variance of the estimated MUF to further reduce the computation time for Problem 1.

The rest of this paper is organized as follows: Section 4.4 discusses relevant background material including important definitions and key concepts related to nuclear safeguards; Section 3.4 contains preliminary technical information; in Sections 3.5 and 3.6, we detail **SOCA** and **MVCM**, respectively; we present and analyze results in Section 4.6 and provide conclusions and discussion of future work in Section 4.8.

### 3.3 Background

The International Atomic Energy Agency implements a group of activities, called nuclear safeguards, which try to ensure that its 140 member states are not using their civilian nuclear fuel cycles to produce nuclear weapons (International Atomic Energy Agency, 2016). One type of nuclear safeguard, material control and accountability (MC&A) attempts to prevent the illicit acquisition of nuclear materials, such as enriched uranium, and the subsequent development of weapons, by detecting and deterring the loss of these materials from within a nuclear fuel cycle (U.S. Department of Energy, 2011). Material control tries to prevent the unapproved removal of nuclear materials
from authorized locations or to detect their absence in a timely manner. Material accountability ensures that there is an accurate record of material within nuclear fuel cycle facilities (U.S. Department of Energy, 2011). Combined, these branches of MC&A establish the measurement and inventory balance of nuclear material at one or more facilities (International Atomic Energy Agency, 2002).

Measurements are the primary means to ensure that nuclear material is not lost from a facility; thus, accountability measurements, which establish initial values of nuclear material, and verification measurements, which authenticate the amount of material present, must be as precise as possible. One of the primary objectives of MC&A is to provide material estimates that enable detecting the loss or diversion of nuclear material despite uncertainties in those values (U.S. Department of Energy, 2011). NUMSO identifies measurement system configurations that provide accurate estimates of material quantities by (i) minimizing the weighted sum of Type I error probabilities for a specific diversion or non-diversion context and (ii) minimizing the population variance of the estimated MUF.

3.3.1 Nuclear Fuel Cycle

To further understand MC&A and its role in safeguarding nuclear material, we describe the primary stages of the current nuclear fuel cycle in the United States: mining and milling, conversion, enrichment, fuel fabrication, reactor power production, spent fuel management, reprocessing (when appropriate), and final disposal. Natural uranium is mined from the ground as ore with approximate isotope concentrations of 0.006 atomic percent (at.%) uranium-234, 0.72 at.% uranium-235, and 99.27 at.% uranium-238 (Smith Jr, 1991). The uranium is milled, usually on-site, into uranium oxide concentrate, also known as “yellowcake,” and then transported to a conversion facility where it is processed into uranium hexafluoride. The uranium-235 in the uranium hexafluoride is then enriched to 3.5-5.0 at.%. Enriched uranium is generally required to generate nuclear power, and highly enriched uranium (>20 at.% uranium-235) is needed to make nuclear weapons.
After enrichment, the uranium is converted back into uranium oxide and formed into ceramic pellets. Fuel rods, i.e., metal tubes packed with ceramic pellets, are arranged into an assembly that comprises part of a reactor core along with several hundred other assemblies. A chain reaction occurs when the uranium-235 fissions, or splits, which heats the water surrounding the fuel rods. The hot water becomes steam, which drives a turbine and generator to produce electricity (World Nuclear Association, 2016a).

Used fuel from the reactor, i.e., a collection of fuel rods with depleted energy value, is placed in a storage pond to reduce the radiation levels and high heat content from radioactive decay. As a storage pond approaches capacity, some of the older used fuel that has been cooling for at least five years is put into dry casks and stockpiled above ground (United States Nuclear Regulatory Commission, 2015). The used fuel remains in storage ponds or dry casks for 40-50 years before it is either reprocessed or permanently disposed. Several countries (including France, the United Kingdom, and Germany) reprocess their used fuel, while other countries (such as Canada, Finland, Sweden, and the United States) plan to permanently dispose of it. Canada and Finland intend to start placing their waste in deep geologic repositories by 2025 and 2023, respectively (World Nuclear Association, 2016b).

### 3.3.2 MC&A Measurement System

A measurement system is used to estimate material entering (i.e., receipts) and exiting (i.e., shipments) one or more nuclear fuel cycle facilities, in addition to deriving estimates for all batch quantities of material present at each facility (i.e., physical inventory). The estimated MUF is the difference between measured shipments and the sum of measured receipt and physical inventory quantities. Even if no material is lost from the system, the estimated MUF is rarely zero because of measurement errors.

It is necessary, therefore, to properly account for the errors that occur when measurements are taken to assess the statistical significance of any differences between what is assumed to be and what is found in a facility (U.S. Department of Energy, 2011). A random error is a positive
or negative fluctuation from the true quantity that is caused by limitations to the precision of the measurement device. A systematic error is a unidirectional bias that can be caused by improper use or function of a measurement device resulting in a shift of the measurement from the true quantity.

To model random errors, we obtain SOCA samples from a uniform distribution associated with each device to compare results with Shugart & King (2016). Many applications, however, use normal distributions to model random measurement errors (Bronshtein & Semendyayev, 2015, p. 849); to maintain flexibility in SOCA, we allow distributions and their parameters (e.g., bounds, mean, variance) to change depending on the properties of the actual devices utilized in a measurement system. We omit systematic errors in our analysis for simplicity.

An MC&A system uses MBAs and key measurement points to identify boundaries and locations, respectively, at which measurements are taken. An MBA represents a facility or subset of a facility provided that (1) the amount transferred into or out of the MBA can be quantified and (2) the physical inventory within the MBA can be quantified “when necessary” (International Atomic Energy Agency, 2002). For example, an MBA can be an entire enrichment facility or an individual centrifuge. In practice, most facilities in a nuclear fuel cycle comprise a single MBA; however, complex manufacturing and reprocessing plants might require two or more MBAs to adequately model activities (International Atomic Energy Agency, 2008).

The ability to recognize a substantial material loss with high probability is required to establish an MC&A system’s effectiveness (de Montmollin & Weinstock, 1979). We analyze a constant, low-level diversion over an extended time horizon because, according to Burr (1994), this is a worst-case loss context in terms of detection probability. To discover a hypothetical worst-case material loss, we estimate CMUF because it may be difficult to detect small diversions with estimated MUF. Statistical tests typically use estimated CMUF to identify material loss (Beedgen, 1988; Leitner et al., 1987; Seifert, 1986).

SOCA evaluates a fixed-period CUMUF test because it yields the maximum detection probability against a worst-case loss context (Avenhaus & Jaech, 1981). SOCA evaluates this test over a single time horizon, which is applicable because in practice, there are usually infrequent material
balance evaluations, e.g., once per year (Burr & Hamada, 2013).

A potential problem with fixed-period tests is that a diversion can occur over multiple time horizons. To address this, Burr & Hamada (2013) use two data-driven tests over multiple time horizons: (i) MUF Shewhart and (ii) standardized, independently transformed MUF. SOCA is able to evaluate these and other statistical tests discussed in Seifert (1986), Gale (1986), Leitner et al. (1987), Beedgen (1988), Jacobson (1992), Burr & Hamada (2013), and Shugart & King (2016).

SOCA uses a material balance equation to estimate the MUF $\tilde{M}_t$ and CMUF $\tilde{C}_t$ at the end of each time period $t$ during a finite, discrete time horizon $\mathcal{T} = \{1, ..., T\}$. Measured receipts, shipments, and physical inventory are random variables $\tilde{R}_t$, $\tilde{S}_t$, and $\tilde{I}_t$, respectively, because measurements introduce random errors. We assume that $\tilde{I}_0$ is the estimated inventory at the beginning of $t = 1$.

\[
\begin{align*}
\tilde{M}_t &= \tilde{I}_{t-1} + \tilde{R}_t - \tilde{S}_t - \tilde{I}_t & \forall t \in \mathcal{T} \\
\tilde{C}_t &= \sum_{\tau=1}^{t} \tilde{M}_\tau & \forall t \in \mathcal{T}
\end{align*}
\]

(3.1) (3.2)

We also assume that the length of the time horizon $T$ is set according to timeliness detection goal limits, which are used in conjunction with significant quantity limits to define the amount of time and material required to signify a consequential diversion. We use a material loss of significant quantity/timeliness goal in each period during the time horizon to represent a constant, low-level diversion. The “target detection times applicable to specific nuclear material categories” define timeliness goals. A significant quantity is “the approximate amount of nuclear material for which the possibility of manufacturing a nuclear explosive device cannot be excluded.” Table 4.2 shows the timeliness detection goal and significant quantity limits provided by the International Atomic Energy Agency for the primary nuclear materials of concern in MC&A (International Atomic Energy Agency, 2002).
Table 3.2: Significant quantities of nuclear materials with their associated timeliness goals

<table>
<thead>
<tr>
<th>Material</th>
<th>Material form</th>
<th>Significant quantity</th>
<th>Timeliness detection goal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plutonium</td>
<td>Metal Irradiated fuel</td>
<td>8 kg</td>
<td>1 month 3 months</td>
</tr>
<tr>
<td>Uranium-233</td>
<td>Metal Irradiated fuel</td>
<td>8 kg</td>
<td>1 month 3 months</td>
</tr>
<tr>
<td>High-enriched uranium (uranium-235 ≥ 20 at.%)</td>
<td>Metal Irradiated fuel</td>
<td>25 kg</td>
<td>1 month 3 months</td>
</tr>
<tr>
<td>Low-enriched uranium (uranium-235 &lt; 20 at.%)</td>
<td>Unirradiated fresh fuel</td>
<td>75 kg uranium-235, 10 metric tons natural uranium, or 20 metric tons depleted uranium</td>
<td>1 year</td>
</tr>
<tr>
<td>Thorium</td>
<td>Unirradiated fresh fuel</td>
<td>20 metric tons</td>
<td>1 year</td>
</tr>
</tbody>
</table>

3.3.3 Enrichment Facility Material Balance Area

We can model different types of nuclear fuel cycle facilities and evaluate the loss of different nuclear materials with NUMSO. For example, we can use a uranium-oxide fuel fabrication or production facility to evaluate uranium loss. To assess plutonium loss, we can model a mixed-oxide fuel fabrication or conversion facility.

Figure 3.1 is a visual representation of material balance components at an example enrichment facility, which is shown as a single MBA with a potential material loss stream and input, output, tails, and cascade key measurement points.
In this example, uranium hexafluoride enters the MBA with naturally occurring uranium isotope concentrations and leaves the MBA with a much higher concentration of uranium-235. The tails stream contains depleted (<0.72 at.%) uranium-235 from the uranium enrichment process and the inventory represents the batch quantity of material currently in the enrichment cascade, i.e., series of centrifuges used to enrich the uranium. We assume that the output stream is the most likely location for a diversion to occur because it contains enriched uranium rather than unenriched uranium present in the other streams. Table 3.3 shows approximate material quantities used in the enrichment facility example.

Table 3.3: Example enrichment facility material quantities

<table>
<thead>
<tr>
<th>Key measurement point</th>
<th>Material quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Input</td>
<td>10.058 kg/day</td>
</tr>
<tr>
<td>Output</td>
<td>6.9237 kg/day</td>
</tr>
<tr>
<td>Tails</td>
<td>3.1341 kg/day</td>
</tr>
<tr>
<td>Cascade</td>
<td>3620.8 kg</td>
</tr>
</tbody>
</table>

3.4 Technical Preliminaries

SOCA uses a hypothesis test based on a discrete stochastic process to identify if there is enough statistical evidence to indicate whether a constant, low-level hypothetical diversion occurs. We assume that the true CMUF $C_t$ is a non-random, but unknown, temporally indexed and non-decreasing function. The non-exhaustive hypotheses are the null hypothesis $H_0$ that there is no material loss in any time period in the time horizon, and the alternate hypothesis $H_1$ that the quantity of material loss is greater than a fixed detection threshold $\lambda > 0$ at some time $k$ in the horizon.

$$H_0 : C_t = 0 \quad \text{for all } t = 1, \ldots, T$$

$$H_1 : C_t \geq \lambda \quad \text{for } t = k, \ldots, T \text{ for some } 1 \leq k \leq T$$

Type I and Type II error probabilities determine the effectiveness of a current or proposed MC&A strategy (e.g., a new measurement system configuration) regarding the detection of a di-
version. To test these hypotheses, we create a rejection rule \( \tilde{C}_t \geq \lambda \). Under this rejection rule, a Type I error occurs if \( \tilde{C}_t \geq \lambda \) for any \( t = 1, \ldots, T \) when \( C_t = 0 \) for all \( t = 1, \ldots, T \), and a Type II error occurs if \( \tilde{C}_t < \lambda \) for all \( t = 1, \ldots, T \) when \( C_t \geq \lambda \), for \( t = k, \ldots, T \) for some \( 1 \leq k \leq T \). We denote the Type I and Type II error probabilities as \( \alpha \) and \( \beta \), respectively.

SOCA indicates that a hypothetical diversion likely occurs if the estimated CMUF exceeds the detection threshold in any period during the time horizon. It is important to note, however, that an actual diversion does not necessarily occur in practice even if the estimated CMUF exceeds the detection threshold; in this case, determining the cause of the alarm requires additional analysis (U.S. Congress, Office of Technology Assessment, 1995). For a worst-case loss context, we use a fixed detection threshold \( \lambda \) that is equivalent to a significant quantity for low-enriched uranium and allow the optimized detection threshold \( \lambda \), in contrast to \( \lambda \), to vary from zero to a significant quantity. We present four modeling paradigms, M1-M4, that SOCA can incorporate to evaluate Type I and Type II error probabilities.

In nuclear safeguards, a Type I error requires time and resources to investigate its cause. It is possible to decrease the probability of a Type I error (\( \alpha \)) by increasing the detection threshold, which undesirably results in a lower probability of identifying an actual diversion (de Montmollin & Weinstock, 1979). Thus, it might be advantageous to limit \( \alpha \) to a sufficiently low value (e.g., \( \leq 0.05 \)) and then maximize the detection probability \( (1 - \beta) \), which reduces the number of Type I errors that must be investigated (International Atomic Energy Agency, 2002); equivalently, we can minimize the probability of Type II errors (\( \beta \)). Others recommend that \( \alpha \) be constrained to 1% or less because, even though lowering the probability of Type I errors decreases the detection probability, the external consequences of a Type I error are higher than of a reduced detection probability (de Montmollin & Weinstock, 1979). We introduce M1 and M2 to identify with high probability the best measurement system configuration by minimizing \( \beta \) and constraining \( \alpha \) to a fixed significance level \( \alpha \).

Minimizing the probability of Type II errors while controlling for the probability of Type I errors is known as the Neyman-Pearson paradigm (Neyman & Pearson, 1933). M1 and M2 deviate from
the Neyman-Pearson paradigm because we minimize Type II errors over a time horizon instead of over a single point in time. We use the following notation in M1 and M2.

Sets
\( \mathcal{X} \) measurement system configurations

Parameters
\( \lambda \) fixed detection threshold (kg)
\( \alpha \) fixed significance level, e.g., 0.05
\( \gamma \) relative importance of Type I and Type II errors; \( 0 \leq \gamma \leq 1 \)

Variables
\( x \) measurement system configuration
\( \lambda \) optimized detection threshold (kg)
\( \alpha(x, \lambda) \) probability of a Type I error at detection threshold \( \lambda \) for measurement system configuration \( x \)
\( \beta(x, \lambda) \) probability of a Type II error at detection threshold \( \lambda \) for measurement system configuration \( x \)

M1

\[
\begin{align*}
\min_{x \in \mathcal{X}} & \quad \beta(x, \lambda) \\
\text{s.t.} & \quad \alpha(x, \lambda) \leq \alpha
\end{align*}
\] (3.5) (3.6)

It is important to choose the fixed detection threshold \( \lambda \) carefully because a universally applied detection threshold cannot adequately meet the needs of individual MBAs. Some researchers note that while the significant quantity values provided by the International Atomic Energy Agency might be “satisfactory,” they can be easily exceeded by accumulating only random errors in large-throughput bulk processing plants, such as reprocessing facilities. They suggest that the detection threshold should be set based on unique measurement system properties (e.g., material quantities), rather than on external consequences (de Montmollin & Weinstock, 1979). Beedgen (1988) uses Monte Carlo methods to estimate a fixed detection threshold based on a significance level \( \alpha \). We use an optimized detection threshold in M2, which provides the threshold that gives the lowest Type II error probability.
A competing paradigm minimizes a weighted sum of Type I and Type II error probabilities (DeGroot & Schervish, 2012, p. 552). On one hand, detecting a diversion can be less detrimental than acting on a Type I error; on the other, identifying a diversion is an important consideration (de Montmollin & Weinstock, 1979). Pericchi & Pereira (2013) note that the downside to the Neyman-Pearson paradigm is that the Type I error probability is always as close to the significance level as possible. They conclude that minimizing a weighted sum of errors is “superior” to the Neyman-Pearson paradigm because both types of errors converge to zero as the evidence for a hypothesis grows, resulting in a consistent method. We introduce M3 and M4 to minimize the weighted sum of Type I and Type II error probabilities.

Some models benefit from having a different relative importance for Type I and Type II error probabilities. Because of the severity of each outcome, Alesina & Ferrara (2011) minimize a weighted average of $\alpha$ and $\beta$ to test for bias in judicial errors based on race. Their model places different importance on the probability of condemning an innocent ($\alpha$) and of letting a guilty person free ($\beta$). In MC&A, $\alpha$ and $\beta$ are also both detrimental outcomes; therefore, M3 considers them simultaneously using a fixed detection threshold.

M3

\[
\min_{x \in \mathcal{X}} \gamma \alpha(x, \lambda) + (1 - \gamma) \beta(x, \lambda) \tag{3.9}
\]

Similarly, M4 minimizes a weighted sum of Type I and Type II error probabilities with an optimized detection threshold.
\[
\min_{x \in \mathcal{X}, \lambda \geq 0} \gamma \alpha(x, \lambda) + (1 - \gamma) \beta(x, \lambda)
\]  

(3.10)

3.5 Simulation Optimization Configuration Algorithm

We develop the Simulation Optimization Configuration Algorithm (SOCA), coded in C++, to find the optimal measurement system configuration with confidence level \(1 - \varepsilon\) based on the constructs in M1-M4. For brevity, we only present pseudocode for incorporating M4; however, SOCA can implement M1-M3 constructs with a few changes. M1 and M2 require a different objective than M4; they also require constraints to ensure that the Type I error probability does not exceed the fixed significance level \(\alpha\). M3 is a simpler version of M4 because it uses a fixed detection threshold \(\lambda\), rather than an optimized detection threshold \(\lambda\).

In addition to including the constructs of M1-M4, SOCA simulates measurement device placement limitations, material balance equations, and Type I and Type II error probabilities. Each feasible measurement system configuration consists of possible device placements at valid key measurement points. Material balance equations estimate CMUF using simulated receipt, shipment, and inventory material measurements. A CUMUF test compares the estimated CMUF to fixed and optimized detection thresholds for various measurement error samples in hypothetical non-diversion and diversion contexts, which yields Type I and Type II error probabilities. SOCA replicates this process and uses components from the BEST algorithm (Sanchez & Wood, 2006) to identify the measurement system configuration that minimizes a weighted sum of Type I and Type II error probabilities with confidence level \(1 - \varepsilon\).

The stochastic nature of SOCA means we can only guarantee that our solution is optimal within a pre-specified confidence level. We capture stochastic behavior in an optimization framework by employing scenario generation, specifically, Monte Carlo sampling using independent and identically distributed random measurement error samples. SOCA implements common random numbers by using the same samples (representing different instances of random measurement errors) to
evaluate each measurement system configuration; this approach reduces variance in a simulation model (Sanchez & Wood, 2006).

To determine an optimized detection threshold, SOCA evaluates a weighted sum of Type I and Type II error probabilities using a series of detection thresholds ranging from zero to a significant quantity, incrementing the thresholds by a pre-defined amount. Section 4.6 compares two different increments to show potential variations in computation time and objective values.

### 3.5.1 SOCA Description

We present pseudocode which details the process by which SOCA obtains the measurement system configuration that minimizes the weighted sum of Type I and Type II error probabilities using an optimized detection threshold. First, we obtain a single replication of measurement error samples. Sanchez & Wood (2006) suggest that the number of replications be at least 1,000 for other applications. They also note that the number of samples included in each replication cannot be determined a priori; however, they point to Efron & Tibshirani (1994) who use a bootstrapping technique with a sample size as small as nine. We use 1,000 independent replications that each contain 1,000 measurement error samples in a diversion context and 1,000 measurement error samples in a non-diversion context. Then, we evaluate the results from each replication with components from the BEST algorithm (Sanchez & Wood, 2006) to provide an optimal measurement system configuration with a pre-specified confidence level $1 - \varepsilon$. We parallelize replications to reduce the computation time.

We add the following notation to describe SOCA:
Sets
\( k \in \mathcal{K} \) key measurement points
\( \mathcal{K}^R \subset \mathcal{K} \) receipt key measurement points
\( \mathcal{K}^S \subset \mathcal{K} \) shipment key measurement points
\( \mathcal{K}^I \subset \mathcal{K} \) inventory key measurement points
\( t \in \mathcal{T} \) time periods, e.g., days over the course of one year
\( \omega \in \Omega \) instances of measurement error samples
\( \Omega^N \subset \Omega \) instances of measurement error samples in a non-diversion context
\( \Omega^D \subset \Omega \) instances of measurement error samples in a diversion context
\( d \in \mathcal{D} \) measurement devices
\( d \in \hat{\mathcal{D}}_k \) measurement devices that can be utilized at key measurement point \( k \)
\( \mathcal{X}^* \subset \mathcal{X} \) optimal measurement system configurations

Parameters
\( R_{kt} \) true receipts at key measurement point \( k \) and time \( t \) (kg)
\( S_{kt} \) true shipments at key measurement point \( k \) and time \( t \) (kg)
\( I_{kt} \) true inventory at key measurement point \( k \) and time \( t \) (kg)
\( \tilde{e}_{k\omega t} \) random error for sample \( \omega \) at key measurement point \( k \) in time \( t \) (kg)
\( \hat{e}_d \) measurement error scaling factor for measurement device \( d \)
\( \hat{\lambda} \) maximum optimized detection threshold, e.g., one significant quantity for uranium-235 (kg)
\( \hat{\lambda} \) optimized detection threshold increment, e.g., one kilogram (kg)
\( 1 - \alpha_1 \) confidence level for the measurement system configuration from Test1 in the BEST algorithm
\( 1 - \alpha_2 \) confidence level for the measurement system configuration from Test2 in the BEST algorithm
\( 1 - \varepsilon \) overall confidence level for the optimal measurement system configuration

Continuous Variables
\( \tilde{R}_{kd\omega t} \) measured receipts for sample \( \omega \) at key measurement point \( k \) utilizing device \( d \) in time \( t \) (kg)
\( \tilde{S}_{kd\omega t} \) measured shipments for sample \( \omega \) at key measurement point \( k \) utilizing device \( d \) in time \( t \) (kg)
\( \tilde{I}_{kd\omega t} \) measured inventory for sample \( \omega \) at key measurement point \( k \) utilizing device \( d \) in time \( t \) (kg)
\( \tilde{M}_{\omega t} \) estimated MUF for sample \( \omega \) in time \( t \) (kg)
\( \tilde{C}_{\omega t} \) estimated CMUF for sample \( \omega \) in time \( t \) (kg)

Integer Variables
\( N^I(x, \lambda) \) number of simulated Type I errors that occur for measurement system configuration \( x \) and detection threshold \( \lambda \)
\( N^H(x, \lambda) \) number of simulated Type II errors that occur for measurement system configuration \( x \) and detection threshold \( \lambda \)
We extend Equations (3.1) and (3.2) to include measurement error samples and multiple key measurement points for receipts, shipments, and inventories in Equations (3.11) and (3.12), respectively. Equation (3.13) shows that the random variable for measured receipts is composed of the true material quantity and a percent-based, scaled random measurement error. Similar equations apply to shipments \( \tilde{S}_{kd\omega t} \) and inventory \( \tilde{I}_{kd\omega t} \). We assume the true material quantities \( R_{kt}, S_{kt}, \) and \( I_{kt} \) are obtained from an independent fuel cycle simulation, such as the Verifiable Fuel Cycle Simulation (VISION) model (Jacobson & Yacout, 2010).

\[
\tilde{M}_{\omega t} = \sum_{k \in \mathcal{X}} \sum_{d \in \tilde{D}_k} \tilde{R}_{kd\omega t} + \sum_{k \in \mathcal{X}} \sum_{d \in \tilde{D}_k} (\tilde{I}_{kd\omega t} - \tilde{I}_{kd\omega t}) - \sum_{k \in \mathcal{X}} \sum_{d \in \tilde{D}_k} \tilde{S}_{kd\omega t} \quad \forall \omega \in \Omega, t \in T \quad (3.11)
\]

\[
\tilde{C}_{\omega t} = \sum_{\tau=1}^{t} \tilde{M}_{\omega \tau} \quad \forall \omega \in \Omega, t \in T \quad (3.12)
\]

\[
\tilde{R}_{kd\omega t} = R_{kt}(1 + \hat{e}_d\hat{e}_{kd\omega}) \quad \forall k \in \mathcal{X}, d \in \tilde{D}_k, \omega \in \Omega, t \in T \quad (3.13)
\]

In the pseudo-code for SOCA, the CUMUF test compares the estimated CMUF to optimized detection thresholds to determine if there are Type I or Type II errors for each measurement error sample in non-diversion and diversion contexts. A simplified version of the Test procedure from the BEST algorithm (further described in Section 3.5.2) identifies the optimal measurement system configuration and optimized detection threshold with confidence level \( 1 - \varepsilon \) by comparing the Type I and Type II error probabilities that result from replicating the CUMUF test.
SOCA Pseudo-code

Description: Replicate CUMUF tests using measurement error samples in diversion and non-diversion contexts
Input: Values for relevant sets and parameters presented in Sections 3.4 and 3.5.1
Output: The measurement system configuration and optimized detection threshold that yield the lowest weighted sum of Type I and Type II error probabilities with confidence level $1 - \varepsilon$

1: // Perform an independent replication of measurement error samples
2: procedure CUMUF Test(All inputs)
3:  for each measurement system configuration $x \in \mathcal{X}$ := \{(k,d) where k \in \mathcal{K} and d \in \mathcal{D}_k\} do
4:   for each instance of measurement error samples $\omega \in \Omega^N \subset \Omega$ or $\Omega^D \subset \Omega$ do
5:      $\delta_{\omega}(x,\lambda) \leftarrow 0$
6:   for each time period $t \in \mathcal{T}$ do
7:      Draw an independent random error $\tilde{e}_{kat} \sim \text{Uniform}(-1,1)$ for every $k$; scale the errors with $\hat{e}_d$
8:      Calculate the measured receipts $\tilde{R}_{katd}$ with Equation (3.13); obtain $\tilde{S}_{katd}$ and $\tilde{I}_{katd}$ similarly
9:      Estimate the MUF $\bar{M}_{kat}$ and CMUF $\bar{C}_{kat}$ using Equations (3.11) and (3.12), respectively
10: // Set a flag if the estimated CMUF exceeds a detection threshold
11: $\lambda \leftarrow 0$
12: while $\lambda < \bar{\lambda}$ do
13:   if $\bar{C}_{kat} > \lambda$ then
14:      $\delta_{\omega}(x,\lambda) \leftarrow 1$
15:      $\lambda \leftarrow \lambda + \hat{\lambda}$
16: // Calculate the number of Type I and Type II errors
17: $N^I(x,\lambda) \leftarrow \sum_{\omega \in \Omega^N} \delta_{\omega}(x,\lambda); N^{II}(x,\lambda) \leftarrow \sum_{\omega \in \Omega^D} (1 - \delta_{\omega}(x,\lambda))$
18: // Perform the Test procedure from BEST; this is a simplified representation
19: procedure SIMPLIFIED Test(Number of replications $R$)
20: $1 - \varepsilon \leftarrow 1 - (\alpha_1 + \alpha_2)$
21: // Test1 from the BEST algorithm
22: for each replication 1,\ldots, $R$ do
23:   Obtain $N^I(x,\lambda)$ and $N^{II}(x,\lambda)$ from CUMUF Test
24: // Calculate the Type I and Type II error probabilities
25: $\alpha(x,\lambda) \leftarrow N^I(x,\lambda)/|\Omega^N|; \beta(x,\lambda) \leftarrow N^{II}(x,\lambda)/|\Omega^D|$
26: Identify all $(x,\lambda)$ that minimize $\gamma \alpha(x,\lambda) + (1 - \gamma) \beta(x,\lambda)$
27: for $x \in \mathcal{X}$ do
28:   if $x$ is optimal in $100 \cdot (1 - \alpha_1)\%$ of replications then
29:      $\mathcal{X}^* \leftarrow \mathcal{X}^* \cup \{x\}$
30: if $|\mathcal{X}^*| = 1$ then
31:   $x \in \mathcal{X}^*$ is optimal with confidence $1 - \alpha_1$
32: else
33:   Implement Test2 from the BEST algorithm to ensure $x$ is optimal with confidence $(1 - \alpha_1)(1 - \alpha_2)$
34: Measurement system configuration $x$ is optimal with confidence $1 - \varepsilon$

3.5.2 BEST Algorithm

In general, the BEST algorithm identifies a probabilistic upper Bound on the optimal objective function value and a deterministic lower-bounding function, Enumerates a set of first-stage solutions, Simulates second-stage outcomes, and Tests the simulated outcomes to identify the first-stage solution with a pre-specified level of confidence. We use the Test procedure from the BEST
algorithm in Sanchez & Wood (2006) to evaluate solutions from SOCA. We obtain measurement system configurations (corresponding to first-stage solutions) and the number of Type I and Type II errors (corresponding to second-stage outcomes) from the CUMUF test in SOCA, which enables us to bypass the Bound, Enumerate, and Simulate steps.

In the Test procedure, we evaluate each measurement system configuration via subset selection to eliminate configurations from $\mathcal{X}$ that are unlikely to be optimal. We assess independent replications of CUMUF tests using a bootstrap screening method, i.e., Test1 in Sanchez & Wood (2006), which ranks each configuration based on the number of replications in which the configuration gives the lowest weighted sum of Type I and Type II error probabilities. The subset of configurations, $\mathcal{X}^* \subset \mathcal{X}$, that yields the best solution in $100 \cdot (1 - \alpha_1)$% of replications contains the optimal solution with a pre-specified confidence level of $1 - \alpha_1$.

If $|\mathcal{X}^*| = 1$, then $x \in \mathcal{X}^*$ is optimal with confidence $1 - \alpha_1$. However, if there is more than one element in $\mathcal{X}^*$, we can use an additional method, i.e., Test2 in Sanchez & Wood (2006), to determine how many additional measurement error samples are needed in the CUMUF test to ensure that the best solution from Test1 is $\varepsilon$-optimal with approximate confidence $(1 - \alpha_1)(1 - \alpha_2)$. We do not show Test2 in the pseudocode because it is unlikely $\mathcal{X}^*$ contains more than one element for the system we analyze in this paper. We choose $\alpha_1$ and $\alpha_2$ so that the fixed, overall confidence level $1 - \varepsilon$ is equivalent to $1 - (\alpha_1 + \alpha_2)$.

3.6 Minimum Variance Configuration Model

The Minimum Variance Configuration Model (MVCM) finds a measurement system configuration that minimizes the population variance of the estimated MUF in a system over a fixed, discrete time horizon. Reducing measurement uncertainty enables us to more accurately estimate true material quantities. The purpose of MVCM is to find a configuration that produces a comparable weighted sum of Type I and Type II error probabilities to the configuration from SOCA. Section 4.6 shows that MVCM obtains the same optimal configuration as SOCA, but more quickly.
MVCM is a deterministic integer program, which simplifies the stochastic complexities present in SOCA, such as samples of random measurement errors. MVCM decreases the number of variables and constraints required in SOCA to find the same measurement system configuration by utilizing the relationship between the population variance of the estimated MUF and the weighted sum of Type I and Type II error probabilities. In addition, MVCM exploits a branch-and-bound algorithm to avoid completely enumerating solutions (Land & Doig, 1960). These attributes enable MVCM to solve faster than SOCA.

Appendix A shows how the population variance of the estimated MUF relates to Type I and Type II error probabilities. We conclude that lowering the random measurement error within $\tilde{C}_t$ provides a lower Type I error probability at a given key measurement point before any time $t$, but may not lower the Type II error probability. However, in Section 4.6, we show empirically that a weighted sum of Type I and Type II error probabilities is lowered for our single enrichment facility example considering one material in a worst-case loss context.

MVCM requires the following notation modifications:

**Additional Sets**
$k \in \tilde{K}_d$ key measurement points at which device $d$ can be utilized

**Additional and Modified Parameters**
$\tilde{e}_{dt}$ random variable corresponding to $\tilde{e}_{d\omega t}$ (kg)
$\sigma_{dt}^2$ variance of error measurements for device $d$ in time period $t$ (kg$^2$)

**Modified Variables**
$\tilde{R}_{kdt}$ random variable corresponding to $\tilde{R}_{k\omega t}$ (kg)
$\tilde{S}_{kdt}$ random variable corresponding to $\tilde{S}_{k\omega t}$ (kg)
$\tilde{I}_{kdt}$ random variable corresponding to $\tilde{I}_{k\omega t}$ (kg)

**Binary Variables**
$x_{kd}$ 1 if measurement device $d$ is utilized at key measurement point $k$; 0 otherwise
MVCM

\[
\min \sum_{t \in \mathcal{T}} \left( \sum_{k \in \mathcal{K}} \sum_{d \in \mathcal{D}_k} R_{kt}^2 \sigma_{d,t}^2 x_{kd} + \sum_{k \in \mathcal{K}^I} \sum_{d \in \mathcal{D}_k} l_{kt}^2 \sigma_{d,s}^2 + \sum_{k \in \mathcal{K}^S} \sum_{d \in \mathcal{D}_k} s_{kt}^2 \sigma_{d,s}^2 x_{kd} \right) \quad (3.14)
\]

Variables in the model are subject to the following constraints:

\[
\sum_{k \in \mathcal{K}_d} x_{kd} = 1 \quad \forall \ d \in \mathcal{D} \quad (3.15)
\]

\[
\sum_{d \in \mathcal{D}_k} x_{kd} = 1 \quad \forall \ k \in \mathcal{K} \quad (3.16)
\]

\[
x_{kd} \text{ binary} \quad \forall \ k \in \mathcal{K}, d \in \mathcal{D} \quad (3.17)
\]

Objective (3.14) minimizes the population variance of the estimated MUF in the measurement system over the time horizon. Equation (3.18) restates Equation (3.11), except that it uses random variables rather than their realizations. Equation (3.19) represents the population variance.

\[
\tilde{M}_t = \sum_{k \in \mathcal{K}^R} \sum_{d \in \mathcal{D}_k} \tilde{R}_{k,d} + \sum_{k \in \mathcal{K}^I} \sum_{d \in \mathcal{D}_k} (\tilde{I}_{k,d},t - 1 - \tilde{I}_{k,d}) - \sum_{k \in \mathcal{K}^S} \sum_{d \in \mathcal{D}_k} \tilde{S}_{k,d} \quad \forall \ t \in \mathcal{T} \quad (3.18)
\]

\[
\sigma^2(\sum_{t \in \mathcal{T}} \tilde{M}_t) = \sigma^2(\sum_{k \in \mathcal{K}^R} \sum_{d \in \mathcal{D}_k} \sum_{t \in \mathcal{T}} \tilde{R}_{k,d} + \sum_{k \in \mathcal{K}^I} \sum_{d \in \mathcal{D}_k} \sum_{t \in \mathcal{T}} (\tilde{I}_{k,d},t - 1 - \tilde{I}_{k,d})) + \sigma^2(\sum_{k \in \mathcal{K}^S} \sum_{d \in \mathcal{D}_k} \sum_{t \in \mathcal{T}} \tilde{S}_{k,d}) \quad (3.19)
\]

Equation (3.20) shows that the random variable for measured receipts is composed of the true material quantity \( R_{kt} \) and a percent-based random measurement error \( \tilde{e}_{dt} \). Equation (3.21) computes the variance of the random measurement error as \( \sigma^2_{d,t} \). The variance for the receipt measurement then simplifies to Equation (3.22), which is based only on the true material quantity and the variance of the random measurement error. The same method follows for shipment and inventory measurements. We assume a constant, non-measured beginning inventory for every time period, which reduces the inventory measurement variance to the single term seen in Objective (3.14), instead of collapsing to \( \sum_{k \in \mathcal{K}^I} \sum_{d \in \mathcal{D}_k} (I_{k,0}^2 \sigma_{k,0}^2 - I_{k,|\mathcal{T}|}^2 \sigma_{k,|\mathcal{T}|}^2) x_{kd} \).
\[
\sum_{k \in K} \sum_{d \in \hat{D}} \sum_{t \in T} \bar{R}_{kdt} = \sum_{k \in K} \sum_{d \in \hat{D}} \sum_{t \in T} R_{kt}(1 + \tilde{e}_{dt})x_{kd}
\] (3.20)

\[
\sigma^2\left(\sum_{k \in K} \sum_{d \in \hat{D}} \sum_{t \in T} \tilde{e}_{dt}\right) = \sum_{k \in K} \sum_{d \in \hat{D}} \sum_{t \in T} \sigma^2_{dt}
\] (3.21)

\[
\sigma^2\left(\sum_{k \in K} \sum_{d \in \hat{D}} \sum_{t \in T} \bar{R}_{kdt}\right) = \sum_{k \in K} \sum_{d \in \hat{D}} \sum_{t \in T} R_{kt}^2 \sigma^2_{dt} x_{kd}
\] (3.22)

Constraints (3.15) ensure that each device is used at only one key measurement point and Constraints (3.16) ensure that there is only one device used at each key measurement point. We assume that each device is utilized in every time period.

3.7 Results

In this section, we show that NUMSO provides comparable results much more quickly than a Monte Carlo simulation of SGA. We note that the purpose of SGA is not to optimize measurement system configurations, but is to be a flexible toolkit that can simulate nuclear material in different hypothetical nuclear fuel cycles and diversion contexts. Therefore, we present computation times to show the benefit of using SOCA and MVCM to specifically optimize measurement system configurations, rather than to provide a direct comparison to SGA. For the remainder of this section, we refer to a Monte Carlo simulation of SGA simply as SGA because all results use this approach.

We use Problems 1-3, introduced in Section 3.2, to demonstrate that SOCA obtains similar Type I and Type II error probabilities compared to Shugart & King (2016), but obtains them at least an order of magnitude faster. We also show MVCM provides the same optimal measurement system configuration in Problem 1 even more quickly than SOCA. We compare results using fixed and optimized detection thresholds in the CUMUF test. SOCA obtains an optimal configuration with a pre-specified confidence level using components of the BEST algorithm.

We show results for a fixed detection threshold of 75 kilograms and a time horizon of 360 days, which correspond to one significant quantity of low-enriched uranium and a timeliness detection goal of one year, respectively. For these problems, we use an equal relative importance \((\gamma = 0.5)\) in Objective (3.10). We use the same uniform random error bounds as Shugart & King (2016);
inventory devices have lower error bounds because they must be more precise to account for much higher material quantities at the Cascade key measurement point. We assume that material quantities are constant over time; therefore, we can scale the population variance of the estimated MUF in Objective (3.14) by the number of time periods to obtain the time-independent population variance.

3.7.1 Computation Times

In SOCA, we model and evaluate CUMUF test replications using the C++11 programming language via the GNU Compiler Collection Version 4.8.4 (Free Software Foundation, 2014). We parallelize replications with GNU Parallel (Tange, 2011). We implement the BEST algorithm in SOCA with Python Version 2.7.6 (Python Software Foundation, 2013). We model and solve MVCM with AMPL Version 20130109 (AMPL Optimization LLC, 2013; Fourer et al., 2003) and CPLEX Version 12.6.0.1 with default settings (IBM, 2014; IBM ILOG AMPL, 2010), respectively. We perform all computations on a Sun Fire x4250 workstation under the Ubuntu 14.04 operating system with two Quad-core CPUs running at 2.83 GHz with 16 GB RAM.

Shugart & King (2016) implement a Monte Carlo simulation of 100 replications of 1,000 SGA process samples with Matlab R2014b (The MathWorks, Inc., 2014). They perform computations on an IMac Pro under the Windows 7 Pro operating system with twelve Dual-core CPUs running at 2.79 GHz with 96GB RAM; however, Shugart & King (2016) use a single core to obtain results.

Table 3.4 shows the total computation time needed for each problem, referenced by the table or figure containing the results, using SGA, SOCA with fixed and optimized detection thresholds, and MVCM. For all problems, SOCA decreases the computation time compared to SGA by over an order of magnitude. For Problem 1, MVCM decreases computation time compared to SGA by nearly 100%.
NUMSO implements parallel processing; however, we only use eight cores to evaluate replications, which provides small improvements compared to our other enhancements. For example, the computation time needed for SOCA in Problem 1 on a single core is approximately 1,500 seconds, compared to 189 seconds on eight cores; this is a marginal reduction compared to the order-of-magnitude improvement the other enhancements provide over SGA. Using an optimized detection threshold in SOCA requires slightly more computation time than employing a fixed threshold, which may be inconsequential compared to the benefits discussed in Section 3.7.2.

### 3.7.2 Problem 1 Results

Problem 1 represents the case in which we seek to determine the configuration of \( n \) devices at \( n \) locations (\( n=3 \)) that gives the lowest weighted sum of Type I and Type II error probabilities, or the lowest population variance of the estimated MUF, provided location-dependent device precisions. The three possible random measurement error distributions for flow measurements are Uniform (-2\%, 2\%), Uniform(-5\%, 5\%), and Uniform(-10\%, 10\%). The measurement error distribution for the single inventory measurement device, which is always utilized at the enrichment cascade key measurement point, is Uniform(-0.02\%, 0.02\%).

In this problem, SOCA estimates the probability of Type I errors to be zero, which indicates that the accumulation of random errors in a non-diversion context never exceeds the detection threshold. Table 3.5 shows that the results from SOCA match those from SGA for all measurement system configurations. The results from MVCM indicate that minimizing the population variance

<table>
<thead>
<tr>
<th>Model</th>
<th>Computation time (s)</th>
<th>Reduction from SGA (%)</th>
<th>Computation time (s)</th>
<th>Reduction from SGA (%)</th>
<th>Computation time (s)</th>
<th>Reduction from SGA (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SGA</td>
<td>73,400</td>
<td>-</td>
<td>61,200</td>
<td>-</td>
<td>171,000</td>
<td>-</td>
</tr>
<tr>
<td>SOCA</td>
<td>189</td>
<td>99.7</td>
<td>176</td>
<td>99.7</td>
<td>4,180</td>
<td>97.6</td>
</tr>
<tr>
<td>SOCA*</td>
<td>284</td>
<td>99.6</td>
<td>275</td>
<td>99.6</td>
<td>5,890</td>
<td>96.6</td>
</tr>
<tr>
<td>MVCM</td>
<td>0.167</td>
<td>100</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
of the estimated MUF yields the same optimal configuration as minimizing a weighted sum of Type I and Type II error probabilities.

Table 3.5: **SOCA** and **MVCM** configuration results with a fixed detection threshold

<table>
<thead>
<tr>
<th>Random error bounds (Input, Output, Tails)</th>
<th>SGA detection probability</th>
<th>SOCA detection probability</th>
<th>MVCM population variance (kg²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>± 2, 5, 10%</td>
<td>0.8569±0.0113</td>
<td>0.8550±0.0112</td>
<td>21.43</td>
</tr>
<tr>
<td>± 2, 10, 5%</td>
<td>0.7771±0.0131</td>
<td>0.7734±0.0136</td>
<td>21.52</td>
</tr>
<tr>
<td>± 5, 2, 10%</td>
<td>0.8481±0.0099</td>
<td>0.8147±0.0124</td>
<td>21.47</td>
</tr>
<tr>
<td>± 5, 10, 2%</td>
<td>0.7457±0.0025</td>
<td>0.7437±0.0142</td>
<td>21.59</td>
</tr>
<tr>
<td>± 10, 2, 5%</td>
<td>0.7143±0.0143</td>
<td>0.7125±0.0144</td>
<td>21.69</td>
</tr>
<tr>
<td>± 10, 5, 2%</td>
<td>0.7061±0.0149</td>
<td>0.7066±0.0147</td>
<td>21.72</td>
</tr>
</tbody>
</table>

Table 3.6 provides Type I and Type II error probabilities using an optimized detection threshold. For the best measurement system configuration, we are able to identify the lost material in every hypothetical diversion context sample, while incurring no Type I errors. These results demonstrate the benefit of using an optimized, rather than a fixed, detection threshold. The threshold for the best configuration is almost three times lower than the International Atomic Energy Agency’s limit for uranium-235 of 75 kilograms.

Table 3.6: **SOCA** configuration results with an optimized detection threshold

<table>
<thead>
<tr>
<th>Random error bounds (Input, Output, Tails)</th>
<th>Type I error probability</th>
<th>Detection probability</th>
<th>Weighted sum of Type I and Type II error probabilities</th>
<th>Average detection threshold (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>± 2, 5, 10%</td>
<td>0.0000±0.0000</td>
<td>1.0000±0.0000</td>
<td>0.0000±0.0000</td>
<td>26.41±1.973</td>
</tr>
<tr>
<td>± 2, 10, 5%</td>
<td>0.0000±0.0000</td>
<td>1.0000±0.0000</td>
<td>0.0000±0.0000</td>
<td>34.59±2.701</td>
</tr>
<tr>
<td>± 5, 2, 10%</td>
<td>0.0000±0.0000</td>
<td>1.0000±0.0000</td>
<td>0.0000±0.0000</td>
<td>38.83±2.909</td>
</tr>
<tr>
<td>± 5, 10, 2%</td>
<td>0.0000±0.0000</td>
<td>1.0000±0.0000</td>
<td>0.0000±0.0000</td>
<td>43.16±2.607</td>
</tr>
<tr>
<td>± 10, 2, 5%</td>
<td>0.0004±0.0006</td>
<td>0.9998±0.0005</td>
<td>0.0006±0.0008</td>
<td>43.73±2.456</td>
</tr>
<tr>
<td>± 10, 5, 2%</td>
<td>0.0006±0.0008</td>
<td>0.9996±0.0006</td>
<td>0.0010±0.0010</td>
<td></td>
</tr>
</tbody>
</table>

We find the optimized detection threshold by identifying which value between 0 and 75 kilograms (using one-kilogram increments) yields the lowest weighted sum of Type I and Type II error probabilities. In certain cases, a finer increment (e.g., 0.1 kilogram) might be required to attain the
optimal solution; however, Table 3.7 shows that we obtain the same solution using an increment of one kilogram as with 0.1 kilogram, while requiring less computation time (284 seconds compared to 3,984 seconds).

Table 3.7: SOCA configuration results for different optimized detection threshold increments

<table>
<thead>
<tr>
<th>Random error bounds (Input, Output, Tails)</th>
<th>1.0 kg increment</th>
<th>0.1 kg increment</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Weighted sum of Type I and Type II error probabilities</td>
<td>Average detection threshold (kg)</td>
</tr>
<tr>
<td>± 2, 5, 10%</td>
<td>0.0000±0.0000</td>
<td>26.41±1.973</td>
</tr>
<tr>
<td>± 2, 10, 5%</td>
<td>0.0000±0.0000</td>
<td>34.59±2.701</td>
</tr>
<tr>
<td>± 5, 2, 10%</td>
<td>0.0000±0.0000</td>
<td>30.04±2.372</td>
</tr>
<tr>
<td>± 5, 10, 2%</td>
<td>0.0000±0.0001</td>
<td>38.83±2.909</td>
</tr>
<tr>
<td>± 10, 2, 5%</td>
<td>0.0006±0.0008</td>
<td>43.16±2.607</td>
</tr>
<tr>
<td>± 10, 5, 2%</td>
<td>0.0010±0.0010</td>
<td>43.73±2.456</td>
</tr>
</tbody>
</table>

3.7.3 Problem 2 Results

Problem 2 finds the key measurement point at which improving device precision reduces objective values the most. For this problem, all random error distributions are initially Uniform(-5%, 5%) for flow measurements and Uniform(-0.01%, 0.01%) for inventory measurements in the base case. Then, we obtain the weighted sums of Type I and Type II error probabilities that result from individually improving each flow measurement distribution to Uniform(-3%, 3%) or the inventory measurement distribution to Uniform(-0.008%, 0.008%).

Table 3.8 shows that SOCA obtains results similar to those obtained by SGA using a fixed detection threshold. In this problem, SOCA also identifies the lost material in every hypothetical diversion sample with an optimized detection threshold and estimates the probability of Type I errors to be zero. We find the best key measurement point at which to decrease a method’s random error bounds is the Input. The lowest average optimized detection threshold corresponds to the highest detection probability using a fixed detection threshold, indicating that it might be better to allocate resources to find the lowest detection threshold for a measurement system than simply to make small improvements to measurement devices to increase the detection probability.
Table 3.8: **SOCA** detection probabilities from decreasing error bounds at each key measurement point

<table>
<thead>
<tr>
<th>Key measurement point</th>
<th>SGA detection probability</th>
<th>SOCA detection probability</th>
<th>Optimized detection threshold</th>
<th>Average detection threshold (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>0.6955±0.0093</td>
<td>0.6936±0.0147</td>
<td>1.0000±0.0000</td>
<td>27.85±2.309</td>
</tr>
<tr>
<td><strong>Input</strong></td>
<td><strong>0.7407±0.0084</strong></td>
<td><strong>0.7393±0.0138</strong></td>
<td><strong>1.0000±0.0000</strong></td>
<td><strong>22.65±1.823</strong></td>
</tr>
<tr>
<td>Inventory</td>
<td>0.6095±0.0105</td>
<td>0.6082±0.0164</td>
<td>1.0000±0.0000</td>
<td>26.12±2.333</td>
</tr>
<tr>
<td>Output</td>
<td>0.7131±0.0094</td>
<td>0.7115±0.0141</td>
<td>1.0000±0.0000</td>
<td>25.56±2.016</td>
</tr>
<tr>
<td>Tails</td>
<td>0.6939±0.0102</td>
<td>0.6969±0.0147</td>
<td>1.0000±0.0000</td>
<td>27.49±2.230</td>
</tr>
</tbody>
</table>

### 3.7.4 Problem 3 Results

Figure 3.2: Type I error and detection probabilities based on measurement frequency for a fixed detection threshold and two different measurement error levels, denoted by (flow %, inventory %)

Problem 3 determines the effect of measurement frequency on measurement system configurations and objective values. We equally segment the time horizon by the number of measurements to determine when devices are utilized as a proxy for time periods. Figures 3.2-3.4 show Type I error and detection probabilities for two levels of uniform random measurement error bounds.
Figure 3.2 depicts similar results to those from Shugart & King (2016) using a fixed detection threshold. The Type I error and detection probabilities decrease and increase, respectively, as the number of measurements increases for the worst-case loss context.

![Graph showing Type I error and detection probabilities](image)

Figure 3.3: Type I error and detection probabilities based on measurement frequency for an optimized detection threshold and two different measurement error levels, denoted by (flow %, inventory %)

Figure 3.3 indicates that by using an optimized detection threshold, the Type I error and detection probabilities reach 1.0 and 0.0, respectively, by measuring far less frequently than using a fixed detection threshold. Measurements must be taken twenty-four times per day to achieve a near perfect detection probability using a fixed detection threshold, but only once every four days using an optimized detection threshold.

Figure 3.4 demonstrates that the optimized detection threshold decreases as the measurement frequency increases. This figure also shows that a larger detection threshold is required for systems that have less precise measurement devices. For this problem, SOCA obtains better detection probabilities using a lower detection threshold and measuring less frequently than the International Atomic Energy Agency significant quantity and timeliness detection goal limits.
3.8 Conclusion

NUMSO uses operations research techniques, specifically, simulation optimization and integer programming, to find the optimal measurement system configuration with a pre-specified level of confidence. We develop SOCA and MVCM to find optimal configurations using two different objectives: minimize (i) a weighted sum of Type I and Type II error probabilities and (ii) population variance of the estimated MUF. We show that these models produce the same optimal configuration for our specific enrichment facility measurement system considering one material in a worst-case loss context. In addition, we are able to find the best key measurement point at which to improve the precision of a measurement device and examine the effect of measurement frequency on the Type I error and detection probabilities using SOCA.

We show that our models obtain similar results to those from Shugart & King (2016), but are able to generate them considerably faster. For each problem, SOCA reduces computation time by at least an order of magnitude. We obtain the same configuration with MVCM almost
instantaneously. This is a considerable improvement over using a Monte Carlo simulation of SGA to optimize configurations.

We also find the optimized detection threshold that gives the lowest objective value in a worst-case loss context using SOCA. We show that an optimized detection threshold lowers the weighted sum of Type I and Type II error probabilities while measuring less frequently compared to a fixed threshold, which indicates that measurement systems should have unique detection thresholds to save the time and resources spent measuring more often than necessary.

Finding the optimal measurement system configuration for a realistic fuel cycle is prohibitive using existing tools, such as SGA, because of the large computation time required to analyze a single facility. We show that NUMSO quickly finds an optimal configuration with high confidence for this simple case, which indicates that it might also obtain the best configuration for a realistic fuel cycle within a reasonable amount of time. However, we need to test NUMSO on a larger measurement system to show that it can be extended for practical applications.

We can add new models to NUMSO to extend its capability to find solutions to other important problems in nuclear safeguards. One potential problem is, provided a measurement system configuration and a fixed budget, determine how to improve measurement devices to reduce the population variance of the estimated MUF in the system the most. Another possible problem is to find the most cost-effective way to reduce population variance of the estimated MUF by a predetermined amount.

3.9 Acknowledgments

We acknowledge Nicolas Shugart, Ph.D. candidate in the Nuclear Engineering Department at the Colorado School of Mines, for developing relevant nuclear engineering problems and giving data support for our models. We thank the National Nuclear Security Administration for providing us support under Grant DE-NA0001730.
4.1 Abstract

The dangerous ability to create nuclear weapons from uranium-235 and plutonium-239 makes it imperative to closely account for these materials as they progress through a nuclear fuel cycle. Improving measurement systems gives more accurate estimates of material quantities and material unaccounted for (MUF). This paper provides solutions to three potential problems in current measurement systems: how to best (i) locate measurement methods given fixed purchase and utilization budgets, (ii) increase the precision of existing methods given a fixed improvement budget, and (iii) reduce measurement uncertainty in the system while limiting the cost of the improvement.

The NUclear Measurement System Optimization (NUMSO) toolkit uses operations research techniques to find optimal solutions to these problems based on minimizing the scaled, estimated MUF variance. The SafeGuards Analysis (SGA) toolkit employs a Monte Carlo simulation to analyze if NUMSO provides good solutions in terms of the Type I error probabilities, i.e., material loss false alarm probabilities, in a measurement system. Solving these problems using a realistic fuel cycle scenario demonstrates the capability of NUMSO and SGA to address representative problems in nuclear safeguards. This paper shows that NUMSO quickly yields similar or better Type I error
probabilities compared to several intuitive analyses that take much longer. However, the authors recommend that a thorough comparison be performed using SGA to ensure that, for a specific application, NUMSO yields acceptable Type I error probabilities.

4.2 Nomenclature

Acronyms
IAEA International Atomic Energy Agency
MC&A material control and accountability
MUF material unaccounted for
MBA mass balance area
HEU high-enriched uranium
CMUF cumulative material unaccounted for
UOX uranium-oxide
LEU low-enriched uranium
MOX mixed-oxide

Toolkits and Models
NUMSO NUclear Measurement System Optimization
MVCM Minimum Variance Configuration Model
MIVM Minimum Improved Variance Model
MICM Minimum Improvement Cost Model
SGA SafeGuards Analysis

Sets
\( t \in \mathcal{T} \) time periods
\( k \in \mathcal{K} \) key measurement points
\( \mathcal{K}^R \subset \mathcal{K} \) receipt key measurement points
\( \mathcal{K}^S \subset \mathcal{K} \) shipment key measurement points
\( \mathcal{K}^I \subset \mathcal{K} \) inventory key measurement points
\( f \in \mathcal{F} \) material forms
\( k \in \mathcal{K}_f \) key measurement points for material form \( f \)
\( d \in \mathcal{D} \) measurement methods
\( d \in \mathcal{D}_f \) measurement methods for material form \( f \)
Parameters

\( \tilde{R}_{kt} \) estimated receipts at key measurement point \( k \) and time period \( t \) (kg)

\( \tilde{S}_{kt} \) estimated shipments at key measurement point \( k \) and time period \( t \) (kg)

\( \tilde{I}_{kt} \) estimated inventory at key measurement point \( k \) and time period \( t \) (kg)

\( \tilde{M}_t \) estimated MUF in time period \( t \) (kg)

\( \tilde{C}_t \) estimated CMUF in time period \( t \) (kg)

\( q_k \) true material quantity at key measurement point \( k \) (kg)

\( \tilde{e}_d \) uncertainty bound for measurement method \( d \) (%)

\( \hat{e}_{kd} \) uncertainty bound conversion factor for measurement method \( d \) at key measurement point \( k \) (%)

\( \hat{\sigma}^2_k \) estimated MUF variance scaling factor for key measurement point \( k \) (unitless)

\( c^p_d \) purchase cost for measurement method \( d \) ($)

\( c^U_d \) utilization cost for measurement method \( d \) ($)

\( p^p_d \) purchase budget ($) 

\( b^U_d \) utilization budget ($)

\( c^I_d \) improvement cost for measurement method \( d \) ($/kg)

\( b^I_d \) improvement budget ($)

\( x^*_{kd} \) fixed measurement system configuration for measurement method \( d \) at key measurement point \( k \) (unitless)

\( i^* \) pre-specified fraction of scaled, estimated MUF variance reduction (unitless)

\( \tilde{e}^+_k \) uncertainty bound increment for key measurement point \( k \) (kg)

\( \hat{c}^I_k \) improvement cost scaling factor for key measurement point \( k \) (unitless)

Binary Variables

\( X_{kd} \) 1 if measurement method \( d \) is utilized at key measurement point \( k \); 0 otherwise (unitless)

Continuous Variables

\( I_{kd} \) uncertainty bound improvement for measurement method \( d \) at key measurement point \( k \) (unitless)

Integer Variables

\( \hat{I}_{kd} \) uncertainty bound improvement scale for measurement method \( d \) at key measurement point \( k \) (kg)

4.3 Introduction

Current nuclear fuel cycles follow uranium and plutonium from the time uranium is mined as ore, the uranium and plutonium are used to produce energy, and the resulting materials are treated, stored, and permanently disposed. Initially, the uranium is not a concern to public safety because
it is only slightly radioactive, but uranium-235 (the isotope used for electricity production) is enriched to a higher concentration to produce nuclear fuel. A nuclear reactor fissions uranium-235 to produce power, which yields plutonium-239 (which can also be fissioned to produce power) and other isotopes. Uranium-235 and plutonium-239 are able to be used to produce nuclear weapons, which makes it imperative to closely account for these materials as they progress through a nuclear fuel cycle.

The International Atomic Energy Agency (IAEA) implements a group of activities, called nuclear safeguards, to ensure its 140 member states are not using their civilian nuclear fuel cycles to produce nuclear weapons (International Atomic Energy Agency, 2016). Nuclear safeguards seek to ensure that nuclear materials are not lost from within a nuclear fuel cycle. Material control and accountability (MC&A) is a type of safeguard that attempts to prevent the development of these weapons by detecting and deterring the theft or, “diversion,” of nuclear material (U.S. Department of Energy, 2011).

It is important to analyze and enhance MC&A methods because nuclear terrorism is an immediate and extreme threat to global security. Terrorists have the desire and ability to turn raw nuclear materials into a weapon; therefore, making it more difficult to acquire these materials improves global security (The White House Office of the Press Secretary, 2016). According to the Nuclear Threat Initiative (2007), there are an increasing number of entities seeking nuclear and/or other radioactive material, i.e., material that emits ionizing radiation but is not capable of a nuclear explosion (International Atomic Energy Agency, 2007).

This paper addresses three representative problems in current MC&A measurement systems: how to (i) best locate measurement methods in a nuclear fuel cycle given fixed purchase and utilization budgets (Problem 1), (ii) increase the precision of existing methods given a fixed improvement budget (Problem 2), and (iii) reduce measurement uncertainty in the system while limiting the cost of the improvement (Problem 3).

The \textit{NUclear Measurement System Optimization} toolkit (NUMSO), extended from Johnson \textit{et al.} (2016a), uses operations research techniques, specifically, integer programming, to find op-
timal solutions to these problems based on minimizing the scaled, estimated material unaccounted for (MUF) variance in the system. **NUMSO uses the Minimum Variance Configuration Model (MVCM), the Minimum Improved Variance Model (MIVM), and the Minimum Improvement Cost Model (MICM)** to obtain solutions to Problems 1-3, respectively. The SafeGuards Analysis toolkit (SGA) from Shugart & King (2016) and Shugart et al. (2016) analyzes if **NUMSO**’s solutions yield lower Type I error probabilities in a measurement system.

Providing optimal solutions to these problems and verifying **NUMSO**’s effectiveness using a realistic fuel cycle scenario demonstrates the capability of **NUMSO** and **SGA** to address potential problems in nuclear safeguards. These toolkits use hypothetical measurement methods because the focus of this paper is to demonstrate their ability to give answers to representative problems. Figure 4.1 shows the relationship between the problems, the **NUMSO** models, and the **SGA** analyses.

---

**Problem | NUMSO Model | SGA Analysis**
---|---|---
Problem 1 | Optimize the measurement system configuration with MVCM | Analyze MVCM’s results with the “manual average start” and “manual cheap start” analyses
Problem 2 | Optimize the measurement system improvement with MIVM | Analyze MIVM and MICM’s results with the “most sensitive” and “cheapest” analyses
Problem 3 | Optimize the measurement system improvement cost with MICM |

Figure 4.1: Relationship between the problems, the **NUMSO** models, and the **SGA** analyses. **SGA** analyses (detailed in Section 4.5) provide intuitive solutions to each problem and indicate if **NUMSO** yields lower Type I error probabilities.

The remainder of the paper is organized as follows: Section 4.4 details general MC&A measurement systems, introduces operations research methodology, and describes **NUMSO** and **SGA** in depth. Section 4.5 explores the specific fuel cycle scenario **NUMSO** and **SGA** enhance in this demonstration, details Problems 1-3, and conveys the rationale of the **SGA** analyses. Sections 4.6
and 4.7 provide results and discussion for each problem using NUMSO and SGA, respectively. Section 4.8 concludes the paper with a summary of results and recommendations for future work.

4.4 Background

The focus of material control within MC&A is to protect nuclear materials and prevent their unapproved removal from authorized locations or to detect their absence in a timely manner. The purpose of material accountability within MC&A is to ensure there is an accurate account of nuclear material within a nuclear fuel cycle (U.S. Department of Energy, 2011). More specifically, MC&A focuses on the material and inventory balance at one or more material balance areas (MBAs) to assess if any nuclear material is missing (International Atomic Energy Agency, 2002).

The theft or loss of nuclear and other radioactive material is an international security concern (International Atomic Energy Agency, 2015). From 1993-2014, there were 714 instances of theft or loss of nuclear and other radioactive material from facilities or during transport reported to the Incident and Trafficking Database (IAEA’s system of tracking illicit incidents involving nuclear and other radioactive material). The majority of these occurrences involved materials from industrial or medical applications, which are mostly harmless. Several instances, however, included high-enriched uranium or plutonium, which, if accumulated in sufficiently large quantities, can be made into nuclear weapons. These events show that people remain able to obtain this dangerous material and underscore the importance of continually improving MC&A methods to help identify its potential theft or loss. Table 4.1 shows the confirmed nuclear material trafficking incidents reported to the Incident and Trafficking Database involving high-enriched uranium (HEU) and plutonium between 1993 and 2007 (Bunn, 2013).
Table 4.1: HEU and plutonium incidents confirmed by the Incident and Trafficking Database, 1993-2007

<table>
<thead>
<tr>
<th>Date</th>
<th>Location</th>
<th>Material</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>05/24/1993</td>
<td>Vilnius, Lithuania</td>
<td>HEU</td>
<td>150 g</td>
</tr>
<tr>
<td>03/??/1994</td>
<td>St. Petersburg, Russian Federation</td>
<td>HEU</td>
<td>2.97 kg</td>
</tr>
<tr>
<td>05/10/1994</td>
<td>Tengen-Wiechs, Germany</td>
<td>Pu</td>
<td>6.20 g</td>
</tr>
<tr>
<td>06/13/1994</td>
<td>Landshut, Germany</td>
<td>HEU</td>
<td>795 mg</td>
</tr>
<tr>
<td>07/25/1994</td>
<td>Munich, Germany</td>
<td>Pu</td>
<td>240 g</td>
</tr>
<tr>
<td>08/10/1994</td>
<td>Munich Airport, Germany</td>
<td>Pu</td>
<td>363 g</td>
</tr>
<tr>
<td>12/14/1994</td>
<td>Prague, Czech Republic</td>
<td>HEU</td>
<td>2.73 kg</td>
</tr>
<tr>
<td>06/??/1995</td>
<td>Moscow, Russian Federation</td>
<td>HEU</td>
<td>1.70 kg</td>
</tr>
<tr>
<td>06/06/1995</td>
<td>Prague, Czech Republic</td>
<td>HEU</td>
<td>415 mg</td>
</tr>
<tr>
<td>06/08/1995</td>
<td>Ceske Budejovice, Czech Republic</td>
<td>HEU</td>
<td>16.9 g</td>
</tr>
<tr>
<td>05/29/1999</td>
<td>Rousse, Bulgaria</td>
<td>HEU</td>
<td>10.0 g</td>
</tr>
<tr>
<td>12/??/2000</td>
<td>Karlsruhe, Germany</td>
<td>Pu</td>
<td>1.00 mg</td>
</tr>
<tr>
<td>07/16/2001</td>
<td>Paris, France</td>
<td>HEU</td>
<td>500 mg</td>
</tr>
<tr>
<td>06/26/2003</td>
<td>Sadahlo, Georgia</td>
<td>HEU</td>
<td>170 g</td>
</tr>
<tr>
<td>03/??/2005 to 04/??/2005</td>
<td>New Jersey, USA</td>
<td>HEU</td>
<td>3.30 g</td>
</tr>
<tr>
<td>06/24/2005</td>
<td>Fukui, Japan</td>
<td>HEU</td>
<td>1.70 mg</td>
</tr>
<tr>
<td>02/01/2006</td>
<td>Tbilisi, Georgia</td>
<td>HEU</td>
<td>79.5 g</td>
</tr>
<tr>
<td>03/30/2006</td>
<td>Hennigsdorf, Germany</td>
<td>HEU</td>
<td>47.5 g</td>
</tr>
</tbody>
</table>

4.4.1 Material Control and Accountability

An MC&A measurement system estimates material entering (i.e., receipts) and exiting (i.e., shipments) one or more nuclear fuel cycle facilities, in addition to deriving estimates for all batch quantities of material present at the facilities (i.e., physical inventory). To do this, a system utilizes measurement methods to quantify a physical attribute of the material. A measurement system configuration is a specific arrangement of these methods and their corresponding parameter settings, which requires the ability to detect a substantial amount of missing material with high probability to establish its effectiveness (de Montmollin & Weinstock, 1979).

In an MC&A measurement system, MBAs and key measurement points identify boundaries and locations, respectively, at which measurements are taken. An MBA is a facility or subset of a facility provided that (1) the amount transferred into or out of the MBA can be quantified and (2) the physical inventory within the MBA can be quantified “when necessary” (International Atomic Energy Agency, 2002). For example, an MBA can be an entire enrichment facility or an individual centrifuge within an enrichment facility. In practice, facilities in a nuclear fuel cycle might comprise a single MBA; however, in complex facilities such as manufacturing and reprocessing
plants, two or more MBAs might be necessary to adequately model activities within the facility. The locations where receipt, shipment, and inventory material can be measured are potential key measurement points (International Atomic Energy Agency, 2008).

One primary MC&A objective is to provide measurements that are able to detect nuclear material loss despite uncertainties in their estimates. To provide assurance that nuclear material is not missing from an MBA, accountability measurements, which establish initial values of nuclear material, and verification measurements, which authenticate the amount of material present, need to be of the highest quality (U.S. Department of Energy, 2011). Estimates of MUF and cumulative material unaccounted for (CMUF) are primary indicators of material loss (Stewart & Jaech, 1970). The estimated MUF is the difference between the measured receipt, shipment, and physical inventory quantities; the estimated CMUF is the estimated MUF accumulated over all previous time periods.

Detecting material loss is difficult because measurement uncertainties result in a non-zero estimated MUF even if no nuclear material is actually missing from the MBA. It is necessary, therefore, to quantify the random and systematic measurement uncertainties to assess the statistical significance of any differences between true and estimated material in an MBA (U.S. Department of Energy, 2011). A random uncertainty is a positive or negative fluctuation from the true quantity, which results from precision limitations of the measurement method. A systematic uncertainty is a constant bias that can be caused by improper use or function of a measurement method, which results in a shift of the measurement from the true quantity. This paper focuses on random uncertainties.

Equations (4.1) and (4.2) estimate the MUF $\tilde{M}_t$ and CMUF $\tilde{C}_t$ at the end of each time period $t$ during a finite, discrete time horizon $\mathcal{T} = \{1, \ldots, T\}$, respectively. Measured receipts $\tilde{R}_{kt}$, shipments $\tilde{S}_{kt}$, and physical inventory $\tilde{I}_{kt}$ are random variables because measurements are uncertain. The toolkits limit each key measurement point $k$ to possible receipt, shipment, and physical inventory locations $\mathcal{K}^R$, $\mathcal{K}^S$, and $\mathcal{K}^I$, respectively. The estimated inventory at the beginning of $t = 1$ defines $\tilde{I}_{k0}$. The timeliness detection goal for the material of concern sets the length of the time
horizon $T$.

$$
\dot{M}_t = \sum_{k \in \mathcal{X}^R} \dot{R}_{kt} + \sum_{k \in \mathcal{X}^I} (\dot{I}_{k,t-1} - \dot{I}_{kt}) - \sum_{k \in \mathcal{X}^S} \dot{S}_{kt} \quad \forall t \in \mathcal{T} \tag{4.1}
$$

$$
\dot{C}_t = \sum_{\tau = 1}^{\mathcal{H}} \dot{M}_\tau \quad \forall t \in \mathcal{T} \tag{4.2}
$$

Figure 4.2 shows an example of an MBA, which represents an enrichment facility with input, output, waste, and cascade key measurement points. The cascade represents a series of centrifuges used to enrich the uranium. In each time period, the material balance equation uses measurements at each key measurement point to obtain an estimate for the MUF. The loss stream represents any actual or estimated MUF from the MBA.

**Example enrichment facility MBA**

Figure 4.2: An example enrichment facility MBA with flow streams, an inventory location, and potential material loss stream

Table 4.2 shows the significant quantity and timeliness detection goal limits provided by the IAEA for the primary nuclear materials relevant to safeguards. Timeliness detection goals are the “target detection times applicable to specific nuclear material categories.” A significant quantity is “the approximate amount of nuclear material for which the possibility of manufacturing a nuclear explosive device cannot be excluded” (International Atomic Energy Agency, 2002). Countries are able to use plutonium, uranium-233, and highly-enriched uranium to create nuclear weapons. Low-enriched uranium and thorium need extra processing before countries can use them in a nuclear weapon, which results in higher significant quantities and longer timeliness detection goals than
those for the other materials (International Atomic Energy Agency, 2002).

Table 4.2: Significant quantities of nuclear materials and their associated timeliness goals

<table>
<thead>
<tr>
<th>Material</th>
<th>Material form</th>
<th>Significant quantity</th>
<th>Timeliness goal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plutonium</td>
<td>Metal</td>
<td>8 kg</td>
<td>1 month</td>
</tr>
<tr>
<td></td>
<td>Irradiated fuel</td>
<td></td>
<td>3 months</td>
</tr>
<tr>
<td>Uranium-233</td>
<td>Metal</td>
<td>8 kg</td>
<td>1 month</td>
</tr>
<tr>
<td></td>
<td>Irradiated fuel</td>
<td></td>
<td>3 months</td>
</tr>
<tr>
<td>High-enriched uranium</td>
<td>Metal</td>
<td>25 kg</td>
<td>1 month</td>
</tr>
<tr>
<td>(uranium-235 ≥ 20 at%)</td>
<td>Irradiated fuel</td>
<td></td>
<td>3 months</td>
</tr>
<tr>
<td>Low-enriched uranium</td>
<td>Unirradiated fresh fuel</td>
<td>75 kg uranium-235, 10 metric tons natural uranium, or 20 metric tons depleted uranium</td>
<td>1 year</td>
</tr>
<tr>
<td>Thorium</td>
<td>Unirradiated fresh fuel</td>
<td>20 metric tons</td>
<td>1 year</td>
</tr>
</tbody>
</table>

A hypothetical material loss likely occurs if the estimated CMUF exceeds a significant quantity over any time period within a timeliness detection goal limit. It is important to note, however, that actual material loss does not necessarily occur in practice even if the estimated CMUF exceeds a significant quantity; in this case, determining the cause of the alarm requires additional analysis (U.S. Congress, Office of Technology Assessment, 1995). A Type I error results from “falsely concluding that nuclear material has been lost when in fact no material has been lost” and a Type II error results from “concluding that a diversion did not occur when in fact it did occur” (International Atomic Energy Agency, 2002). Figure 4.3 summarizes Type I and Type II error outcomes.

4.4.2 Introduction to Optimization

Operations research is a field that uses various analytical techniques to make better, more informed decisions. Operations research combines methods such as statistical analysis and mathematical modeling, specifically, optimization, to arrive at optimal or near-optimal solutions to complex problems.
Mathematical models require input parameters, decision variables, an objective function, and problem-specific constraints. Input parameters are fixed values that depict physical aspects of reality, such as the material flow in a fuel cycle. Parameters can also include physical or desired limits on system variable values, e.g., the random uncertainty bounds of a measurement method. Decision variables represent continuous or discrete aspects of the problem that are initially unknown and are determined by finding the optimal or near-optimal solution to the problem, such as where to locate a measurement method. The objective function is a combination of parameters and decision variables that describes the goal of the problem, e.g., minimizing estimated MUF variance. Constraints are needed to ensure that limitations imposed by the nature of the problem are upheld, e.g., budget restrictions.

Integer programming is a branch of optimization that restricts at least some of the decision variables in the problem to be integer. The primary benefit of integer programming compared to other optimization methods is the ability to model binary decisions, represented by a value of one if a decision is to be made and zero if a decision is not to be made, e.g., one if a measurement method is utilized at a key measurement point; zero otherwise. Binary variables also allow for logical constructs, e.g., if-then statements. Mixed-integer programs include continuous, in addition to integer, variables. Algorithms for integer programs enumerate a subset of feasible, non-dominated solutions to determine an optimum. The limitation of integer programs is that they are non-convex, which makes them more difficult to solve than their convex, linear counterparts. Linear programs search extreme point solutions, i.e., vertices in a convex set, for a local optimum, which is guaranteed to be the global optimum due to convexity. A drawback of linear programs is that they only contain linear constraints and continuous variables, which limits their applicability to many problems.

Integer and linear programming MC&A applications in the literature are sparse. However, this paper provides examples of these techniques used elsewhere in nuclear energy. Fourcade et al. (1997) develop an integer program to plan nuclear reactor shutdowns and demonstrate that their methods quickly solve a four-reactor, single-site scenario. Johnson et al. (2016b) use a mixed-
integer program to sequence the disposal of high-level nuclear waste; they greatly reduce the heat load concentration in a repository compared to intuitive methods. Silvennoinen et al. (1980) use a linear program to determine that the optimal strategy to minimize the economic risk and the proliferation hazard of a light water reactor fuel cycle is to recycle plutonium in discontinuous batches and to introduce an economic penalty based on fuel cycle costs. Lehtveer et al. (2015) analyze multiple criteria of nuclear power in a linear program to minimize the total discounted energy system costs over an extended time horizon; they find that nuclear power is important to mitigate climate change based on energy security and affordability.

4.4.3 NUclear Measurement System Optimization

The NUclear Measurement System Optimization (NUMSO) toolkit uses operations research techniques, specifically, integer programming, to quickly find solutions to the three nuclear safeguards problems introduced in Section 4.3 and detailed in Section 4.5. These techniques can solve complex problems much more quickly than other methods used in nuclear energy applications (Johnson et al., 2016a,b), such as Monte Carlo simulations (Gul et al., 2016; Haghighat & Wagner, 2003; Lewis & Böhm, 1984; Nuttin et al., 2005). Another benefit is that NUMSO provides assurance of globally optimal solutions using a branch-and-bound algorithm (Atamtürk & Savelsbergh, 2005; Land & Doig, 1960). This paper extends the previously published capabilities of NUMSO by modifying MVCM from Johnson et al. (2016a) and implementing two new mixed-integer quadratic programs, MIVM and MICM.

MVCM obtains an optimal measurement system configuration by minimizing the scaled, estimated MUF in a measurement system. Previously, Stewart (1970) identifies how many measurements should be taken at each location of a hypothetical fuel cycle facility by approximately minimizing the estimated MUF variance subject to a cost constraint. Bouchey et al. (1971) use a multi-stage dynamic program to solve the same problem but without using Stewart’s variance approximation. Rather than finding how many measurements to take at a location, MVCM determines where to locate measurements. Suzuki & Ihara (2008) use linear programming to compare
the trade-off between cost and probability of detecting a hypothetical diversion of two specific measurement methods, destructive and non-destructive analysis. **MIVM** and **MICM** find the best scaled, estimated MUF improvement in a system given a budget constraint and the most cost-effective way to reduce the scaled, estimated MUF variance in a system by a pre-specified amount, respectively.

Johnson *et al.* (2016a) show that lowering the random measurement uncertainty within $\tilde{C}_t$ provides a lower Type I error probability at a given key measurement point before any time $t$. They obtain the same measurement system configuration by minimizing the estimated MUF variance and weighted sum of Type I and Type II error probabilities at a single, example enrichment facility considering only uranium. This paper considers an entire fuel cycle with multiple MBAs and nuclear materials, which have different significant quantity and timeliness detection goal limits. Therefore, there is no guarantee that minimizing the estimated MUF variance yields the “optimal” configuration based on minimizing Type I error probabilities. However, by scaling the estimated MUF variance to account for materials with different significant quantity and timeliness detection goal limits, Section 4.6 shows that the optimal scaled, estimated MUF variance configuration is also a good, but perhaps not optimal, configuration based on minimizing Type I error probabilities.

**Minimum Variance Configuration Model**

The *Minimum Variance Configuration Model* (**MVCM**) identifies an optimal measurement system configuration by minimizing the scaled, estimated MUF variance in a measurement system. In this paper, **MVCM** finds the best configuration for an entire fuel cycle, as opposed to the single facility considered by Johnson *et al.* (2016a). **MVCM** also introduces budget constraints and costs for measurement methods. Section 4.5 discusses the relevant material forms used in the fuel cycle. This paper modifies the notation presented in Johnson *et al.* (2016a) to better address the larger measurement system. **NUMSO** uses uppercase and lowercase letters to denote variables and parameters, respectively.
Sets

- $f \in F$ material forms
- $k \in K$ key measurement points
- $k \in K_f$ key measurement points for material form $f$
- $d \in D$ measurement methods
- $d \in D_f$ measurement methods for material form $f$

Parameters

- $q_k$ true material quantity at key measurement point $k$ (kg)
- $\bar{e}_d$ uncertainty bound for measurement method $d$ ($\%$)
- $\hat{e}_{kd}$ uncertainty bound conversion factor for measurement method $d$ at key measurement point $k$ ($\%$)
- $e_{k_i}^+$ uncertainty bound increment for key measurement point $k$ (kg)
- $\hat{\sigma}^2_k$ estimated MUF variance scaling factor for key measurement point $k$ (unitless)
- $c_{d_i}$ purchase cost for measurement method $d$ ($\$)
- $c_{U_d}$ utilization cost for measurement method $d$ ($\$)
- $b^P$ purchase budget ($\$)
- $b^U$ utilization budget ($\$)

Binary Variables

- $X_{kd}$ 1 if measurement method $d$ is utilized at key measurement point $k$; 0 otherwise (unitless)

MVCM

$$\min \sum_{f \in F} \sum_{k \in K_f} \sum_{d \in D_f} \frac{1}{12} q_k^2 \left( \frac{2\bar{e}_d}{\hat{e}_{kd}} \right)^2 \hat{\sigma}^2_k X_{kd}$$ (4.3)

Variables in the model are subject to the following constraints:

$$\sum_{d \in D_f} X_{kd} = 1 \quad \forall f \in F, k \in K_f$$ (4.4)

$$\sum_{f \in F} \sum_{k \in K_f} \sum_{d \in D_f} c_{d_i}^P X_{kd} \leq b^P$$ (4.5)

$$\sum_{f \in F} \sum_{k \in K_f} \sum_{d \in D_f} c_{d_i}^U X_{kd} \leq b^U$$ (4.6)

$$X_{kd} \text{ binary} \quad \forall f \in F, k \in K_f, d \in D_f$$ (4.7)
Objective (4.3) minimizes the scaled, estimated MUF variance of a measurement system, which is a combination of the assumed, true material quantity and the variance associated with the method used to obtain its estimate. **MVCM** scales the estimated MUF variance to place equal weighting on key measurement points that have lower variance contributions because of the required precision of the methods utilized there. If there is no scaling, **MVCM** places more importance on key measurement points that have higher variance contributions, but might not have higher Type I error probabilities because of different significant quantity and timeliness detection goal limits.

**MVCM** uses uniform distributions for random uncertainties. A uniform distribution is described by its bounds $a$ and $b$, which form the interval $[a, b]$. The variance of a uniform distribution is $\frac{1}{12}(b-a)^2$ (Ross, 2014, p. 162). Equation (4.8) shows the variance for each measurement method $d$ based on its uniform uncertainty bounds $\pm \bar{e}_d$:

$$
\frac{1}{12} \left( \frac{\bar{e}_d}{100\%} - \frac{-\bar{e}_d}{100\%} \right)^2 = \frac{1}{12} \left( \frac{2\overline{\bar{e}}_d}{100\%} \right)^2 \quad \forall \; d \in \mathcal{D}
$$

(4.8)

For readability, **MVCM** uses uncertainty bounds rated on a scale of zero to ten percent and then converts them using $\hat{e}_{kd}$ to realistic values (Appendix B). The following mathematical expression shows the variance for the measurement method’s random uncertainty distribution:

$$
\frac{1}{12} \left( \frac{2\bar{e}_d}{\hat{e}_{kd}} \right)^2 \quad \forall \; f \in \mathcal{F}, k \in \mathcal{K}_f, d \in \mathcal{D}_f
$$

(4.9)

Constraints (4.4) ensure that there is exactly one method used at each key measurement point. **MVCM** in Johnson et al. (2016a) uses each method only once; here, **MVCM** allows measurement methods to be utilized at multiple key measurement points that consider the same material form $f$. Constraints (4.5) and (4.6) ensure that the purchase and utilization costs of measurements do not exceed their respective budgets.

**Minimum Improved Variance Model**

The **Minimum Improved Variance Model (MIVM)** identifies by how much to increase the precision of measurement methods within a fixed budget by minimizing the scaled, estimated MUF var-
ance of the improved system. **MIVM** assumes **MVCM**’s optimal measurement system configuration. Here, the precision of measurement methods increases as their uniform random uncertainty bounds decrease. If a different distribution characterizes the random measurement uncertainty of a method, the improvement can be based on a defining characteristic of the distribution, e.g., mean or variance for a normal distribution. This model uses existing notation and the following additions:

**Additional Parameters**

\[c^f_d\] improvement cost for measurement method \(d\) (\$/kg)

\[b^f\] improvement budget ($)

\[x^*_kd\] fixed measurement system configuration for measurement method \(d\) at key measurement point \(k\) (unitless)

**Continuous Variables**

\[I_{kd}\] uncertainty bound improvement for measurement method \(d\) at key measurement point \(k\) (unitless)

**Integer Variables**

\[\hat{I}_{kd}\] uncertainty bound improvement scale for measurement method \(d\) at key measurement point \(k\) (kg)

**MIVM**

\[
\min \sum_{f \in \mathcal{F}} \sum_{k \in \mathcal{K}_f} \sum_{d \in \mathcal{D}_f} \frac{1}{12} q_k^2 \left( \frac{2\hat{e}_{kd}}{\hat{e}_{kd} - I_{kd}} - I_{kd} \right)^2 \hat{\sigma}_{kd}^2 x^*_kd 
\]

(4.10)

Variables in the model are subject to the following constraints:

\[
\sum_{f \in \mathcal{F}} \sum_{k \in \mathcal{K}_f} \sum_{d \in \mathcal{D}_f} c^f_d q_k I_{kd} \leq b^f 
\]

(4.11)

\[q_k I_{kd} - \hat{I}_{kd} = 0 \quad \forall \ f \in \mathcal{F}, k \in \mathcal{K}_f, d \in \mathcal{D}_f \]

(4.12)

\[I_{kd} \geq 0 \quad \forall \ f \in \mathcal{F}, k \in \mathcal{K}_f, d \in \mathcal{D}_f \]

(4.13)

\[\hat{I}_{kd} \geq 0, \text{ integer} \quad \forall \ f \in \mathcal{F}, k \in \mathcal{K}_f, d \in \mathcal{D}_f \]

(4.14)

Objective (4.10) minimizes the scaled, estimated MUF variance in a measurement system by reducing the uncertainty bounds on one or more methods. Constraints (4.11) ensure that the cost
to improve the methods does not exceed the budget. The expression \( q_k I_{kd} \) converts the unitless uncertainty bound improvement to kilograms, which is necessary to correspond to the improvement cost. Constraints (4.12) ensure that the uncertainty bound reduction is on an integer scale.

**Minimum Improvement Cost Model**

The *Minimum Improvement Cost Model* (MICM) determines the most cost-effective way to reduce the scaled, estimated MUF variance in a system by a pre-specified fraction. MICM incurs an improvement cost for each kilogram decrease in uncertainty bound for a measurement method. MICM assumes MVCM’s optimal measurement system configuration as the basis for its system. This model uses existing notation and the following additions:

### Additional Parameters

- \( i \): pre-specified fraction of scaled, estimated MUF variance reduction (unitless)
- \( c_k^l \): improvement cost scaling factor for key measurement point \( k \) (unitless)

**MICM**

\[
\min \sum_{f \in \mathcal{F}} \sum_{k \in \mathcal{K}_f} \sum_{d \in \mathcal{D}_f} c_k^l q_k I_{kd} \tag{4.15}
\]

Variables in the model are subject to the following constraints:

\[
\sum_{f \in \mathcal{F}} \sum_{k \in \mathcal{K}_f} \sum_{d \in \mathcal{D}_f} \frac{1}{12} q_k^2 \left( \frac{2 \bar{e}_d}{\hat{e}_{kd}} - I_{kd} \right)^2 \hat{\sigma}_{kd}^2 \leq (1 - i) \sum_{f \in \mathcal{F}} \sum_{k \in \mathcal{K}_f} \sum_{d \in \mathcal{D}_f} \frac{1}{12} q_k^2 \left( \frac{2 \bar{e}_d}{\hat{e}_{kd}} \right)^2 \hat{\sigma}_{kd}^2 \tag{4.16}
\]

\[
q_k I_{kd} - \hat{I}_{kd} = 0 \quad \forall f \in \mathcal{F}, k \in \mathcal{K}_f, d \in \mathcal{D}_f \tag{4.17}
\]

\[
I_{kd} \geq 0 \quad \forall f \in \mathcal{F}, k \in \mathcal{K}_f, d \in \mathcal{D}_f \tag{4.18}
\]

\[
\hat{I}_{kd} \geq 0, \text{ integer} \quad \forall f \in \mathcal{F}, k \in \mathcal{K}_f, d \in \mathcal{D}_f \tag{4.19}
\]

Objective (4.15) minimizes the cost to decrease measurement method uncertainty bounds. MICM scales the improvement cost to place more importance on key measurement points that SGA determines have higher Type I error probabilities. Constraints (4.16) ensure that the scaled, estimated MUF variance in a system improves by a pre-specified fraction \( i \). Constraints (4.17) ensure that the uncertainty bound reduction is on an integer scale.
4.4.4 SafeGuards Analysis

SafeGuards Analysis (SGA) enables safeguards engineers to evaluate uncertainty across multiple MBAs. Several other software programs also use simulated uncertainty to estimate material quantities at various stages in a nuclear fuel cycle (Cipiti & McDaniel, 2012; Cipiti & Zinaman, 2010a,b; Cipiti et al., 2011; Riley et al., 2016; Wilkey & Whitty, 1995). SGA can simulate measurements using multiple forms of uncertainty, although this paper only examines basic random error. This section gives an overview of SGA.

SGA is a toolkit, not a specific model, which ensures SGA is flexible enough to apply to a wide range of problems and nuclear fuel cycles. MATLAB Simulink provides an intuitive visual interface in SGA for users without extensive scientific computing expertise. SGA estimates MUF values at one or more MBAs based on simulated measurements that include a range of uncertainties. Figure 4.4 shows the basic data flow for a single MBA in SGA.

Figure 4.4: Data flow for a measurement in SGA

Initially, the user translates a source “signal” into an SGA-compatible form using the Input Interface Block, which represents a single material quantity provided by a separate fuel cycle flow model. The signal requires either manual or automated translation via a script if the process is steady-state or time-dependent, respectively. In the Measurement Block, SGA adds uncertainty to the flow or inventory material quantity to produce a simulated measurement signal; the uncertainty
is an additive offset to the flow model value.

In the MUF Calculation block, SGA estimates MUF by incorporating the flow and inventory measurements in a material balance equation. Finally, SGA evaluates the estimated MUF value in the Statistical Analysis block by using various tests, and generates an alarm signal if a material loss is indicated. Shugart & King (2016) and Shugart et al. (2016) describe the individual blocks in detail, including the MUF estimate and different statistical tests, such as the cumulative-material-unaccounted-for, cumulative-sum, and exponential-weighted-moving-average tests. Beedgen (1988) also uses a cumulative-material-unaccounted-for test in the PROgram for Statistical Analysis (PROSA) software program to identify potential uranium loss from the Allied General Nuclear Services Barnwell Nuclear Fuels Plant.

SGA models an individual realization of this process for a given MC&A system using Simulink and the SGA library. A Monte Carlo simulation, using Matlab, evaluates multiple realizations of the SGA process, which provides Type I and Type II error probabilities. In addition, independent batches of SGA realizations provide error bounds on the Type I and Type II error probabilities. The user can define how many realizations and batches are run in the simulation.

4.5 Scenario Description

This paper examines a closed fuel cycle scenario. Figure 4.5 displays the primary facilities in the fuel cycle, which are labeled based on the materials of concern to safeguards. This scenario does not include the reactor facility, on-site storage facilities at the reactor, storage locations, or final repositories for used-nuclear-fuel because material remains in these facilities longer than the time horizon analyzed in this paper.

NUMSO and SGA obtain material quantities from VISION, which is a software program that groups facilities into single, black-box MBAs. The downside to this method is that high-fidelity material tracking is unavailable, which means VISION does not output waste material flows for many of the MBAs in this fuel cycle scenario (Jacobson & Yacout, 2010).
Because of the gap in material flow information at the reactor, the fuel cycle scenario exists in two parts: the fresh-fuel section, which produces low-enriched uranium (LEU) for use in LEU reactors, and the separations section, which manufactures mixed-oxide (MOX) fuel. Each part has materials with different significant quantities and timeliness detection goals. The first three MBAs monitor LEU while the second section of the fuel cycle considers plutonium (in both the used and MOX fuels) as the material of safeguards concern. Plutonium has a much shorter timeliness detection goal than LEU (three months for the Separations MBA, and one month for the PuO$_2$ and MOX Fuel Fabrication MBAs). Furthermore, all MBAs are distinguished based on the material form they contain.

### 4.5.1 MC&A Measurement System Problems

Obtaining solutions to the three problems introduced in Section 4.3 demonstrates the capabilities of NUMSO and SGA. Problem 1 places measurement methods in a nuclear fuel cycle given
fixed purchase and utilization budgets; Problem 2 increases the precision of the methods selected in Problem 1 given a fixed improvement budget; and Problem 3 reduces measurement uncertainty in the system while limiting improvement costs. For each problem, NUMSO considers the scaled, estimated MUF variance, instead of Type I error probabilities, because it is a metric NUMSO can use to minimize measurement system uncertainty and decrease solution times. SGA obtains Type I error probabilities because they are more meaningful and actionable to a safeguards engineer than the mathematical concept of variance.

To provide a solution to Problem 1, NUMSO enhances MVCM to find the best measurement system configuration based on a pre-defined set of hypothetical measurement methods and purchase and utilization budgets, provided in Sections 4.5.2 and 4.6.1, respectively. This scenario uses budgets that are limiting based on approximate total average costs, i.e., the product of the average of all available methods’ costs and the number of key measurement points. These budgets represent “average” methods, in terms of cost, being utilized at every key measurement point in the system. In order to ensure that the purchase and utilization budgets are limiting, MVCM also generates results with an unlimited budget to show that it yields a different solution than with a fixed budget.

SGA calculates the Type I error probabilities at each MBA that result from NUMSO’s configuration. These probabilities are compared to those from two manual analyses to ensure that there is no obvious configuration that provides a lower total Type I error probability in the system than NUMSO’s. The “manual average start” analysis initially selects methods with purchase costs closest to $500 (the approximate average cost), and then replaces them with more precise methods, where possible, while remaining under budget. The “manual cheap start” analysis initially uses methods with the lowest purchase costs, and then replaces them with more precise methods as resources allow. Combined, these analyses demonstrate that this problem does not have an obvious optimal configuration and that NUMSO’s solution is non-intuitive.

In Problem 2, MIVM minimizes the scaled, estimated MUF variance of the measurement system configuration obtained in Problem 1 by increasing the precision (i.e., decreasing the uniform
random uncertainty bounds) of measurement methods with a budget that is half of the total average improvement cost. In this problem, the estimated MUF variance scaling factor $\hat{\sigma}_k^2$ input values change from those provided in Section 4.5.2 to place more importance on the highest Type I error probabilities SGA outputs in Problem 1 for each key measurement point $k$. Section 4.6.2 provides these new scaling factor values.

To verify NUMSO’s results, the “most sensitive” analysis calculates the sensitivity of each method to determine which ones have the greatest potential Type I error probability reduction. Method sensitivity is the change in the Type I error probability obtained using each method’s initial uncertainty bounds and the initial bounds reduced by $\pm 0.05$ kg. The analysis decreases the uncertainty bounds of the most sensitive method as much as possible within the budget, and then, the most sensitive subsequent methods as resources allow. The “cheapest” analysis reduces the uncertainty bounds of each method by one unit in their order of sensitivity until there can be no additional improvements.

In Problem 3, MICM finds the most cost-effective way to reduce the scaled, estimated MUF variance of the measurement system configuration obtained in Problem 1 by 25%. In this problem, the improvement cost scaling factor $\hat{c}_k$ input values reflect the relative importance of the Type I error probabilities SGA outputs in Problem 1 for each key measurement point $k$. Section 4.6.2 provides the improvement cost scaling factors.

Instead of evaluating the scaled, estimated MUF variance, SGA examines the change in Type I error probabilities between MICM’s improved configuration and the original configuration from Problem 1 to observe the impact of increasing measurement method precision. SGA calculates the Type I error probabilities of the configurations that the most sensitive and cheapest analyses provide to verify MICM’s results.

This paper presents results from MVCM, MIVM, and MICM modeled in AMPL Version 20130109 (AMPL Optimization LLC, 2013; Fourer et al., 2003) and solved with CPLEX Version 12.6.0.1 with default settings (IBM, 2014; IBM ILOG AMPL, 2010). A Sun Fire x4250 workstation under the Ubuntu 14.04 operating system with two Quad-core CPUs running at 2.83 GHz.
GHz with 16 GB RAM performs the computations. SGA is implemented in Matlab R2014b (The MathWorks, Inc., 2014) running on a Mac Pro under the Windows 7 Pro operating system with twelve Dual-core CPUs running at 2.79 GHz with 96GB RAM. Unless otherwise noted, SGA uses a Monte Carlo simulation with 100 batches of 1,000 realizations. NUMSO and SGA both utilize a single core for computations.

4.5.2 Key Measurement Point and Measurement Method Characteristics

A number of traits define each key measurement point in the fuel cycle scenario: the material type under MC&A control (uranium or plutonium), the material form, and the flow or inventory material quantity. Differentiating each key measurement point by these three traits prevents them from appearing nearly identical to another. Having unique key measurement points is important so that NUMSO does not produce an overabundance of alternate optimal solutions for which SGA must calculate Type I error probabilities. Table 4.3 shows input values for the material type, form, and quantity, the uniform random uncertainty bounds and their associated increments $e_k^+$, and the variance scaling factor $\hat{\sigma}_k^2$ for each key measurement point $k$ in the fuel cycle scenario.

Each method’s uniform random uncertainty bounds are rated on a scale of zero to ten for ease of presentation. However, these methods require distinct error bound ranges depending on the MBA where they are utilized, which accounts for the significant quantity and timeliness detection goal limits of isotopes at different facilities in the fuel cycle scenario. Methods utilized at the Separations MBA, PuO$_2$ and MOX-based MBAs, and uranium-based MBAs have measurement uncertainty ranges between 0.1-0.5, 0.1-0.75, and 1.0-3.0 kilograms, respectively. Appendix B details the process by which the zero-ten scale is converted into the specific error bounds NUMSO and SGA use. It is also necessary to ensure that the improvement costs are based on these ranges. This paper uses ten segments for each range, which corresponds to the unitless, zero-ten uncertainty bound scale. Separations, PuO$_2$ and MOX, and uranium-based key measurement points $k$ have error bound segment increments $e_k^+$ of 0.04, 0.065, and 0.2 kilograms, respectively.

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Table 4.3: Key measurement point characteristics

<table>
<thead>
<tr>
<th>Material type</th>
<th>Material form</th>
<th>Key measurement point</th>
<th>Material quantity (kg)</th>
<th>Uncertainty bounds (kg)</th>
<th>Uncertainty bound increments (kg)</th>
<th>Variance scaling factor (unitless)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Enrichment Input</td>
<td>119858.2</td>
<td>±1.0-3.0</td>
<td>0.2</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Enrichment Output</td>
<td>13643.1</td>
<td>±1.0-3.0</td>
<td>0.2</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Enrichment Waste</td>
<td>106215.0</td>
<td>±1.0-3.0</td>
<td>0.2</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>UO₂ Conversion Input</td>
<td>13643.1</td>
<td>±1.0-3.0</td>
<td>0.2</td>
<td>0.44</td>
</tr>
<tr>
<td>Uranium</td>
<td>UO₂ Flow</td>
<td>Enrichment Inventory</td>
<td>43029080.4</td>
<td>±1.0-3.0</td>
<td>0.2</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>UO₂ Conversion Inventory</td>
<td>4911521.2</td>
<td>±1.0-3.0</td>
<td>0.2</td>
<td>0.44</td>
</tr>
<tr>
<td></td>
<td>UO₂ Flow</td>
<td>UO₂ Conversion Output</td>
<td>136431.0</td>
<td>±1.0-3.0</td>
<td>0.2</td>
<td>0.44</td>
</tr>
<tr>
<td></td>
<td></td>
<td>UOX Fuel Fabrication Input</td>
<td>136431.0</td>
<td>±1.0-3.0</td>
<td>0.2</td>
<td>0.44</td>
</tr>
<tr>
<td></td>
<td>UO₂ Inventory</td>
<td>UOX Fuel Fabrication Inventory</td>
<td>4911521.2</td>
<td>±1.0-3.0</td>
<td>0.2</td>
<td>0.44</td>
</tr>
<tr>
<td></td>
<td>U Fuel Rods</td>
<td>UOX Fuel Fabrication Output</td>
<td>136431.0</td>
<td>±1.0-3.0</td>
<td>0.2</td>
<td>0.44</td>
</tr>
<tr>
<td>Plutonium</td>
<td>Pu Fuel Rods</td>
<td>Separations Input</td>
<td>308484.0</td>
<td>±0.1-0.5</td>
<td>0.04</td>
<td>36</td>
</tr>
<tr>
<td></td>
<td></td>
<td>MOX Fuel Fabrication Output</td>
<td>147084.0</td>
<td>±0.1-0.75</td>
<td>0.065</td>
<td>7.1</td>
</tr>
<tr>
<td></td>
<td>Aqueous Solution Flow</td>
<td>Separations Waste</td>
<td>161400.0</td>
<td>±0.1-0.5</td>
<td>0.04</td>
<td>36</td>
</tr>
<tr>
<td></td>
<td>Aqueous Solution Inventory</td>
<td>Separations Inventory</td>
<td>147084.0</td>
<td>±0.1-0.5</td>
<td>0.04</td>
<td>36</td>
</tr>
<tr>
<td></td>
<td>Pu Nitrate Flow</td>
<td>Separations Output</td>
<td>147084.0</td>
<td>±0.1-0.5</td>
<td>0.04</td>
<td>36</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PuO₂ Production Input</td>
<td>147084.0</td>
<td>±0.1-0.75</td>
<td>0.065</td>
<td>7.1</td>
</tr>
<tr>
<td></td>
<td>Pu Nitrate Inventory</td>
<td>PuO₂ Production Inventory</td>
<td>5295013.5</td>
<td>±0.1-0.75</td>
<td>0.065</td>
<td>7.1</td>
</tr>
<tr>
<td></td>
<td>PuO₂ Flow</td>
<td>PuO₂ Production Output</td>
<td>147084.0</td>
<td>±0.1-0.75</td>
<td>0.065</td>
<td>7.1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>MOX Fuel Fabrication Input</td>
<td>147084.0</td>
<td>±0.1-0.75</td>
<td>0.065</td>
<td>7.1</td>
</tr>
<tr>
<td></td>
<td>PuO₂ Inventory</td>
<td>MOX Fuel Fabrication Inventory</td>
<td>5295013.5</td>
<td>±0.1-0.75</td>
<td>0.065</td>
<td>7.1</td>
</tr>
</tbody>
</table>

The variance scaling factor places a greater importance on MBAs with more key measurement points (i.e., Enrichment and Separations) to reflect the higher Type I error probabilities that result from those MBAs due to increased measurement uncertainty. NUMSO also places more weight on plutonium-based MBAs because they have a lower estimated MUF variance contribution than uranium-based MBAs, even though they have approximately the same Type I error probabilities. This method is justified by the use a uniform distribution for each measurement method, because the variance of a uniformly distributed random variable only changes based on its interval. Therefore, the least precise measurement methods yield the highest variance contributions and the most precise methods yield the lowest. This scaling method can also be used for any shift-invariant distribution, i.e., a distribution in which the mean can be shifted without any change to the variance. Normal distributions, which are often used to model random measurement errors (Bronshtein & Semendyayev, 2015, p. 849), are also shift-invariant.
Tables 4.4 and 4.5 show the various hypothetical measurement methods available with which to estimate different forms of uranium and plutonium material quantities at each stage in the fuel cycle scenario. Each method has different uniform random uncertainty bounds and associated purchase, utilization, and improvement costs to reflect the trade-offs between being precise and being more expensive to purchase, utilize, or both. Without loss of generality, this paper uses dollars to denote cost units.

**Table 4.4: Hypothetical uranium measurement methods and their properties**

<table>
<thead>
<tr>
<th>Material form</th>
<th>Measurement method</th>
<th>Uniform random error bounds</th>
<th>Purchase cost ($)</th>
<th>Utilization cost ($)</th>
<th>Improvement cost ($/e⁻ᵏ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>UF₆ Flow</td>
<td>AC20</td>
<td>±5</td>
<td>668</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>RSFF</td>
<td>±4</td>
<td>855</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>TIFD</td>
<td>±10</td>
<td>145</td>
<td>10</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>RPD</td>
<td>±2</td>
<td>909</td>
<td>2</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td>CED</td>
<td>±7</td>
<td>659</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>UF₆ Inventory</td>
<td>RDD2</td>
<td>±6</td>
<td>573</td>
<td>5</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>TIED</td>
<td>±9</td>
<td>195</td>
<td>10</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td>RSL</td>
<td>±3</td>
<td>814</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>UO₂ Flow</td>
<td>D5</td>
<td>±8</td>
<td>245</td>
<td>10</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>T1D</td>
<td>±9</td>
<td>559</td>
<td>2</td>
<td>9</td>
</tr>
<tr>
<td>UO₂ Inventory</td>
<td>RDD1</td>
<td>±7</td>
<td>523</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>RSB</td>
<td>±4</td>
<td>809</td>
<td>2</td>
<td>5</td>
</tr>
<tr>
<td>U Fuel Rods</td>
<td>CTMS5</td>
<td>±6</td>
<td>573</td>
<td>5</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>CTMS1</td>
<td>±8</td>
<td>518</td>
<td>4</td>
<td>6</td>
</tr>
</tbody>
</table>

**Table 4.5: Hypothetical plutonium measurement methods and their properties**

<table>
<thead>
<tr>
<th>Material form</th>
<th>Measurement method</th>
<th>Uniform random error bounds</th>
<th>Purchase cost ($)</th>
<th>Utilization cost ($)</th>
<th>Improvement cost ($/e⁻ᵏ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pu Fuel Rods</td>
<td>FWS</td>
<td>±10</td>
<td>100</td>
<td>11</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td>AC21</td>
<td>±6</td>
<td>573</td>
<td>5</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>EES</td>
<td>±2</td>
<td>955</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>A8I</td>
<td>±8</td>
<td>291</td>
<td>9</td>
<td>6</td>
</tr>
<tr>
<td>Aqueous Solution</td>
<td>CTMS4</td>
<td>±8</td>
<td>518</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>Flow</td>
<td>ST</td>
<td>±2</td>
<td>500</td>
<td>11</td>
<td>11</td>
</tr>
<tr>
<td>Aqueous Solution</td>
<td>A9I</td>
<td>±6</td>
<td>482</td>
<td>7</td>
<td>6</td>
</tr>
<tr>
<td>Inventory</td>
<td>RT5</td>
<td>±7</td>
<td>477</td>
<td>6</td>
<td>9</td>
</tr>
<tr>
<td>Pu Nitrate Flow</td>
<td>TIID</td>
<td>±9</td>
<td>195</td>
<td>10</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>D3IG8</td>
<td>±8</td>
<td>200</td>
<td>11</td>
<td>10</td>
</tr>
<tr>
<td>Pu Nitrate Inventory</td>
<td>RSI</td>
<td>±2</td>
<td>909</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>A92</td>
<td>±7</td>
<td>341</td>
<td>9</td>
<td>10</td>
</tr>
<tr>
<td>PuO₂ Flow</td>
<td>A8</td>
<td>±8</td>
<td>382</td>
<td>7</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>D3HE7</td>
<td>±4</td>
<td>200</td>
<td>11</td>
<td>9</td>
</tr>
<tr>
<td>PuO₂ Inventory</td>
<td>D6</td>
<td>±9</td>
<td>241</td>
<td>9</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td>A1I</td>
<td>±6</td>
<td>300</td>
<td>11</td>
<td>11</td>
</tr>
</tbody>
</table>
4.6 NUMSO Results and Analysis

This section provides NUMSO’s results and analyses for Problems 1-3. This paper uses a realistic fuel cycle scenario with hypothetical measurement methods to convey the capabilities of NUMSO and presents examples of the relative differences and trends that it can provide.

4.6.1 Problem 1 NUMSO Results

Table 4.6 shows the optimal measurement system configuration results for unlimited and fixed budgets. This table also provides the optimal placement of measurement methods for the scaled and unscaled, estimated MUF variance objectives with a fixed budget. NUMSO takes 1.5 seconds to generate solutions for Problem 1, compared to 8 hours per SGA analysis.

Table 4.6: Optimal measurement system configuration for unlimited and fixed budgets with scaled or unscaled, estimated MUF variance objectives. Shaded rows denote key measurement points at which the same, most precise method is utilized for unlimited and fixed budgets.

<table>
<thead>
<tr>
<th>Material</th>
<th>Key measurement point</th>
<th>Unlimited budget</th>
<th>Fixed budget</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Measurement method</td>
<td>Scaled variance (kg²)</td>
</tr>
<tr>
<td>Enrichment Input</td>
<td>RPD</td>
<td>0.65</td>
<td>RSFF 1.1</td>
</tr>
<tr>
<td>Enrichment Output</td>
<td>RPD</td>
<td>0.65</td>
<td>RSFF 1.1</td>
</tr>
<tr>
<td>Enrichment Waste</td>
<td>RPD</td>
<td>0.65</td>
<td>RSFF 1.1</td>
</tr>
<tr>
<td>Enrichment Inventory</td>
<td>RSL</td>
<td>0.85</td>
<td>RSL 0.85</td>
</tr>
<tr>
<td>UO₂ Conversion Input</td>
<td>RPD</td>
<td>0.29</td>
<td>TIFD 1.3</td>
</tr>
<tr>
<td>UO₂ Conversion Output</td>
<td>D5</td>
<td>1.0</td>
<td>T1D 1.2</td>
</tr>
<tr>
<td>UO₂ Conversion Inventory</td>
<td>RSL</td>
<td>0.38</td>
<td>TIED 1.2</td>
</tr>
<tr>
<td>UOX Fuel Fabrication Input</td>
<td>D5</td>
<td>1.0</td>
<td>T1D 1.2</td>
</tr>
<tr>
<td>UOX Fuel Fabrication Output</td>
<td>CTMS5</td>
<td>0.72</td>
<td>CTMS1 1.0</td>
</tr>
<tr>
<td>UOX Fuel Fabrication Inventory</td>
<td>RSB</td>
<td>0.48</td>
<td>RDD1 0.85</td>
</tr>
<tr>
<td>Separations Input</td>
<td>EES</td>
<td>0.39</td>
<td>EES 0.39</td>
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<td>Separations Output</td>
<td>D3IG8</td>
<td>2.1</td>
<td>D3IG8 2.1</td>
</tr>
<tr>
<td>Separations Waste</td>
<td>ST</td>
<td>0.39</td>
<td>CTMS4 2.1</td>
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<tr>
<td>Separations Inventory</td>
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<td>1.4</td>
<td>A9I 1.4</td>
</tr>
<tr>
<td>PuO₂ Production Input</td>
<td>D3IG8</td>
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<td>D3IG8 0.91</td>
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<td>D3IE7</td>
<td>0.31</td>
<td>D3IE7 0.31</td>
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<td>PuO₂ Production Inventory</td>
<td>RSI</td>
<td>0.13</td>
<td>A9I2 0.73</td>
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<tr>
<td>MOX Fuel Fabrication Input</td>
<td>D3IE7</td>
<td>0.31</td>
<td>D3IE7 0.31</td>
</tr>
<tr>
<td>MOX Fuel Fabrication Output</td>
<td>EES</td>
<td>0.13</td>
<td>FWS 1.3</td>
</tr>
<tr>
<td>MOX Fuel Fabrication Inventory</td>
<td>AII</td>
<td>0.56</td>
<td>D6 1.1</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>13</td>
<td>21</td>
</tr>
</tbody>
</table>

Every key measurement point utilizes the most precise measurement methods with an unlimited budget, as opposed to only 35% and 10% of the key measurement points with a fixed budget.
considering scaled or unscaled, estimated MUF variance, respectively. This means that many trade-offs are necessary to balance the budget while minimizing the scaled or unscaled, estimated MUF variance. Table 4.7 shows that the purchase and utilization budgets are limiting in Problem 1 because, although the budgets are not met exactly, there are not enough resources to purchase or utilize an additional measurement method. The measurement system configuration with a fixed budget contains methods that are more expensive to use than with an unlimited budget, which helps offset the scaled, estimated MUF variance reduction from purchasing more imprecise methods.

Table 4.7: Input budgets and output costs to purchase and utilize measurement methods for Problem 1

<table>
<thead>
<tr>
<th>Context</th>
<th>Purchase budget ($)</th>
<th>Purchase cost ($)</th>
<th>Utilization budget ($)</th>
<th>Utilization cost ($)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unlimited budget</td>
<td>∞</td>
<td>12,037</td>
<td>∞</td>
<td>118</td>
</tr>
<tr>
<td>Fixed budget - Scaled</td>
<td>9,316</td>
<td>9,315</td>
<td>126</td>
<td>124</td>
</tr>
<tr>
<td>Fixed budget - Unscaled</td>
<td>9,316</td>
<td>9,274</td>
<td>126</td>
<td>126</td>
</tr>
</tbody>
</table>

Plutonium has lower significant quantity and timeliness detection goal limits than uranium, which indicates that plutonium measurements have a smaller unscaled, estimated MUF variance contribution than uranium measurements to obtain similar Type I error probabilities. The scaled, estimated MUF variance contribution at key measurement points containing uranium (11 kg) is approximately equal to the contribution at plutonium-based key measurement points plutonium (10 kg). This shows the scaling factor is necessary to prevent the unscaled, estimated MUF variance contribution of uranium (15 kg) from dominating that of plutonium (1.0 kg).

4.6.2 Problem 2 NUMSO Results

Table 4.8 provides the estimated MUF variance and improvement cost scaling factors based on the Type I error probabilities SGA generates in Problem 1 (presented in Section 4.7). The estimated MUF variance scaling factors are obtained by weighting the Type I error probability for each key measurement point (grouped by MBA) based on the highest Type I error probability in the system (UO$_2$ Conversion). Plutonium-based MBAs have scaling factors greater than one because they have lower estimated MUF variance contributions than uranium-based MBAs. The
Improvement cost scaling factors are determined similarly, but are based on the lowest Type I error probability in the system (PuO$_2$ Production), rather than the highest.

Table 4.8: Estimated MUF variance and improvement cost scaling factors for each MBA

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Enrichment</th>
<th>UO$_2$ Conversion</th>
<th>UOX Fuel Fabrication</th>
<th>Separations</th>
<th>PuO$_2$ Production</th>
<th>MOX Fuel Fabrication</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\hat{\sigma}^2_k$</td>
<td>0.2887</td>
<td>1.000</td>
<td>0.7555</td>
<td>23.79</td>
<td>1.062</td>
<td>6.942</td>
</tr>
<tr>
<td>$\hat{c}_k^I$</td>
<td>0.1022</td>
<td>0.02950</td>
<td>0.03905</td>
<td>0.04466</td>
<td>1.000</td>
<td>0.1530</td>
</tr>
</tbody>
</table>

Table 4.9 shows which measurement methods to improve and how much to reduce their uncertainty bounds given a budget of $66. MIVM only increases the precision of methods utilized at the UO$_2$ Conversion and Separations MBAs because they have two of the three highest scaled, estimated variance contributions, and similarly, the highest Type I error probabilities. These improvements reduce the scaled, estimated MUF variance by 13%. NUMSO takes 0.13 seconds to generate solutions for Problem 2, compared to 8.5 hours per SGA analysis.

Table 4.9: Optimal measurement method improvements for a fixed budget of $66

<table>
<thead>
<tr>
<th>Key measurement point</th>
<th>Measurement method</th>
<th>Improvement amount (kg)</th>
<th>Improvement cost ($)</th>
<th>Scaled variance reduction (kg$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>UO$_2$ Conversion Output</td>
<td>T1D</td>
<td>0.80</td>
<td>24</td>
<td>0.57</td>
</tr>
<tr>
<td>UO$_2$ Conversion Inventory</td>
<td>TIED</td>
<td>0.80</td>
<td>24</td>
<td>0.57</td>
</tr>
<tr>
<td>Separations Waste</td>
<td>CTMS4</td>
<td>0.24</td>
<td>18</td>
<td>1.7</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>1.8</td>
<td>66</td>
<td>2.9</td>
</tr>
</tbody>
</table>

MIVM uses the most resources to reduce the uncertainty bounds of the methods utilized at the UO$_2$ Conversion MBA because they are very imprecise with uncertainty bounds of Uniform(-9, 9). Even though these methods are fairly expensive to improve, reducing their uncertainty bounds has the largest potential reduction to Type I error probabilities. Section 4.7 shows that the UO$_2$ Conversion and Separations MBAs have two of the three highest Type I error probabilities for the optimal measurement system configuration obtained in Problem 1. These results indicate that it might be more beneficial to enhance imprecise, rather than the cheapest, measurement methods because they give the highest Type I error probabilities.
4.6.3 Problem 3 NUMSO Results

Table 4.10 shows which measurement methods to improve and how much to reduce their uncertainty bounds to reduce the scaled, estimated MUF variance by at least 25% in the most cost-effective manner. MICM reduces the scaled, estimated MUF variance by just over 25% with an improvement cost of $90. NUMSO takes 0.35 seconds to generate solutions for Problem 3, compared to 8.0 hours per SGA analysis.

Table 4.10: Optimal measurement method improvements to reduce the scaled, estimated MUF variance by 25%

<table>
<thead>
<tr>
<th>Key measurement point</th>
<th>Measurement method</th>
<th>Improvement amount (kg)</th>
<th>Improvement cost ($)</th>
<th>Scaled variance reduction (kg²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Enrichment Input</td>
<td>RSFF</td>
<td>0.6</td>
<td>6</td>
<td>0.60</td>
</tr>
<tr>
<td>Enrichment Output</td>
<td>RSFF</td>
<td>0.4</td>
<td>4</td>
<td>0.43</td>
</tr>
<tr>
<td>Enrichment Waste</td>
<td>RSFF</td>
<td>0.4</td>
<td>4</td>
<td>0.43</td>
</tr>
<tr>
<td>UO₂ Conversion Output</td>
<td>T1D</td>
<td>0.4</td>
<td>12</td>
<td>0.31</td>
</tr>
<tr>
<td>UO₂ Conversion Inventory</td>
<td>TIED</td>
<td>0.2</td>
<td>6</td>
<td>0.16</td>
</tr>
<tr>
<td>Separations Input</td>
<td>EES</td>
<td>0.08</td>
<td>6</td>
<td>0.27</td>
</tr>
<tr>
<td>Separations Output</td>
<td>D3IG8</td>
<td>0.04</td>
<td>10</td>
<td>0.38</td>
</tr>
<tr>
<td>Separations Waste</td>
<td>CTMS4</td>
<td>0.32</td>
<td>24</td>
<td>2.0</td>
</tr>
<tr>
<td>Separations Inventory</td>
<td>A9I</td>
<td>0.12</td>
<td>18</td>
<td>0.81</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>3.0</td>
<td>90</td>
<td>5.4</td>
</tr>
</tbody>
</table>

Similar to Problem 2, MICM uses a large portion of the improvement cost to reduce the uncertainty bounds of methods at the UO₂ Conversion MBA. In addition, MICM allocates a large portion of resources at the Separations MBA, which has very imprecise methods (except for EES) and the third highest Type I error probability. However, these results also show that MICM improves methods at the Enrichment MBA, which has fairly precise, but cheap-to-improve methods, indicating that it is also beneficial to reduce the uncertainty bounds of methods with a low improvement cost.

Figure 4.6 shows that there is a nonlinear relationship between the scaled, estimated MUF variance and the improvement cost. This result indicates that there might be a point at which an additional percent reduction in the scaled, estimated MUF variance is no longer worth the cost.
Figure 4.6: Relationship between the scaled, estimated MUF variance reduction and improvement cost

4.7 SGA Results and Analysis

This section illustrates the comparative analysis done in SGA to examine NUMSO’s results. For Problems 1-3, SGA manually creates intuitive solutions using several analyses and compares them to NUMSO’s results. There is no guarantee that minimizing the scaled, estimated MUF variance in a multi-material measurement system yields the same configuration and improvements as minimizing Type I error probabilities. Unlike NUMSO, SGA’s ability to calculate Type I error probabilities for each MBA, or any combination of MBAs, makes it an ideal tool to analyze if minimizing the scaled, estimated MUF variance yields good results.

4.7.1 Problem 1 SGA Results

Table 4.11 shows the configurations from the manual average start and manual cheap start SGA analyses and NUMSO are very different, which implies that the optimal configuration based on the scaled, estimated MUF variance is not intuitive. Only 25% of the key measurement points contain the same measurement method for all three analyses.
Table 4.11: Measurement system configurations obtained from two SGA analyses and NUMSO. Shaded rows denote key measurement points at which the same method is utilized.

<table>
<thead>
<tr>
<th>Material</th>
<th>Key measurement point</th>
<th>Manual average start analysis</th>
<th>Measurement methods</th>
<th>NUMSO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uranium</td>
<td>Enrichment Input</td>
<td>CED</td>
<td>CED</td>
<td>RSFF</td>
</tr>
<tr>
<td></td>
<td>Enrichment Output</td>
<td>RSFF</td>
<td>RPD</td>
<td>RSFF</td>
</tr>
<tr>
<td></td>
<td>Enrichment Waste</td>
<td>TIFD</td>
<td>CED</td>
<td>RSFF</td>
</tr>
<tr>
<td></td>
<td>Enrichment Inventory</td>
<td>RDD2</td>
<td>T1D</td>
<td>RSL</td>
</tr>
<tr>
<td></td>
<td>UO₂ Conversion Input</td>
<td>RSFF</td>
<td>CED</td>
<td>TIFD</td>
</tr>
<tr>
<td></td>
<td>UO₂ Conversion Output</td>
<td>T1D</td>
<td>T1D</td>
<td>T1D</td>
</tr>
<tr>
<td></td>
<td>UO₂ Conversion Inventory</td>
<td>RDD2</td>
<td>RDD2</td>
<td>TIED</td>
</tr>
<tr>
<td></td>
<td>UOX Fuel Fabrication Input</td>
<td>T1D</td>
<td>D5</td>
<td>T1D</td>
</tr>
<tr>
<td></td>
<td>UOX Fuel Fabrication Output</td>
<td>CTMS1</td>
<td>CTMS1</td>
<td>CTMS1</td>
</tr>
<tr>
<td></td>
<td>UOX Fuel Fabrication Inventory</td>
<td>RDD1</td>
<td>RDD1</td>
<td>RDD1</td>
</tr>
<tr>
<td>Plutonium</td>
<td>Separations Input</td>
<td>FWS</td>
<td>A8I</td>
<td>EES</td>
</tr>
<tr>
<td></td>
<td>Separations Output</td>
<td>D3IG8</td>
<td>TIID</td>
<td>D3IG8</td>
</tr>
<tr>
<td></td>
<td>Separations Waste</td>
<td>ST</td>
<td>ST</td>
<td>CTMS4</td>
</tr>
<tr>
<td></td>
<td>Separations Inventory</td>
<td>A9I</td>
<td>RT5</td>
<td>A9I</td>
</tr>
<tr>
<td></td>
<td>PuO₂ Production Input</td>
<td>D3IG8</td>
<td>TIID</td>
<td>D3IG8</td>
</tr>
<tr>
<td></td>
<td>PuO₂ Production Output</td>
<td>A8</td>
<td>D3IE7</td>
<td>D3IE7</td>
</tr>
<tr>
<td></td>
<td>PuO₂ Production Inventory</td>
<td>A92</td>
<td>A92</td>
<td>A92</td>
</tr>
<tr>
<td></td>
<td>MOX Fuel Fabrication Input</td>
<td>A8</td>
<td>A8I</td>
<td>D3IE7</td>
</tr>
<tr>
<td></td>
<td>MOX Fuel Fabrication Output</td>
<td>AC21</td>
<td>AC21</td>
<td>FWS</td>
</tr>
<tr>
<td></td>
<td>MOX Fuel Fabrication Inventory</td>
<td>D6</td>
<td>D6</td>
<td>D6</td>
</tr>
</tbody>
</table>

Table 4.12 shows the Type I error probabilities that result from the configurations produced using the most (best possible) and least (worst possible) precise measurement methods, each SGA analysis, and NUMSO. For some of the individual MBAs, the SGA analyses yield lower Type I error probabilities than the NUMSO measurement system configuration, such as for the UO₂ Conversion and MOX Fuel Fabrication MBAs. However, this comes at the cost of having higher Type I error probabilities for nearly every other MBA. The SGA analyses do not provide an intuitive solution that is objectively better than NUMSO’s. This result reinforces that for a simplified example, such as this, NUMSO is able to generate a comparable solution far faster than intuitive analyses (1.5 seconds compared to 8.0 hours per SGA analysis).

4.7.2 Problem 2 SGA Results

For Problem 2, SGA uses the most sensitive and cheapest analyses to compare the Type I error probabilities that result from their improvements to those from NUMSO. Table 4.13 shows the sensitivity of Type I error probabilities at each key measurement point; the probabilities are calcu-
lated by improving the random uncertainty bounds of each method by ±0.05 kg. Because of the inherently small difference between the original and improved Type I error probabilities, the sensitivity analysis uses a Monte Carlo method with 200 batches of 4,000 SGA realizations. Even with this increase in the number of realizations, there are only four key measurement points at which the difference in Type I error probabilities in the sensitivity analysis exceeds three standard deviations with a 99% confidence interval. These are Separations Output and Waste, PuO\(_2\) Production Input, and MOX Fuel Fabrication Output.

Table 4.13: SGA sensitivity analysis on the Type I error probabilities at each key measurement point. Shaded rows denote the key measurement points SGA uses in the most sensitive analysis.
Based on these values, the most sensitive analysis focuses on improving the uncertainty bounds of methods at these four key measurement points. The cheapest analysis increases each of the lowest improvement cost methods with the process described in Section 4.5.1. Table 4.14 shows the cost expenditures and uncertainty bound improvement amounts for NUMSO and the two SGA analyses.

Table 4.14: Measurement method uncertainty bound improvement amounts and cost expenditures at key measurement points for a fixed budget of $66 using NUMSO and two SGA analyses

<table>
<thead>
<tr>
<th>Key measurement point</th>
<th>NUMSO</th>
<th>Most sensitive analysis</th>
<th>Cheapest analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Improvement amount (kg)</td>
<td>Improvement cost ($)</td>
</tr>
<tr>
<td>Enrichment Input</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Enrichment Output</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Enrichment Waste</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Enrichment Inventory</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>UO₂ Conversion Input</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>UO₂ Conversion Output</td>
<td>0.80</td>
<td>24</td>
<td>0.00</td>
</tr>
<tr>
<td>UO₂ Conversion Inventory</td>
<td>0.80</td>
<td>24</td>
<td>0.00</td>
</tr>
<tr>
<td>UOX Fuel Fabrication Inventory</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Separations Input</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Separations Output</td>
<td>0.00</td>
<td>0.08</td>
<td>20</td>
</tr>
<tr>
<td>Separations Waste</td>
<td>0.24</td>
<td>18</td>
<td>0.08</td>
</tr>
<tr>
<td>PO₂ Production Input</td>
<td>0.00</td>
<td>0.13</td>
<td>20</td>
</tr>
<tr>
<td>MOX Fuel Fabrication Output</td>
<td>0.00</td>
<td>0.13</td>
<td>20</td>
</tr>
</tbody>
</table>

Table 4.15 shows the Type I error probabilities for each SGA analysis and NUMSO at each MBA. The base analysis represents the original configuration without improvements. This table shows that for a budget of $66, NUMSO provides the best improvement, although it is only slightly better than the solution from the cheapest analysis. This result occurs because NUMSO focuses on improving UO₂ Conversion, which has the highest Type I error probability. The limitation of the most sensitive analysis is that the key measurement points with the highest sensitivity in this configuration have relatively low Type I error probabilities. Hence, while these improvements have a large relative impact on Type I error probabilities, this analysis uses much of the budget at key measurement points that have a comparatively low total Type I error probability in the system, which limits their effectiveness.
Table 4.15: Problem 2 Type I error probabilities at each MBA for SGA analyses and NUMSO

<table>
<thead>
<tr>
<th>Analysis</th>
<th>Enrichment</th>
<th>UO&lt;sub&gt;2&lt;/sub&gt; Conversion</th>
<th>UOX Fuel Fabrication</th>
<th>Separations</th>
<th>PuO&lt;sub&gt;2&lt;/sub&gt; Production</th>
<th>MOX Fuel Fabrication</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>2.74±0.58</td>
<td>9.49±0.92</td>
<td>7.17±0.88</td>
<td>6.27±0.37</td>
<td>0.28±0.18</td>
<td>1.83±0.40</td>
<td>27.78±1.5</td>
</tr>
<tr>
<td>Most sensitive</td>
<td>2.65±0.56</td>
<td>9.32±0.85</td>
<td>7.07±0.70</td>
<td>1.51±0.38</td>
<td>0.01±0.04</td>
<td>0.28±0.16</td>
<td>20.84±1.3</td>
</tr>
<tr>
<td>Cheapest</td>
<td>0.01±0.02</td>
<td>9.61±0.91</td>
<td>6.90±0.76</td>
<td>1.09±0.30</td>
<td>0.28±0.18</td>
<td>1.84±0.43</td>
<td>19.73±1.3</td>
</tr>
<tr>
<td>NUMSO</td>
<td>2.69±0.55</td>
<td>5.60±0.64</td>
<td>7.23±0.80</td>
<td>0.97±0.29</td>
<td>0.23±0.16</td>
<td>1.90±0.43</td>
<td>18.62±1.3</td>
</tr>
</tbody>
</table>

4.7.3 Problem 3 SGA Results

For Problem 3, SGA uses the most sensitive and cheapest analyses to compare Type I error probabilities against those that result from NUMSO’s measurement system configuration. For each analysis, the improvement is bounded by the cost incurred by NUMSO of $90. Table 4.16 shows the cost expenditures and uncertainty bound improvement amounts for NUMSO and the two SGA analyses.

Table 4.16: Measurement method uncertainty bound improvement amounts and cost expenditures at key measurement points for a fixed budget of $90 using NUMSO and two SGA analyses

<table>
<thead>
<tr>
<th>Key measurement point</th>
<th>NUMSO</th>
<th>Most sensitive analysis</th>
<th>Cheapest analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Improvement amount (kg)</td>
<td>Improvement cost ($)</td>
<td>Improvement amount (kg)</td>
</tr>
<tr>
<td>Enrichment Input</td>
<td>0.60</td>
<td>6</td>
<td>0.00</td>
</tr>
<tr>
<td>Enrichment Output</td>
<td>0.40</td>
<td>4</td>
<td>0.00</td>
</tr>
<tr>
<td>Enrichment Waste</td>
<td>0.40</td>
<td>4</td>
<td>0.00</td>
</tr>
<tr>
<td>Enrichment Inventory</td>
<td>0.00</td>
<td>0</td>
<td>0.00</td>
</tr>
<tr>
<td>UO&lt;sub&gt;2&lt;/sub&gt; Conversion Input</td>
<td>0.00</td>
<td>0</td>
<td>0.00</td>
</tr>
<tr>
<td>UO&lt;sub&gt;2&lt;/sub&gt; Conversion Output</td>
<td>0.40</td>
<td>12</td>
<td>0.00</td>
</tr>
<tr>
<td>UO&lt;sub&gt;2&lt;/sub&gt; Conversion Inventory</td>
<td>0.20</td>
<td>6</td>
<td>0.00</td>
</tr>
<tr>
<td>UOX Fuel Fabrication Inventory</td>
<td>0.00</td>
<td>0</td>
<td>0.00</td>
</tr>
<tr>
<td>Separations Input</td>
<td>0.08</td>
<td>6</td>
<td>0.00</td>
</tr>
<tr>
<td>Separations Output</td>
<td>0.04</td>
<td>10</td>
<td>0.12</td>
</tr>
<tr>
<td>Separations Waste</td>
<td>0.32</td>
<td>24</td>
<td>0.12</td>
</tr>
<tr>
<td>Separations Inventory</td>
<td>0.12</td>
<td>18</td>
<td>0.00</td>
</tr>
<tr>
<td>PO&lt;sub&gt;2&lt;/sub&gt; Production Input</td>
<td>0.00</td>
<td>0</td>
<td>0.13</td>
</tr>
<tr>
<td>MOX Fuel Fabrication Output</td>
<td>0.00</td>
<td>0</td>
<td>0.20</td>
</tr>
</tbody>
</table>

Table 4.17 shows the Type I error probabilities for each SGA analysis and NUMSO at each MBA. The base analysis represents the original configuration without improvements. NUMSO obtains the best total Type I error probability in the system. Similar to the results in Problem 2, the configuration from the most sensitive analysis does not provide the greatest improvement. These results indicate that NUMSO is able to provide a better total Type I error probability than two
Table 4.17: Problem 3 Type I error probabilities at each MBA for SGA analyses and NUMSO

<table>
<thead>
<tr>
<th>Analysis</th>
<th>Enrichment</th>
<th>UO₂ Conversion</th>
<th>Type I error Probabilities</th>
<th>MOX Fuel Fabrication</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>UOX Fuel Fabrication</td>
<td>PuO₂ Production</td>
<td></td>
</tr>
<tr>
<td>Base</td>
<td>2.74±0.58</td>
<td>9.49±0.92</td>
<td>7.17±0.88</td>
<td>6.27±0.37</td>
<td>1.83±0.40</td>
</tr>
<tr>
<td>Most sensitive</td>
<td>2.76±0.54</td>
<td>9.50±0.99</td>
<td>7.00±0.77</td>
<td>0.50±0.23</td>
<td>0.01±0.03</td>
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<td>0.11±0.10</td>
<td>0.23±0.15</td>
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intuitive analyses, although there is no guarantee that it is optimal.

4.8 Conclusion

The dangerous ability to make nuclear weapons from uranium-235 and plutonium-239 makes it imperative to account closely for these materials as they progress through a nuclear fuel cycle. Many instances of theft or loss of nuclear and other radioactive material have occurred in the last two decades, which indicate that the potential loss of this material is still a threat. Improving MC&A methods gives a more accurate estimate of material quantities and MUF in the system.

This paper provides solutions to three potential problems in MC&A measurement systems: how to (i) locate measurement methods in a nuclear fuel cycle given fixed purchase and utilization budgets (Problem 1), (ii) increase the precision of existing methods given a fixed improvement budget (Problem 2), and (iii) reduce measurement uncertainty in the system while limiting improvement costs (Problem 3). NUMSO uses operations research techniques, specifically, integer programming, to find optimal solutions to these problems based on minimizing the scaled, estimated MUF variance in the system. SGA employs a Monte Carlo simulation to analyze if NUMSO provides good solutions in terms of the Type I error probabilities in a measurement system.

This paper examines a closed fuel cycle scenario that does not include the reactor facility, on-site storage facilities at the reactor, storage locations, or final repositories for used-nuclear-fuel because material remains in these facilities longer than the time horizon analyzed in this paper. NUMSO and SGA use hypothetical measurement methods because the focus of this paper is to demonstrate their ability to provide answers to representative problems.
Results from SGA analyses show that NUMSO provides a measurement system configuration in Problem 1 and improvements in Problems 2-3 that not only minimize the scaled, estimated MUF variance, but also yield similar or better total Type I error probabilities compared to intuitive analyses. For every problem, NUMSO has a much smaller solution time than the SGA analyses. The quick solution times also indicate that much larger, more complicated fuel cycle scenarios can be examined using NUMSO.

SGA provides accurate Type I error probabilities for each MBA in the fuel cycle, which is a more meaningful metric to safeguards engineers than estimated MUF variance. This paper shows that for this fuel cycle scenario, NUMSO yields similar or better solutions in terms of Type I error probabilities much faster than several intuitive analyses. However, the authors recommend that a thorough comparison be performed using SGA to ensure that, for a specific application, NUMSO yields acceptable Type I error probabilities.

Further research could examine whether there is a mathematical relationship between significant quantity and timeliness detection goal limits for different isotopes and the estimated MUF variance in a measurement system. Such a connection could provide a better justification for the variance scaling factors to relate the scaled, estimated MUF variance and the Type I error probabilities. Additionally, SGA and NUMSO could evaluate a larger, more complex fuel cycle scenario to show their extensibility.

4.9 Acknowledgments

This paper is made possible thanks to the insights provided by Dr. Aaron Porter of the Department of Applied Mathematics and Statistics at the Colorado School of Mines and Dr. R. Kevin Wood of the Operations Research Department at the Naval Postgraduate School regarding MVCM, and Jake Jacobson at the Center for Advanced Energy Studies at the University of Idaho for helping develop the fuel cycle scenario. The National Nuclear Security Administration provides funding for this paper under Grant DE-NA0001730.
CHAPTER 5
CONCLUSION

This dissertation shows that operations research techniques yield solutions that provide better objective values and are able to be obtained faster than solutions from existing and intuitive methods in nuclear waste disposal and nuclear safeguards. Our results highlight the benefit of using operations research techniques to solve complex nuclear energy problems and indicate that larger, more complicated applications can be examined with these techniques.

In the first paper, we develop a mixed-integer programming model that creates an optimal, reproducible schedule for nuclear waste placement, using the Yucca Mountain repository in Nevada as a case study. The optimal solution determines where to place each waste package of a specific type in a given time period with the goal of minimizing heat load concentration within a repository. Existing filling methods give at least a 17% to an 873% higher, i.e., worse, heat load concentration in the repository with respect to these objectives than do optimal methods. The performance enhancements incorporated in the model increase the solvable model size. This research can be applied to any of the repositories planned for operation around the world with slight modifications to incorporate site-specific objectives and constraints.

In the second paper, we use a simulation-optimization algorithm and an integer-programming model to find the optimal measurement system configuration with a pre-specified level of confidence. We obtain similar results to existing outcomes, but are able to generate them at least an order of magnitude faster. In the third paper, we develop two mixed-integer quadratic programming models to increase the precision of existing measurement methods given a fixed improvement budget and to reduce the measurement uncertainty in the system while limiting improvement costs. We quickly obtain similar or better solutions compared to several intuitive analyses that take much longer to perform.
REFERENCES CITED


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APPENDIX A - MVCM PROPERTIES

In this appendix we derive the properties of the MVCM formulation for a single key measurement point. We begin by considering a continuous time \( \tilde{C}_t \) modeled by a Gaussian Process.

Type I error case:

Let \( \tilde{C}_{1t} \) be a Gaussian Process without drift, and \( \text{Var}(\tilde{C}_{1,t+\tau} - \tilde{C}_{1t}) = \sigma_1^2 \tau \) with independent increments. Let \( T_{\lambda} \) be the first time \( \tilde{C}_{1t} = \lambda \).

Let \( \tilde{C}_{2t} \) be a Gaussian Process without drift, and \( \text{Var}(\tilde{C}_{2,t+\tau} - \tilde{C}_{2t}) = \sigma_2^2 \tau \) with independent increments where \( \sigma_2^2 < \sigma_1^2 \). Let \( S_{\lambda} \) be the first time \( \tilde{C}_{2t} = \lambda \).

\[
P(\tilde{C}_{1t} \geq \lambda) = P(\tilde{C}_{1t} \geq \lambda | T_{\lambda} \leq t)P(T_{\lambda} \leq t) + P(\tilde{C}_{1t} \geq \lambda | T_{\lambda} > t)P(T_{\lambda} > t) \tag{A.1}
\]

note \( P(\tilde{C}_{1t} \geq \lambda | T_{\lambda} \leq t) = \frac{1}{2} \) and \( P(\tilde{C}_{1t} \geq \lambda | T_{\lambda} > t) = 0 \) \tag{A.2}

\[\Rightarrow P(T_{\lambda} \leq t) = 2P(\tilde{C}_{1t} \geq \lambda) \tag{A.3}\]

Similarly,

\[
P(S_{\lambda} \leq t) = 2P(\tilde{C}_{2t} \geq \lambda) \tag{A.4}\]

Now, we have:

\[
P(\tilde{C}_{1t} \geq \lambda) = \int_{-\infty}^{\lambda/\sqrt{\sigma_1}} \frac{1}{\sqrt{2\pi\sigma_1^2t}} \exp\left(-\frac{x^2}{2\sigma_1^2t}\right)dx
\]

\[> \int_{-\infty}^{\lambda/\sqrt{\sigma_2}} \frac{1}{\sqrt{2\pi\sigma_2^2t}} \exp\left(-\frac{y^2}{2\sigma_2^2t}\right)dy = P(\tilde{C}_{2t} \geq \lambda) \tag{A.5}\]

Therefore, reducing the variance at a single key measurement point reduces the Type I error probability for a device at that key measurement point before any time \( t \).
Type II error case:

Let \( \tilde{C}_t \) be a Gaussian Process with drift \( C_t \), and \( \text{Var}(\tilde{C}_{1,t} - \tilde{C}_t) = \sigma_1^2 \tau \) with independent increments. Let \( T_{\Lambda} \) be the first time \( \tilde{C}_{1,t} = \Lambda \).

Let \( \tilde{C}_t \) be a Gaussian Process with drift \( C_t \), and \( \text{Var}(\tilde{C}_{2,t} - \tilde{C}_t) = \sigma_2^2 \tau \) with independent increments where \( \sigma_2^2 < \sigma_1^2 \). Let \( S_{\Lambda} \) be the first time \( \tilde{C}_{2,t} = \Lambda \).

\[
P(\tilde{C}_{1,t} \geq \Lambda) = P(\tilde{C}_{1,t} \geq \Lambda | T_{\Lambda} \leq t)P(T_{\Lambda} \leq t) + P(\tilde{C}_{1,t} \geq \Lambda | T_{\Lambda} > t)P(T_{\Lambda} > t) \quad (A.6)
\]

\[
\Rightarrow P(\tilde{C}_{1,t} - C_t \geq \Lambda - C_t | T_{\Lambda} \leq t) = \int_{\Lambda}^{\infty} \frac{1}{\sqrt{2\pi \sigma_1^2 t}} \exp\left(-\frac{(x - C_t)^2}{2\sigma_1^2 t}\right) dx \quad (A.7)
\]

\[
\Rightarrow P(T_{\Lambda} \geq t) = \int_{\Lambda}^{\infty} \frac{1}{\sqrt{2\pi \sigma_1^2 t}} \exp\left(-\frac{(x - C_t)^2}{2\sigma_1^2 t}\right) P(\tilde{C}_{1,t} \geq \Lambda) \quad (A.8)
\]

Similarly,

\[
P(S_{\Lambda} \geq t) = \int_{\Lambda}^{\infty} \frac{1}{\sqrt{2\pi \sigma_2^2 t}} \exp\left(-\frac{(y - C_t)^2}{2\sigma_2^2 t}\right) dx \quad (A.9)
\]

Now, we have:

\[
P(T_{\Lambda} \geq t) = \frac{\int_{\Lambda}/(\sqrt{\tau} \sigma_1) \frac{1}{\sqrt{2\pi \sigma_1^2 t}} \exp\left(-\frac{(x - C_t)^2}{2\sigma_1^2 t}\right) dx}{\int_{\Lambda}^{\infty} \frac{1}{\sqrt{2\pi \sigma_1^2 t}} \exp\left(-\frac{(x - C_t)^2}{2\sigma_1^2 t}\right) dx} \quad (A.10)
\]

which is not uniformly related to

\[
\int_{\Lambda}^{\infty} \frac{1}{\sqrt{2\pi \sigma_2^2 t}} \exp\left(-\frac{(y - C_t)^2}{2\sigma_2^2 t}\right) dy = \int_{\Lambda}^{\infty} \frac{1}{\sqrt{2\pi \sigma_2^2 t}} \exp\left(-\frac{(y - C_t)^2}{2\sigma_2^2 t}\right) dy = P(S_{\Lambda} \geq t) \quad (A.11)
\]

This implies no guarantee of a lower Type II error probability at a given key measurement point and before any time \( t \) by lowering the measurement error at that key measurement point, as was seen in SOCA simulations. We can, therefore, conclude that, lowering the measurement error generating \( \tilde{C}_t \) provides a lower Type I error probability at a given key measurement point before any time \( t \), but may not lower the Type II error probability. However, we note that the Type II
error probability is oftentimes lowered in SOCA simulations. Because these results hold for every $t$ denoting continuous time, they also hold for $\tilde{C}_t$ where $t = 1, \ldots, T$, indexing discrete time by means of integration with respect to $t$. Finally, these results are suggestive of a general pattern for $T$ large enough, as $\tilde{C}_t$ will converge to a Gaussian random variable as $t \to \infty$ by the Central Limit Theorem.
NUMSO directly translates the uncertainty bounds in Tables 4.4 and 4.5 into percent values (e.g., a bound of 4 is 4%) and then scales them to correspond to the kilogram-based bounds in SGA. Table B.1 shows the scaling factors used to translate the initial uncertainty bounds to percent-based bounds. Equation B.1 shows how to relate the percent-based uncertainty bounds in NUMSO to the kilogram-based uncertainty bounds $e_{kd}^\dagger$ in SGA:

$$e_{kd}^\dagger = \frac{q_k \cdot \bar{e}_d}{\bar{e}_kd} \quad \forall f \in \mathcal{F}, k \in \mathcal{K}_f, d \in \mathcal{D}_f$$ (B.1)

For example, consider measurement method TIFD at the Enrichment Input key measurement point. TIFD has an uncertainty bound of 10, which results in the upper bound of 3.0 kg for the Enrichment Input.

$$e_{Enrichment \ Input, \ TIFD}^\dagger = \frac{119858.200 \text{ kg} \cdot 10\%}{399527.333\%} = 3.0 \text{ kg}$$
Table B.1: Scaling factors for each measurement method and key measurement point

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<th>Enrichment Input</th>
<th>Enrichment Output</th>
<th>Enrichment Waste</th>
<th>UO₂ Conversion Input</th>
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