

Safeguards Modeling for Advanced Nuclear Facility Design

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Abstract

Future nuclear fuel cycle facilities will see a significant benefit from considering materials accountancy requirements early in the design process. The Material Protection, Accounting, and Control Technologies (MPACT) working group is demonstrating Safeguards and Security by Design (SSBD) for a notional electrochemical reprocessing facility as part of a 2020 Milestone. The idea behind SSBD is to consider regulatory requirements early in the design process to provide more optimized systems and avoid costly retrofits later in the design process. Safeguards modeling, using single analyst tools, allows the designer to efficiently consider materials accountancy approaches that meet regulatory requirements. However, safeguards modeling also allows the facility designer to go beyond current regulations and work toward accountancy designs with rapid response and lower thresholds for detection of anomalies. This type of modeling enables new safeguards approaches and may inform future regulatory changes. The Separation and Safeguards Performance Model (SSPM) has been used for materials accountancy system design and analysis. This paper steps through the process of designing a Material Control and Accountancy (MC&A) system, presents the baseline system design for an electrochemical reprocessing facility, and provides performance metrics from the modeling analysis. The most critical measurements in the electrochemical facility are the spent fuel input, electrorefiner salt, and U/TRU product output measurements. Material loss scenario analysis found that measurement uncertainties (relative standard deviations) for Pu would need to be at 1% (random and systematic error components) or better in order to meet domestic detection goals or as high as 3% in order to meet international detection goals, based on a 100 metric ton per year plant size.

Introduction

The MPACT working group, funded through the U.S. Department of Energy, Office of Nuclear Energy, conducts research on technologies and concepts to improve safeguards and security in the civilian nuclear fuel cycle. This program area is focused on domestic regulatory requirements. The MPACT program has developed a Virtual Facility Distributed Test Bed as part of a 2020 milestone to demonstrate advanced SSBD.^{1,2,3,4} A notional electrochemical facility design was used for the demonstration due to recent research and development on related safeguards technologies. The Virtual Test Bed is described in more detail in reference 1.

The “Virtual Facility” aspect of the milestone refers to the use of systems-level modeling tools to design the plant and monitoring systems. Flowsheet modeling is the first step in the design process, used to define an initial plant design, flowrates, process steps, and timing of operations.⁵ The flowsheet modeling information feeds into safeguards modeling tools, which are presented

here. The SSBD process is inherently iterative, so identified gaps can be used to impact the design of the flowsheet. Likewise, operational constraints can define the safeguards approaches that must be used for a facility.

MC&A Design Process

The DEPO (Design and Evaluation Process Outline)⁶ methodology has been used as the basis for designing an MC&A system, as shown in Figure 1. The process starts with defining system requirements. This includes determining regulatory requirements, characterizing the facility, and determining the materials and forms present. Then the MC&A system is designed by establishing Material Balance Areas (MBAs), Key Measurement Points (KMPs), and Material Balance Periods (MBPs), which are described in later sections. The difference between item and bulk accounting MBAs are identified, and containment and surveillance are applied depending on the location. Then modeling and simulation tools are used to evaluate the MC&A system focusing on error propagation and loss scenario analysis. Based on identified gaps, the system will be redesigned (for example, higher precision measurement technologies may be needed). Once applied, Safeguards by Design (SBD) recommendations may affect the flowsheet and facility design. The process is iterative until achieving an effective yet cost-optimized final design.

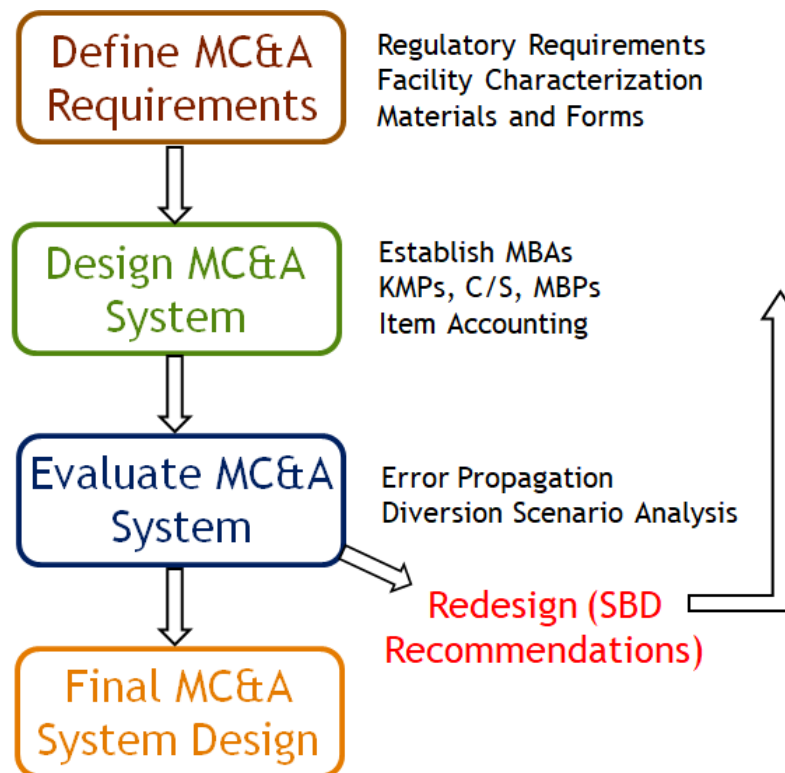


Figure 1: MC&A system design process.

The following sections show how the Virtual Facility Distributed Test Bed capabilities are used to step through the design process toward a finalized MC&A design.

Regulatory Requirements

The process for designing a safeguards and security system for a new facility begins with regulatory requirements. In the U.S., MC&A is outlined in the Code of Federal Regulations (CFR)⁷ 10 CFR Part 74. The regulations follow a graded approach depending on the category of the facility. A commercial reprocessing facility is considered a Category I facility. One difficulty with applying Part 74 is that it specifically excludes reprocessing, so it has only been used as a guide for the design process, as described below.

10 CFR Part 74 covers all aspects of MC&A requirements including reporting requirements for normal operations and anomalies, inventory timing, detection probabilities, item monitoring requirements, alarm resolution, quality assurance. Category I facilities need to perform at least 3 bimonthly inventories at startup until the approach is acceptable to the NRC, and then semi-annual inventories after that, the results of which need to be reported within 45 days. The facility must have a statistical test capable of detecting the loss of five formula kilogram quantities within 7 working days (Category Ib requirement) with a 95% detection. Trend analysis must be performed, and any inventory difference (ID) greater than three times the standard error of the inventory difference (SEID) must be evaluated. The SEID should be less than 0.1% of active inventory, or the current inventory of the facility. For item accounting areas, the plant must have a sampling plan that provides a greater than 99% chance of detecting the loss of five formula kilograms within 60 days for vaults and within 7 days from processing areas.

The statistical and timeliness requirements were not written for large reprocessing plants, and the goals/requirements are difficult for a large throughput reprocessing plant to achieve simply due to the limitations of measurement uncertainties. For this reason, and in the absence of new rulemaking by the Nuclear Regulatory Commission (NRC), this modeling study also used International Atomic Energy Agency (IAEA) regulations as a goal since they were developed for large throughput reprocessing facilities. IAEA regulations are based on detecting the loss of 8 kg of Pu within one month with a 95% detection probability.⁸ Note that IAEA's timeliness requirement can be up to 3 months for Pu in mixed solutions, but a one-month detection requirement was chosen for this work for conservatism since it is not clear yet how the mixed U/TRU product from electrochemical processing would be viewed. In addition, detection goals are easier to achieve in a shorter material balance period due to the lower absolute throughput during a shorter MBP.

Electrochemical Facility Characterization and Safeguards Challenges

Electrochemical processing facilities use molten salts and electrochemical operations to separate actinides from spent nuclear fuel (SNF). The technology was originally designed for processing metallic fuels but, with modifications, can also be used for oxide fuels. Variation in the flowsheet design, beyond what is used as the basis for this work, is certainly possible and depends somewhat on operator/country needs, engineering issues, and any safeguards or security considerations. Additional information on electrochemical flowsheets can be found in references 9 and 10, but a brief description is provided here.

The flowsheet is based on a 100 metric ton per year (MT/yr) throughput of SNF, with the Pu comprising approximately 1% by weight. Fuel assemblies are initially disassembled in a hot cell, and the fuel rods are de-clad to liberate the fuel. The SNF is chopped into small particle sizes and loaded into porous metal baskets for processing.

Oxide fuel first goes through an oxide reduction (OR) step to convert most of the fuel to a metallic form while liberating oxygen and some of the gases in the SNF. This is accomplished by lowering the baskets into a molten salt and applying a potential across the basket and a cathode. As current is passed, the metal oxides reduce to metals, and the oxide ions are dissolved into the molten salt and transported to the cathode where they are oxidized to produce oxygen gas.

The metallic fuel in the baskets is then transferred to an electrorefiner (ER) vessel, where the baskets are lowered into another molten salt. An electric potential is applied between the basket and a cathode; this potential dissolves fuel components into the salt phase, and extracts actinides in the salt onto the cathode. Separate cathodes are used to recover the majority of the uranium (U) and uranium/transuranics (U/TRU). These two products (U and U/TRU) are ultimately purified and consolidated into metal ingots for storage and/or future use for fuel fabrication.

Separate recovery processes are used to remove active metals (group I and II elements) from the OR salt and rare earth fission products from the ER salt. Residual noble metals stay in the basket and are also recovered and placed into a metal waste form along with cladding and assembly hardware.

Safeguards Challenges

As part of this modeling work, several safeguards challenges have been identified for electrochemical processing, and most of them relate to the unique environment, material forms present, and lack of large-scale operational experience. Because large-scale aqueous reprocessing plants exist, they can be compared to electrochemical plants.

- **Plant Flushouts** – In aqueous reprocessing plants, processing solutions are typically drained to select vessels for interim inventory measurements or completely flushed from all vessels and pipes every 6 or 12 months to facilitate a physical inventory. By contrast, completely flushing out an electrochemical facility is not as feasible since the process is designed to maintain a steady-state actinide content in the ER salt. Actinide concentrations in the salt can be reduced through a drawdown process, but materials accountancy approaches generally need to consider interim measurements of the salts.
- **Input Accountability** – Aqueous plants establish input accountancy by dissolving fuel and taking samples of well-mixed solutions. This input accountability tank allows the operator to take precision measurements due to the homogeneity of the solution. Electrochemical plants face a difficult challenge in establishing input accountancy of the solid fuel, which is inhomogeneous. Options may include representative sampling of the solid fuel followed by some type of analytical measurement.
- **Representative Salt Samples** – ER salts may be difficult to measure accurately because they can include fine solids throughout the salt, dross or scum in a layer on top of the salt, and/or solid debris on the bottom of the ER vessel. Obtaining replicable representative samples can be challenging and may require unique engineering approaches.

- Accountability of Metallic Products – The U and U/TRU metallic products require measurement approaches that differ from output accountancy measurements for aqueous plants. Sampling and destructive analysis (DA) of melts is possible but may be difficult for routine measurements. Non-destructive analysis (NDA) measurements can also be considered.
- Holdup – Every bulk handling facility needs to identify both process and residual holdup locations. Electrochemical plants are no exception; operators will need to determine how to account for material held up in these locations.
- Confirmatory Measurements – Due to the need for greater reliance on interim inventory measurements in electrochemical plants compared to aqueous plant, confirmatory measurements (of empty vessels, or those with low quantities of actinides) are needed to fully close out a material balance. However, confirmatory measurements would need to be performed in a hot cell using NDA techniques, and such measurements can be particularly challenging inside a hot cell.
- Process Monitoring – Electrochemical facilities have unique processing signals that can be used for monitoring the process. Current, voltage, or voltammetry measurements can be used for overall process control and/or safeguards, but these measurements need to be understood better and will require training data from a real facility.

MC&A System Design

Material Balance Areas

The next step in the design process is to define the MBAs for the notional electrochemical facility. The MBAs are logical boundaries placed around processing or storage areas in which inputs, outputs, and the change of inventory are tracked. MBAs are often chosen to coincide with physical boundaries, such as all within the same hot cell or within the same building. They may also be chosen based on grouping material of similar attractiveness as well as ease of measurement. For example, most reprocessing facilities set MBA 1 to include fuel receipt and all front-end operations (disassembly and fuel chopping) up until the accountability tank. The front end is difficult to measure until the accountability tank, so the MC&A system in MBA 1 relies more on item accounting and containment and surveillance (C/S). The overall error attributed to MBA 1 is driven mostly by the uncertainty in the estimates of actinide content in the incoming spent fuel assemblies. MBA 2 typically goes from the input accountability tank (or equivalent) up through product processing because the bulk material can be sampled and measured throughout this area. The switch back to item accounting on the back end usually means another MBA will be defined for product and waste storage.

The Separation and Safeguards Performance Model (SSPM) has been used for design and performance testing of the MC&A system.^{11,12} The SSPM uses MATLAB® Simulink and tracks material flows and inventories through the various unit operations in the plant. The SSPM tracks elemental and isotopic inventories for all species along with flow rates for bulk liquids and solids. Mathematical operations are used to simulate tank filling and emptying and realistic timing of process unit operations. This detail is needed to support the main function of the model, which is simulating material measurements. The model simulates bulk and elemental

measurements with user-defined measurement errors. Error propagation and statistical tests are used to determine if material losses can be detected.

The MBA structure in the SSPM architecture is shown in Figure 2. MBA 1 covers front end operations inside an air hot cell. The front end includes fuel receipt and storage, disassembly of the fuel assemblies, decladding, and chopping of the fuel. The plant design assumes that some type of (undefined) sampling or NDA measurement is used to establish input accountancy for the fuel either before or within the fuel baskets, just before the baskets are transferred to the argon hot cell.

MBA 2 covers all operations in the argon hot cell. These operations include oxide reduction, electrorefining, distillation steps, cathode processing, rare earth drawdown, active fission product removal, and metal waste form processing. The outputs of MBA 2 are the U and U/TRU products, fission product waste form (combined active metal and rare earth fission products), and the metallic waste form.

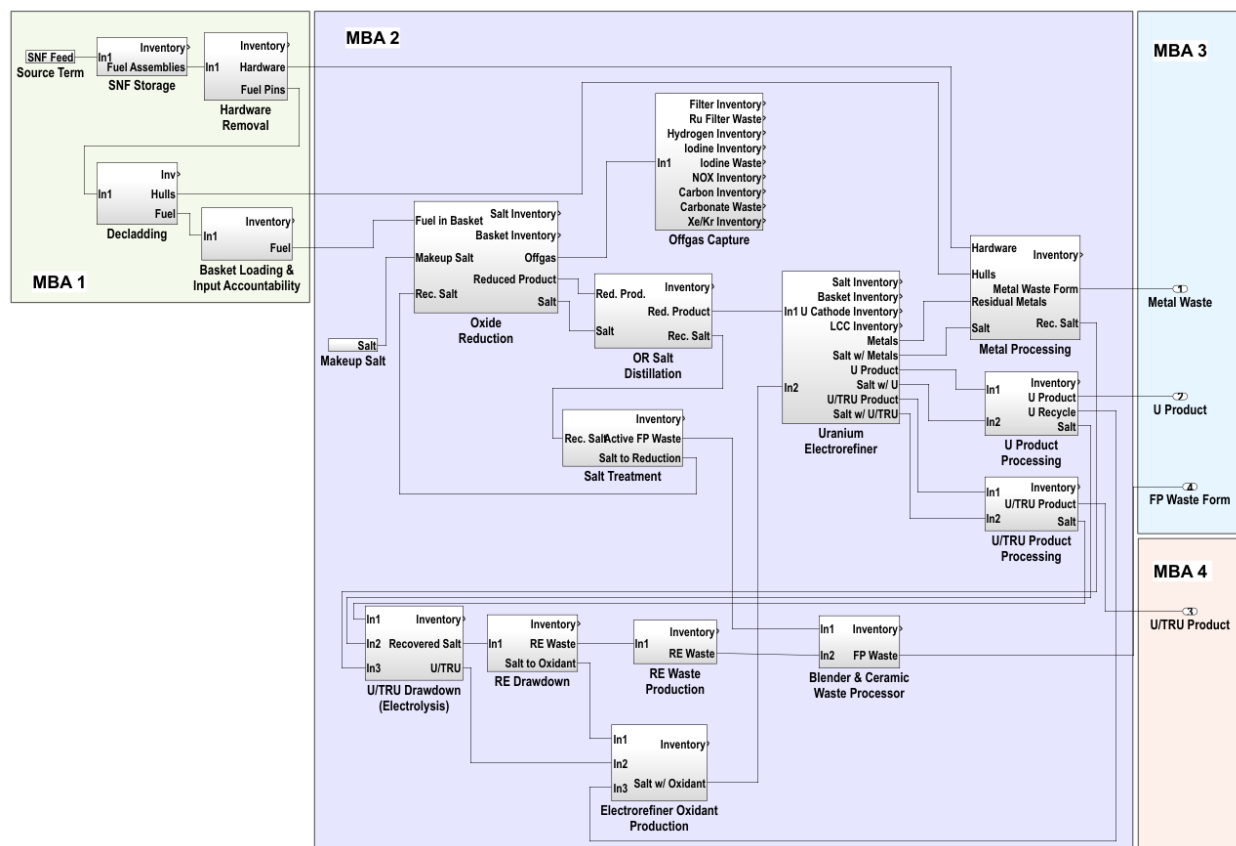


Figure 2. MBA structure for the generic electrochemical facility

MBAs 3 and 4 are item accounting MBAs. MBA 3 includes storage of the U product and waste forms. MBA 4 includes the U/TRU vault, in which the U/TRU ingot products are securely stored until they are shipped out of the facility. In an actual facility, MBA 3 will likely be a separate building.

Figure 3 shows the timing sequence for the reference flowsheet. These plots show the Pu content in twenty unit operations as a function of time out to 3000 hours of simulation time. There is a startup period before assemblies start processing through the system, and then the Pu content in the ER vessel builds up until steady-state is achieved. The plots show the quantities of Pu in each unit operation for this notional flowsheet—actual values may differ for a real facility.

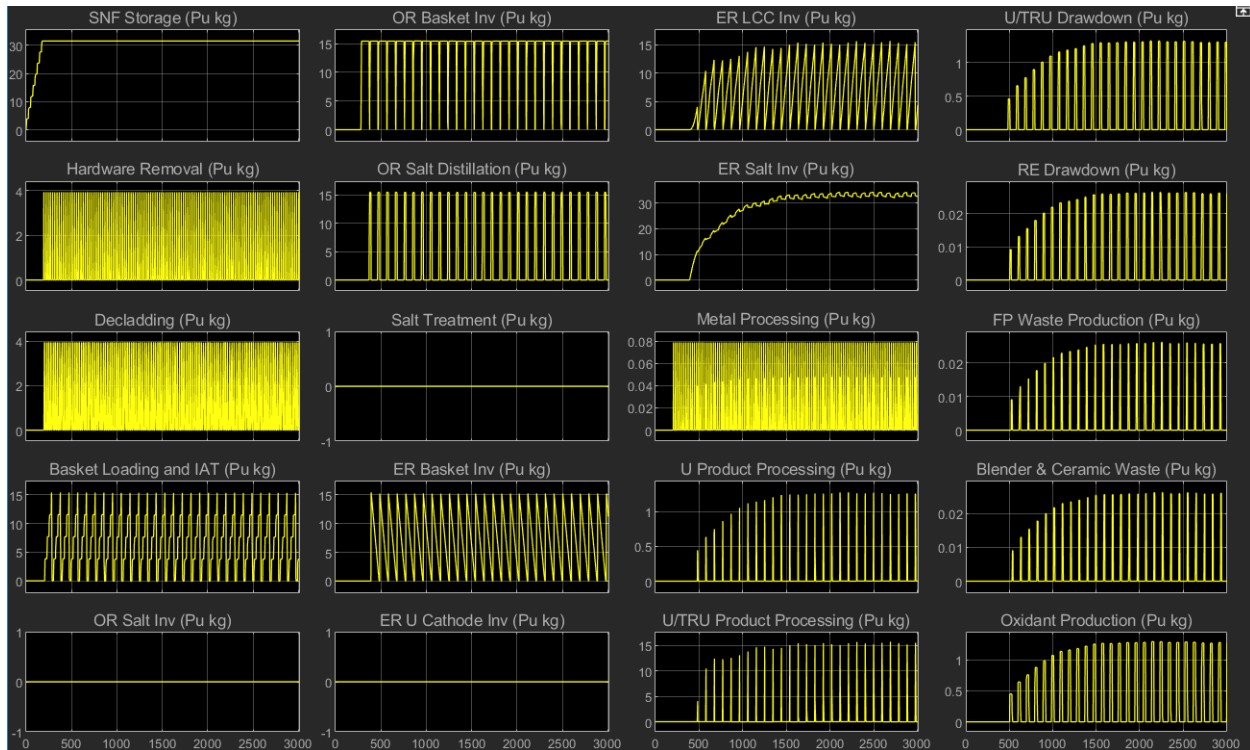


Figure 3: Time-dependent Pu quantities for various unit operations simulated by the SSPM.

C/S is an integral part of the overall safeguards system and is relied upon more heavily when material measurements would have higher uncertainty. For example, front end operations including decladding and chopping of the fuel present difficult material forms to measure with low uncertainty, so C/S is used to ensure that these materials are not removed or accessed during processing. C/S is not explicitly modeled in the SSPM other than simulating a gross measurement that looks at whether nuclear material is present. However, C/S is used throughout the facility as part of the plant's PPS system, so many of these aspects are covered in an article accompanying this issue.¹³ C/S has not been a focus of the work in the MPACT program because many existing technologies can be applied. These technologies include surveillance cameras, entry control, locks on hatches to the hot cell, tags, and seals.

Reporting requirements are also a significant part of the regulatory requirements and include material status reports, material transaction reports, reporting on loss or theft, and inventory summary reports. Since these tasks are more administrative, they are not covered here, but they do represent an important part of the overall MC&A system.

Key Measurement Points

The MBA structure stipulates the locations of KMPs, which include both flow and inventory measurements. Flow measurement points are performed when nuclear material transfers into or out of the MBA. Inventory measurements are performed periodically for interim or physical inventory taking. A significant part of the MPACT campaign has focused on measurement technologies that can be used for KMPs. The overall goal of these measurements is to provide material tracking for reporting to a regulatory body, and ultimately to provide assurance that material has not gone missing.

Table 1 summarizes the KMPs, measurement technologies, and assumed measurement uncertainties, based upon the work on measurement technologies in the MPACT program. The modeling work focused on MBA 2 since the front end relies mainly on C/S like existing large aqueous reprocessing plants. Table 1 provides current best estimates of measurement capabilities, but it is possible that measurements could improve with more research. In all cases, the relative errors from the R&D or references were rounded to the nearest integer percent.

Table 1. Key Measurement Points and Pu measurement uncertainties.

MBA 2	Measurement Technology	δ_r	δ_s	Reference
Input Fuel	Microcalorimetry (bulk mass and sampling errors are assumed to be included in these measurement uncertainties)	1%	1%	14
Input Hulls & Hardware	NDA	10%	10%	15
OR Salt Inv.	OR Voltammetry (confirmatory measurements do not contribute significantly to the material balance)	10%	10%	16
ER Salt Inv.	Bulk Mass	1%	1%	16
	ER Voltammetry (uncertainties are an extrapolated best-case estimate)	1%	1%	17
Drawdown Inv.	Bulk Mass	1%	1%	16
	Voltammetry or Other (measurement does not drive overall error due to small actinide quantities-less precise measurements can be used)	5%	5%	17
U Product	Bulk Mass	1%	1%	Assumption for use of scales.
	High Dose Neutron Detector (Note that measurement only needs to confirm low or trace Pu content for the Pu balance)	5%	5%	14
U/TRU Product	Bulk Mass	1%	1%	Assumption for use of scales.

	Microcalorimetry (sampling errors are assumed to roll up into these measurement uncertainties)	1%	1%	14
Metal Waste Form	NDA	10%	10%	15
Fission Product Waste Form	NDA	10%	10%	15

The relative standard deviations (RSDs) in Table 1 represent results from experimental work in the MPACT program, if available. In other cases, references on international safeguards for large aqueous reprocessing plants were used for measurements that could be applied with little or no modification. Note that measurement uncertainties are broken down into random (δ_r) and systematic (δ_s) error components. Random error results from statistical variation in the measurement system and will vary around a mean value. Systematic error is due to repeated measurement biases and usually leads to a persistent positive or negative bias in the result. In all cases random and systematic errors are currently assumed to be the same based on experimental performance. Application on real systems and proper measurement control is required to more accurately estimate RSDs.

The MPACT program did not examine sampling uncertainties for KMPs. In reality, sampling uncertainty is a significant challenge for getting representative measurements of the input spent fuel and the ER salt. Sampling error is probably less of a challenge for the U/TRU product. Table 1 assumes some of those sampling errors are included in the best-case estimates, but additional research and development will need to address this component of the uncertainty.

For the most critical measurements in MBA 2 (input fuel, ER salt inventory, and U/TRU output), the best-case measurements uncertainties could potentially be 1%. However, in most cases these uncertainties are an extrapolation of experimental work and represent a best estimate of what may be possible with the technology. Sampling and DA with a well-calibrated analytical laboratory should be able to achieve these values or possibly better, but there are still engineering challenges in measuring the unique materials from electrochemical facilities. The modeling work assumed 1% RSDs in the random and systematic errors as the best case, but also evaluated the effect of 3% and 5% RSDs in case these technologies do not perform as well on higher-throughput facilities.

Material Balance and Timing

The SSPM automatically calculates the material balance during model runs. The material balance equation is:

$$ID = \sum inputs - \Delta inventory - \sum outputs$$

The inventory difference (ID) for a particular MBP is determined by summing the inputs over that time period, subtracting all the outputs during that time period, and subtracting the change of inventory. Thus, all material movement across MBAs needs to be measured, and inventories of nuclear material in the process units are measured when each material balance is closed.

The material balance can be optimized by appropriate timing of unit operations to minimize the overall measurement error. Material balances should be chosen at times when the inventory is contained in as few processing vessels as possible in order to limit the number of precision nuclear measurements needed. The timing also needs to be chosen at a time when all inputs and outputs to that MBA can be accounted for. This is one area where SBD recommendations may indicate changes to a flowsheet or individual unit operation timing in order to make safeguards more efficient.

The timing sequences for MBA 2 are shown in Figure 4. The red lines show one example material balance time, or strike time, (at hour 2122) for when the balance is calculated. Strike times can and may need to be at slightly different times in the same MBA due to delays in getting samples and the analytical measurement turn around time. Appropriate strike times can also help to keep the balance over a batch of material. The example shown in Figure 4 was chosen to minimize the number of low uncertainty inventory measurements. At the time shown, all operations are clear of material except for a batch of fuel in the OR vessel, a batch of fuel in the OR salt distillation process, the ER salt, and the drawdown vessel. The two batches of fuel in the OR vessel and salt distillation vessel can be estimated based on the original input accountancy measurement since that measurement is done for each basket. A low-uncertainty measurement is needed of the ER salt, and a measurement is needed for the drawdown salt (but note that the quantity of Pu in the drawdown vessel is very small, so higher uncertainty measurements are adequate). Thus, the only low uncertainty inventory measurement needed is for the ER vessel. The inputs and outputs also require low uncertainty measurements.

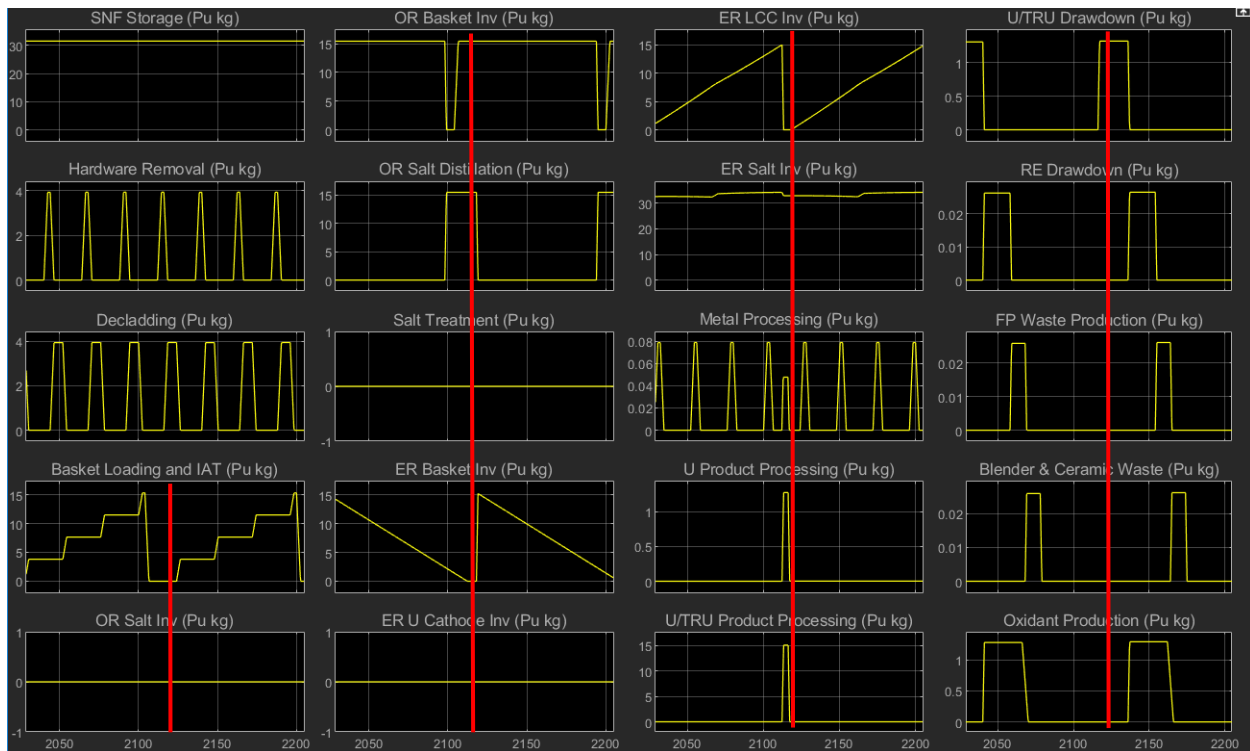


Figure 4: Conceptual material balance strike time

The MBP differed depending on whether the IAEA or NRC timeliness goal was being considered for the modeling runs. For the IAEA timeliness goal of one month, the model calculates a material balance every 672 hours in order to achieve a roughly one-month balance period. For the NRC goal, a 192-hour balance period is used. The facility operates on a 96-hour cycle, so in order to keep the strike time at a similar point in the process each time, a multiple of 96 hours is required. A real facility may need to have flexibility of exact closure times because operations do not always follow a clockwork cycle.

Error Propagation and Statistical Tests

The SSPM allows the user to change the assumed measurement uncertainties for the various measurement locations. Upon running the model, the error propagation (SEID) is calculated based on all the random and systematic errors. Several statistical tests are used to monitor for material loss, but the Page's test on SITMUF (Standardized Independently Transformed Material Unaccounted For) was used for the results. Material Unaccounted For (MUF) is a term used in the international safeguards community and is the same as ID. The ID sequence from subsequent material balances are transformed into a standardized and independent series (SITMUF), and the Page's trend test is applied to this sequence for alarm detection. Reference 18 describes error propagation and the statistical tests in more detail.

Page's test has been found to be a good choice detecting material loss.¹⁹ The SSPM uses a joint Page's test that improves the ability to detect both abrupt and protracted losses.²⁰ The joint test includes one test that is optimized to detect abrupt or rapid loss and another that is optimized to

detect protracted loss over longer time periods. The Page's test is set up by specifying parameters (k, h). In general, the k value sets the sensitivity of the test and the h value is the threshold for an alarm condition. These parameters are determined by choosing values for normal simulations (no loss modeled) that keep the false alarm probability below 5% per year. Simulations are used to select h for a given k value.

The SSPM can be used to set up material loss from a variety of locations within the plant model for loss scenario analysis. The user can specify the fraction of material removed, the length of the loss period (which determines whether it is an abrupt or protracted loss), and whether material is directly removed or if a substitution loss is being modeled. Substitution means that material is removed and replaced with something similar in order to deceive a bulk mass balance. Example results from the loss scenario analysis are shown in the evaluation section of this paper.

Process Monitoring and Machine Learning

Process monitoring (PM) may also be used to help the operator account for the material. Process monitoring is not specifically defined in 10 CFR 74, but the requirements were summarized previously in this paper. A better definition is given in a U.S. DOE Standard²¹ as, "a methodology to ensure that special nuclear material (SNM) is in its authorized location and when effectively implemented, it is a useful tool to detect anomalous process conditions and indicate losses of SNM well before the scheduled physical inventory." PM is particularly useful to the operator who has a large amount of facility data. Electrochemical facilities contain different types of PM data and technologies (compared to other fuel cycle facilities) such as current, voltage, and voltammetry, all of which can be used to monitor relevant processes.

PM measurements encompass certain types of data that can be difficult to directly incorporate into a material balance, but that could still be used to indicate off-normal conditions. Machine learning (ML), which can potentially use disparate data-streams (such as traditional materials accountancy measurements along with current and voltage monitoring), is being evaluated for safeguards applications.^{22,23} These concepts establish a normal pattern of behavior for a facility. Deviations from that established normal pattern could then indicate off-normal conditions and inform follow-up investigations by relevant stakeholders. This contrasts with traditional safeguards approaches where measurements are made to infer mass of actinides in an area of interest. Recent work has suggested that detecting changes in PM data rather than inferred mass, could prove more effective.²⁴

As part of this modeling work, some limited investigations were conducted to determine the feasibility of integrating ML approaches into the overall safeguards system. One investigation examined NDA measurements of the ER salt to help detect substitution loss scenarios. The goal of these investigations was to significantly reduce the need for sampling and DA by only monitoring bulk mass balances and NDA measurements.

A direct loss of ER salt could be detected through simple bulk measurements such as tank levels. However, in a substitution loss scenario, an adversary may try to trick bulk mass measurement systems by replacing diverted salt with an equal mass of clean salt. Under normal operations, there should be little or no removal of rare earths from the ER salt during the U/TRU extraction

and drawdown stages for this flowsheet design. The more difficult-to-detect substitution loss would show a decrease in rare earth concentration for the ER salt.

Figure 5 shows a comparison of a particular rare earth gamma peak from a normal run compared to a loss scenario. In the normal run, if measured both before and after U/TRU extraction steps, the peak should not change much, but in a loss scenario the peak drops as the fission product-bearing salt is replaced with a clean salt.

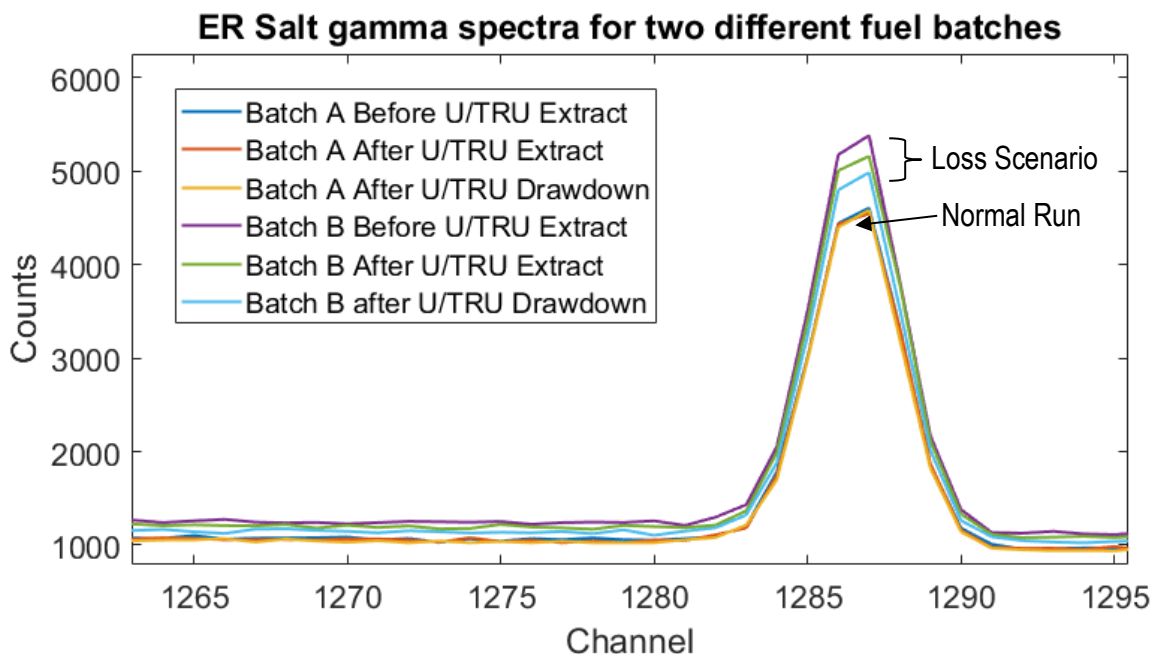


Figure 5. Use of NDA measurements to indicate substitution loss of the ER salt.

It is important to note that the fission product gamma peaks vary with time due to the variation in fuel going into the reprocessing plant. Therefore, the relative change needs to be monitored as opposed to a total change from batch to batch. ML techniques can be applied to this peak change to develop detection strategies.

While not explored extensively in this work, research in other areas^{22,23} suggests that the use of predictive algorithms could help monitor relative peak changes. Long Short Term Memory networks²⁵ have been shown to successfully predict the output of downstream vessels provided input measurements are made. The prediction becomes poor under anomalous conditions, such as a material loss. In this case, a poor prediction would indicate a potential anomaly and provides a means for detection. This approach could potentially be applied to gamma measurements on ER salt in the future to further improve facility safeguards.

Related work in the MPACT program through university partnerships²⁶ considered additional PM measurements, such as the (alpha,n) reaction, that could improve safeguards for electrochemical facilities.

The application of PM and ML approaches was limited in this modeling work, but some general lessons were learned. First, modeling and simulation is required to examine these approaches due to the large volume of data needed both for training and testing under loss or misuse scenarios. Second, this area of research can quickly require a significant effort due to the large number of different types of algorithms that could be tested. Third, unsupervised techniques would be more useful to plant operators since testing on a lot of actual plant data (including loss events) would be difficult in practice. Finally, interpretation of ML and PM approaches is critical. ML approaches are often criticized as black-box approaches, and given the high consequence nature of safeguards, adequate explanations will be required for widespread adoption.

MC&A System Evaluation

The SSPM was used to evaluate the overall MC&A system design by both analyzing material loss and determining SEID (the overall error on the measurement for MBA 2). To provide more clarity, the work simply looks at the ability of the system to detect losses from material streams or process vessels and does not evaluate a full diversion scenario analysis (which would include how the material is removed from the facility). These performance metrics provide an indication of how well the system responds to material loss.

Material loss analysis determines the probability of detecting both abrupt and protracted loss. Due to the random nature of the model and how measurement uncertainties are applied, every run will provide slightly different results. Multiple iterations are required to determine detection probabilities. In all cases, approximately 100 iterations of the various loss scenarios were run in order to estimate detection probabilities using the joint Page's test applied to SITMUF. The use of 100 iterations does not provide highly accurate results, but 1000 or more iterations per scenario would have been time prohibitive given the current modeling setup.

In all cases, a range of random and systematic RSDs (1%, 3%, 5%) were examined. The less important measurement points (such as waste forms and vessels that are empty at the time of the material balance) remained at the same value (5%) for all runs. Only the more critical measurement points (input fuel, ER salt inventory, and product outputs) were modified for the different cases. Bulk mass measurements were all kept the same at 1% for random and systematic RSDs. The h,k values were chosen to keep the false alarm probability below 5% per year.

Both NRC and IAEA detection goals were examined. NRC regulations are more stringent and were not written for reprocessing facilities, so examining both goals provides more information for potential future regulatory changes. Results are shown in Tables 2 through 4.

Table 2 shows detection probabilities as a function of RSD for the loss of 2 kg of Pu within 7 days, consistent with NRC regulations. Fuel was removed from the OR baskets in this scenario so that 2 kg of total Pu was removed. The material balance was performed every 8 days in order to be close to the 7 day goal while also on a consistent cycle for the plant. The system was only able to achieve a high detection probability (>95%) for the abrupt loss scenario with 1% RSDs. The detection probability dropped below the goal for protracted loss and significantly dropped off for the 3% and 5% RSD assumptions.

Table 2. Conceptual fuel loss scenario results based on NRC goal (2 kg loss in 7 days)

Loss Scenario	Detection Probabilities as a Function of Measurement Uncertainty (RSD)		
	All 1%	All 3%	All 5%
Abrupt Loss	97%	14%	7%
Protracted Loss	83%	7%	5%
SEID (kg Pu)	1.2	3.0	4.9

Table 2 also shows the overall SEID (one standard deviation) for one balance period. With 1% measurement uncertainties, the SEID equals 1.2 kg of Pu, and because the loss is almost twice this value, the detection probability was high. The alarm threshold for this case was about 50% higher than the SEID, which is why the detection probability was high. However, for the SEID of 3.0 kg and 4.9 kg, the material loss is well below the SEID, so the loss of material is lost in the noise. These results illustrate how difficult the NRC regulation is, if applied to reprocessing facilities.

Table 3 shows the detection probability as a function of measurement uncertainty for the loss of 8 kg of Pu (an IAEA significant quantity) within 30 days for loss of fuel from the OR basket. The results highlighted in green show when the detection probability was above or near the 95% goal. A high detection probability was seen in all loss scenarios at the 1% measurement uncertainty assumption and for the first two scenarios at the 3% measurement uncertainty assumption. These results show that if the technologies examined as part of the MPACT program are able to reach 3% measurement uncertainty, the MC&A system will still do reasonably well detecting material loss. These results are all notional for a 100 MT/yr facility, and different facility sizes will have different requirements in order to reach the goal. Table 2 also shows the SEID for each assumption. As the SEID gets closer to the loss amount, the detection probability drops off more.

Table 3. Conceptual fuel loss scenario results based on IAEA goal (8 kg loss of Pu in 30 days)

Loss Scenario	Detection Probabilities and SEID as a Function of Measurement Uncertainty (RSD)		
	All 1%	All 3%	All 5%
Abrupt Loss	100%	99%	63%
Protracted Loss 1	100%	93%	31%
Protracted Loss 2	100%	66%	13%
SEID (kg Pu)	1.9	5.5	9.1

Table 4 shows detection probabilities as a function of measurement uncertainty for the loss of 8 kg of Pu within 30 days of the U/TRU product. The results are very similar to the previous case, which is expected since the scenarios in Table 3 and 4 involve the same total amount of Pu removed in the same MBA, but just from different locations. There are slight differences likely due to the fact that this material loss occurs close to the end of the MBA. The SEID values remain the same.

Table 4. Conceptual fuel loss scenario results based on IAEA goal (8 kg loss of Pu in 30 days)

Loss Scenario	Detection Probabilities and SEID as a Function of Measurement Uncertainty (RSD)		
	All 1%	All 3%	All 5%
Abrupt Loss	100%	100%	75%
Protracted Loss 1	100%	90%	32%
Protracted Loss 2	100%	79%	21%
SEID (kg Pu)	1.9	5.5	9.1

The MPACT measurement technologies described in Table 1 suggest that 1% random and systematic measurement uncertainties for Pu accountability are likely best-case assumptions for the most critical measurement points. However, measurement uncertainties as high as 3% could still meet IAEA detection goals unless material loss is protracted over very long periods. The results show the challenge of meeting NRC's detection goals and should be taken into account should future rule-making be considered in this area.

Safeguards by Design Recommendations

As a result of the safeguards modeling work, the following list presents SBD recommendations for electrochemical facilities. Note that some of these conclusions are specific to the plant size examined here (100 MT/yr) and will change if different plant sizes are considered.

- The front end of an electrochemical processing facility (MBA 1) will likely primarily rely on C/S like other reprocessing facilities. It makes sense to make the MBA 1 boundary the same as the physical boundary for the air hot cell. Material accountancy is established with item accounting of spent fuel assemblies entering the facility (input), C/S of head end operations, the accountancy measurement of fuel in baskets (output), and NDA measurements of hulls and hardware (output).
- The boundary of MBA 2 aligns with the boundary of the argon hotcell, which contains most of the electrowinning and cathode processing operations. This area relies more on accountancy measurements (than C/S) since the material is in bulk form.
- Flushing out the facility may not be realistic given the way ER vessels operate. However, the material balance can be performed at a time when most of the nuclear material is in a small number of vessels. Physical inventories would require measurements of inputs and outputs, along with a precision measurement on the ER vessel only. Other locations can use less precise NDA or PM measurements to quantify small quantities of actinides or to simply verify the presence of only trace amounts.
- Based on the potential best case of 1% measurement uncertainties for the input SNF, ER salt inventory, and U/TRU product output, the modeled plant can meet IAEA detection and timeliness goals for abrupt and loss scenarios (assuming a one month MBP). The results also showed that an increase in measurement uncertainty to 3% allowed the system to achieve the detection goal for all but the most protracted loss scenario

examined. However, the plant could only meet NRC requirements as currently written in 10 CFR Part 74 for abrupt loss scenarios with 1% measurement uncertainty assumptions.

- Due to low actinide quantities at the time of the measurement, NDA or PM measurements such as voltammetry were assumed for the drawdown inventory, confirmatory measurements of all empty vessels, and waste form measurements. High measurement uncertainties (10-20%) are adequate and will not impact overall detection probabilities. Hot cell design which can facilitate simple gamma or neutron measurements should be considered.
- Holdup was not examined in detail in this work other than assuming small quantities of residual holdup in vessels. Future work will need to examine holdup (both in-process and residual) in more detail.
- Electrochemical facilities have the potential to include unique PM measurements, such as current and voltage monitoring. A small effort examined the use of ML algorithms to tie together PM, NDA, and DA measurements. More research would be needed to determine the impact these approaches could have.

Conclusion

The SSPM was used for designing and analyzing the materials accountancy system for a notional electrochemical facility. This work outlined the material balance areas, the material balance period, measurement performance, and the key safeguards metrics including the overall SEID (measurement error) and detection probabilities for various material loss scenarios. The SSPM is one modeling tool being used within the Virtual Facility Distributed Test Bed and pulls in information from the rest of the MPACT program to examine safeguards by design. This modeling approach provides an efficient way to develop a safeguards approach for future fuel cycle facilities.

For the notional 100 MT/yr facility used for this work, a range of RSDs were examined to determine whether the facility could meet both NRC and IAEA timeliness and detection goals. The best-case measurements for the most critical measurement points may be able to achieve 1% random and systematic RSDs for Pu measurements in MBA 2. At this level, the materials accountancy system would be able to meet IAEA detection and timeliness goals for abrupt and protracted material loss. The RSDs could be as high as 3% and still meet IAEA detection goals, except for very protracted material loss. However, NRC regulations cannot be met if RSDs are greater than 1%. NRC regulations were not written for large reprocessing plants, so the limitations of measurement uncertainties should be taken into account if future rule-making efforts are considered.

The 1% assumption was based on best-case approaches for measurement technologies explored in the MPACT program. An important caveat is that the sampling error was assumed to be included in this overall measurement uncertainty. In reality, sampling error can be a significant source of error, particularly for electrochemical processing, due to the difficulties of getting representative samples of spent fuel and ER salts. Future work should explore this sampling error in more detail.

The front end of the reprocessing plant, MBA 1, would likely perform similarly to existing reprocessing plants since the error on the incoming spent fuel assemblies drives the overall error.

Therefore, MBA 1 would rely more on C/S. Additional MBAs for product and waste storage would be item accounting areas and can likely use existing technologies and approaches.

Higher throughput facilities will have a more difficult time meeting regulatory goals and so may need to consider decreasing the material balance period or adding process monitoring or C/S to make up for the deficit.

Keywords

Electrochemical; Safeguards; Safeguards and Security by Design; Pyroprocessing; MPACT 2020 Milestone

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