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High Reliability Safeguards approach to remotely handled nuclear processing facilities: Use of discrete event simulation for material throughput in fuel fabrication



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ABSTRACT

The future, sustainable use of nuclear energy will require transition to advanced nuclear energy systems. Some of these systems will utilize remotely-handled facilities in which batch-type processing will occur in hot cells. These handling procedures, as well as differences in physical and chemical composition of the special nuclear material, create new challenges to safeguardability. The focus area of the High Reliability Safeguards is the continual development of methodologies and approaches which address the safeguardability of the advanced fuel cycle from a design-driven perspective. There is a need to develop models that can quantitatively assess the safeguardability of proposed facility designs. Herein is presented progress made in regards to a first-build, material-throughput model using a discrete event simulation modeling framework for the fuel fabrication system in a pyroprocessing facility. This model takes advantage of the synergy between safeguards, safety, and security when designing a nuclear handling facility. A commercial pyroprocessing facility is used as an example system. The intent of the model is to determine if nuclear materials accounting can potentially serve as a metric for safeguardability in facility designs.

1. Introduction

1.1. Motivation

Many nations are expanding nuclear power in order to enhance energy security, grow the economy, or address climate change (GIF, 2002; IAEA, 2013). Ensuring resource sustainability will require transition to advanced nuclear energy systems (NESs). Nuclear fuel for some of the advanced NESs will be fabricated in remotely-handled facilities in which batch-type processing will occur in heavily-shielded hot cells. For the advanced NESs, special nuclear material (SNM) is in both different physical and chemical form than that of the contemporary fuel cycle. This gives rise to new challenges in terms of integrating safeguards, safety, and security with facility design; i.e., safeguardability, or safeguards- and security-by-design (Ehinger and Johnson, 2009; Johnson and Ehinger, 2010). To this end, the High Reliability Safeguards (HRS) focus area is continuing to develop research directions in order to address the safeguardability of advanced fuel cycle concepts from a design-driven perspective (Borrelli, 2014a,b). A commercial pyroprocessing facility is used as an example system. The intent is to build a model for material throughput that is flexible in terms of accommodating multiple facility designs, where each can be tested in terms of safeguardability.

Designing a safeguardable model is a complex. The use of hot cells to process materials provides passive security, and other security measures from analogous facilities can also be applied to a pyroprocessing facility. For safety, a standard probabilistic risk assessment will be performed and likely required as part of the licensing process. This is discussed briefly at the end of this paper as part of future work. While there are issues with the pyroprocessing facility perhaps with lack of knowledge in terms of new failure modes and failure frequencies, or how materials might be transferred if there are multiple hot cells, the risk assessment framework is well known and an established tool for safety analysis. Here, the focus is primarily on safeguards-by-design and how materials accounting can be applied within the context of safeguardability.

Nearly all of the safeguards knowledge and experience for commercial facilities is largely based on aqueous materials processing facilities. The pyroprocessing facility will not have an accountability tank to determine SNM concentration in the materials, nor can the system be flushed out in order to 'reset' plant inventory. Held-up material then becomes a unique challenge. It must be removed from equipment and

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Fig. 1. Pyroprocessing flowsheet. Pyroprocessing converts used uranium oxide fuel to a metal alloy. The main subsystems in a pyroprocessing facility are voloxidation, electroreduction, electrorefining, electrowinning/cadmium distillation, and metal fuel fabrication, as indicated by the yellow boxes. The primary material flow is shown by the red arrows. Material losses are shown for each subsystem. Treatment and recycle of eutectic salts from the electroreduction and electrorefining processes are a major design consideration. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

accurately accounted for periodically in a way that does not impinge on operational goals.

As part of HRS, a quantitative assessment measure of the safeguardability of proposed designs that will be widely acceptable and based on established principles common to safeguards, safety, and security is needed. Prior HRS-related work focused on functional components of facility design by modeling the spontaneous fission of ²⁴⁴Cm (Borrelli, 2013, 2014c, 2016). Results for the dose rate of processed materials in the system fell below the IAEA self-protecting standard. This is a non-negligible physical protection risk for the facility that should be addressed during conceptual design phases, thus highlighting the importance of facility design to safeguardability. Additionally, study of the hot cell wall design showed that occupational safety can be maintained for the pyroprocessing facility comparable to analogous facilities. Therefore, storage buffers, maintenance, or even personnel areas can be designed near process cells. This can considerably reduce the overall facility footprint if physical space is a design constraint.

1.2. Current work

The overall intent of HRS is to provide a systematic methodology that can integrate proliferation resistance and physical protection measures, equally weighted with safety and physical security, while optimizing practical design approaches and operational goals. The primary operational goal is that the operator will have a target quantity as to the amount of material that would need to be processed over a given time period; e.g., for the Rokkasho reprocessing facility in Japan, it is expected that 800 tons of used fuel would be processed over a year. That is not to imply that a pyroprocessing facility would process the same amount, but that there would be a similar goal.

For a pyroprocessing facility, each subsystem processes batches with

different weights for different lengths of time. This will be a challenge to nuclear materials accounting (NMA). Poor accounting could result in numerous false alarms; while resolvable, subsequent time delays will affect operational goals. Additionally, poor accounting could fail to detect an actual diversion event. A discrete event simulation (DES) modeling framework is useful for safeguardability assessment. A discrete event model describes a state space that contains state variables. The occurrence of an 'event' drives the transition of the state variable (Wainer and Mosterman, 2011). The transition occurs in a discrete time interval, and the state space remains unaffected in between occurrences. The state transition is assumed to be instantaneous. Events can be triggered sequentially and can occur asynchronously in the state space. DES lends itself to modeling batch-type processes like pyroprocessing. DES can model materials flow for arrival, storage, processing, and transfer, as well as disrupted equipment and material flow states that result from maintenance or off-normal events of varying frequency.

This paper presents the first build of a facility process model using DES. The purpose is twofold. First, the model is established for bulk flow in the fuel fabrication process based on DES principles. This will serve as the architecture for the eventual, full system model. Second, with this model, the use of the probability of the false alarm anomalies; i.e., the Type I error (Avenhaus, 1977; IAEA, 2002), as a metric for safeguardability assessment is tested. The Type I error is already widely applied as a safeguards measure for nuclear materials accounting. A Type I error occurs when an analysis of the accounting system indicates that some quantity of nuclear material is missing; i.e., diverted, but in actuality no diversion has occurred. There are not yet any suggested IAEA goals for use of this metric for the advanced fuel cycle. This allows for some latitude in studying how to use it within the context of safeguardability. (Borrelli, 2014a,b).

Initiating events, which can lead to a false alarm, arise from a breach in safeguards, safety, or security. Here, the focus is on equipment failures, which occur during normal operation. If such an event leads to a false alarm, an IAEA inspection and facility mass balance would likely be required to resolve the anomaly, costing time and resources (Borrelli, 2014a). At a high-level, therefore, the facility operator then would have a strong interest in designing the facility to achieve low false alarm probabilities. Criteria for a safeguardability metric is also discussed in this paper. Use of the Type I error as a metric for safeguardability assessment takes advantage of the synergy between all three when designing a nuclear materials handling facility. Therefore, in the larger context, our overall intent is to provide a process model that allows for different conceptual facility designs, where each could exhibit different frequencies for the Type I error, and this can provide a measure of the safeguardability of each design.

2. Background

2.1. Pyroprocessing technical details

Used uranium oxide fuel is treated electrochemically by anodic dissolution at high temperatures in order to produce a metal fuel alloy. Materials are pyrophoric and must be processed in hot cells with an inert atmosphere. The pyroprocessing flowsheet used to build this model is shown in Fig. 1. The main subsystems are voloxidation, electroreduction, electrorefining, electrowinning/cadmium distillation, and metal fuel fabrication. Used fuel is first chopped, and cladding is mechanically stripped. Voloxidation then transforms UO2 pellets to U3O8 powder. Subsequently, electroreduction converts the powder to metal by dissolution in LiCl-LiO2 salt at 650 °C, where alkali metal and alkaline earth fission products remain in the salt (Herrmann et al., 2006, 2012; Herrmann and Li, 2010; Phongikaroon et al., 2011; Herrmann et al., 2012). Cs, Sr, and all volatile species are removed. Electrorefining extracts uranium metal on a cathode (Herrmann and Li, 2010), and graphite is typically used. Electrowinning extracts TRU metal on a liquid cadmium cathode (Li et al., 2009, 2010; Herrmann et al., 2012). Noble metal fission products remain on the anode. Both processes require anodic dissolution in LiCl-KCl salt at 500 °C. Lanthanides remain in the salt.

Injection casting is currently assumed for the fuel fabrication process due to cost efficiency, capacity to mass produce metal slugs, and remote operability (Trybus et al., 1993; Burkes et al., 2009; Lee et al., 2016). It is shown in Fig. 2. Injection casting was used in the past for the Integral Fast Reactor program for EBR-II (Battles et al., 1992; McFarlane and Lineberry, 1997) and is being considered as the fuel fabrication method for some Generation IV systems (Lee et al., 2016; Kuk et al., 2017). However, when scaling up to the commercial level, process losses potentially could be prohibitively high. Materials are first melted in a graphite crucible. Quartz molds are inserted into the molten alloy, and a vacuum is induced. This results in the injection of alloy into the molds. Some of the metal will remain in the crucible. This is called the 'heel' and can be recycled. The molds are removed and sheared. Because they have to be broken to obtain the slugs, they are a waste stream. The crucible will also be a waste stream as it will suffer from eventual wear. Safeguardability in fuel fabrication is important because the process includes a large amount of special nuclear material, approximately 4 kg of transuranic elements, half of which is ²³⁹Pu (Borrelli, 2013). A full technical discussion and literature review for the pyroprocessing system applied in this study is contained in Borrelli (2014a).

2.2. Prior use of DES for pyroprocessing

There has been scant use of DES modeling for pyroprocessing. Previously, DES has been be applied to nuclear facilities to study performance measures of used fuel handling (Houshyar, 1998; Garcia and Houshyar, 1998; Garcia, 2000). DES also has been used to model the receipt of used fuel assemblies and separation of individual fuel pins (Lee et al., 2009). DES modeling has also shown that for batch processing, storage buffer capacity will be a key feature governing bottlenecks (Lee et al., 2011, 2013). Material congestion will occur if the buffer is too small. However, increasing buffer size is dependent on practical design considerations, such as cost and physical space. The challenge in developing a realistic model is that each subsystem requires a different batch size and processing time. For pyroprocessing, large quantities of salt are required for electroreduction, electrorefining, and electrowinning. To avoid lengthy process idleness, fresh salt must be available to load into these subsystems when needed. Operational scheduling is therefore, vital (Lee et al., 2011, 2013). Most recently, DES has been used to develop a nuclear materials accounting model to identify potential diversion using a high-level MATLAB model (Riley et al., 2016). The head-end processes were modeled but not fuel fabrication. Similarly, Garcia et al. (2013, 2017) used DES for process monitoring to detect anomalies using multiple sensor data for the headend subsystems in pyroprocessing.

2.3. Safeguardability assessment

A quantitative assessment for safeguardable facility designs has not been developed. Much of the research into safeguardability over the short history of the field has been qualitative. Initially, the Proliferation Resistance and Physical Protection Evaluation Methodology Working Group of the Generation IV International Forum (PRPPWG) promulgated high-level principles for establishing safeguardability (PRPPWG,

> Fig. 2. Injection casting process to fabricate metal fuel slugs. U and TRU are melted with zirconium to form metal feedstock for slug fabrication by injection casting and eventual fuel element assembly. The metal feedstock is first melted in a graphite crucible, and a vacuum is induced to inject the molten alloy into quartz molds. The 'heel' is a coating of metal that will remain on the crucible. The molds are then sheared and broken to obtain slugs. The sheared casting ends are called the 'scrap.' The crucible will suffer from eventual wear and is a waste stream, along with the quartz molds. The scrap will have to be recovered and accounted for, as well as the heel, prior to disposal.



2011). A case study was developed for an Example Sodium Fast Reactor Full System (PRPPWG, 2009). Four sodium fast reactors co-located with various storage facilities and a pyroprocessing facility were analyzed for several diversion and physical protection scenarios. Other studies addressed different components of the Example Sodium Fast Reactor Full system based on a pathway analysis for additional scenarios (Bari, 2012; Boyer et al., 2012; Cojazzi et al., 2012; Peterson, 2012; Pilat, 2012a,b; Whitlock et al., 2012; Zentner et al., 2012). From a conceptual design analysis perspective within the context of safeguardability, several other studies outside of the PRPPWG are summarized in Borrelli (2014a). These studies discuss safeguardability from a high-level, qualitative point of view. However, facility design as a process is not addressed in these studies. Engineering design approaches for a safeguardable facility are now needed. Therefore, because there are not yet any widely accepted metrics for safegurdability assessment, there is considerable latitude to develop one within this context.

3. Conceptual model and context

3.1. Relevance of materials accounting and facility design to safeguardability assessment

There is not yet a full system model that can enhance safety, security, and safeguards from a design-driven perspective. This preliminary process model presented here is not site specific and will be flexible and adaptable to varying facility designs. It can offer user-directed conceptual facility designs with a safeguardability assessment metric for each. It is *design-driven* in that proliferation risk reduction is part of the design strategy. A top-down approach to pyroprocessing is applied here for facility design. That is, the whole system is considered as a 'big picture' first. The system is decomposed into first level elements called subsystems. It is described in Fig. 1. Each system is refined to its 'base elements.' Then, these are studied as to how they interact with one another in order to produce the system output. This is further explained in Section 4.1. The model for fuel fabrication is built in this way, and eventually, this design approach will be applied to the full pyroprocessing system.

There are pyroprocessing models with similar goals in terms of process modeling (Cipiti et al., 2012; Gonzalez et al., 2015). These are developed from a bottom-up perspective, where the chemistry and physics that govern processes in the base elements are applied in the model first, and then the full system is assembled from there. These research efforts apply different flowsheets from Fig. 1. This approach is considered to be complementary to these models in that the focus first is on the facility design aspect inherent in the initial formulation of the safeguards- and security-by-design concept (Ehinger and Johnson, 2009; Johnson and Ehinger, 2010). Eventually, for a truly realistic process model that can be used to evaluate safeguardability, these approaches should be integrated. This is a long term goal as part of HRS.

The main focus of this study is to determine if the false alarm probability can be applied as a quantitative metric for safeguardability assessment. There are no current formalized International Atomic Energy Agency (IAEA) goals for the Type I error probability for an advanced fuel cycle concept. Therefore, there is considerable latitude in studying this metric within the context of safeguardability (Borrelli, 2014a,b). The occurrence of a false alarm during facility operation would indicate a diversion has occurred, when in actuality it did not. For the model presented here, this could happen due to equipment failures. Equipment failures require repair and cleaning to remove SNM, and these are potential diversion risks. False alarms would have to be resolved by a facility inspection and subsequent inventory accounting. Facility operations would cease in the meantime. This would be costly for the facility operator, both in terms of operation throughput goals and possible compensatory penalties.

3.2. The role of nuclear materials accounting

Quantitative assessment of safeguardability is ultimately based on nuclear materials accounting (NMA). Poor accounting could fail to detect an actual diversion event. In order to establish an accurate mass balance for SNM in the facility, material balance areas (MBAs); i.e., the configuration of hot cells in the facility, have to be established appropriately. NMA would be performed at designated key measurement points (KMPs) at the interface of the MBAs. For pyroprocessing, two main challenges to safeguardability are: (1) lack of an accountability tank in order to determine SNM concentration and (2) inability to flush out the entire system and entirely clear the inventory. For NMA, the following well-known relationship is used (Avenhaus, 1977):

$$\Phi^{-1}(1-\alpha) + \Phi^{-1}(1-\beta) = \frac{SQ}{\sigma},$$
(1)

where α is the false alarm probability, $1-\beta$ is the detection probability, SQ is the significant quantity of SNM, σ is the standard error of the inventory difference (SEID), and Φ^{-1} is the inverse Gaussian function. A instructive example is commonly used (IAEA, 2002): for $\alpha = 0.05$ and $1-\beta = 0.95$, an SQ of 8 kg of Pu allows for an uncertainty in measurement of 2.4 kg in order to detect a diversion.

In the interval $t = (t_0, t_1)$, over a material balance area, the inventory difference (ID) is formally defined as Avenhaus (1977):

$$ID = I_0 + D - I_1,$$
 (2)

where $I_0 =$ initial physical inventory, $I_1 =$ final physical inventory or the inventory at $t = t_1$, and D = material throughput over the time interval across the material balance area. Ideally, ID = 0 over any time interval, but in reality $ID \neq 0$ due to material hold up and process losses. Typically, in materials accounting, the three quantities defined in Eq. (2) are treated as random variables. Therefore, measurements are obtained in terms of the expected value of the ID with associated deviation due to persistent systematic errors; i.e., SEID (Avenhaus, 1977).

A possible pyroprocessing facility conceptual design is depicted by the flow diagram shown in Fig. 1. For large MBAs containing many of the subsystems, based on standard NMA techniques, the SEID could exceed detection limits for a possible diversion attempt. With small MBAs, the SEID may be low due to more KMPs. There could be frequent Type I errors. Additionally, with more KMPs, more time is needed for accounting, and operation time would be affected. The formation of MBAs and resulting NMA are clearly interrelated with material throughput and operational goals. Both are a function of the facility design. Safeguardability therefore, is invariably a function of facility mass balance. These considerations should be optimized as part of the conceptual design strategy and safeguardability assessment.

3.3. Fuel fabrication intracell activity

Here, a systematic method that has been established to consider the activities included in each subsystem is described, and therefore it provides a framework for conceptual facility design. This framework then has informed how the DES modeling architecture was constructed for the fuel fabrication system. This conceptual modeling framework was established for overall hot cell and facility design, and material throughput (Borrelli, 2014a). It is shown in Fig.3a. Five activities will occur during normal operation of any process in the system: (1) process activity, (2) byproduct, (3) in-situ recycling, (4) final product, and (5) ancillary activity. Not all of these activities will be performed in a single cell, however, the prior study has determined that these five are essential.

Fig.3b shows how these activities apply to fuel slug fabrication. Injection casting will process the largest amount of SNM in the pyroprocessing facility, and material is always left in the crucible; i.e., heel (Borrelli, 2013). The heel will contribute to the SEID and could pose a diversion risk upon equipment failure. The process activity (1) includes





(b) Assay:



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Fig. 3. Conceptual fuel fabrication facility design overlay. A minimum of five activities are assumed to occur in order to complete a process. These are shown notionally in (a) and applied to the injection and casting of metal alloy fuel slug in (b). The five activities defined in (a) are contained each within the red dotted box in (b). Material arrives from the electrorefining (ER) and electrowinning (EW) processes. The process activity (1) is the injection casting system in which U and TRU metal, rare earth fission products, and Zr are melted into an alloy and injected into quartz molds to form fuel slugs and then trimmed. Material, such as americium, may be held up in the equipment. The recycled (2) material (scrap) is the leftover alloy from the mold trimming process. The heel could be recycled with the scrap. The byproducts (3) are the graphite crucibles. This is treated as waste. The heel could also be collected and returned to head end processes for recycle or stored in a buffer. The quartz molds, after being trimmed and broken to obtain the alloy, cannot be recycled and are treated as waste. The alloy products are fuel slugs (4). Additional analysis may be necessary, as an ancillary activity (5), for in-situ quality control; e.g., slug straightness. Assay both upon entry and exit is critical because U and TRU enter as separate batches, but after fabrication the single alloy will exit the cell. These materials could be assaved by visual inspection, neutron detection, weight, or potentially other destructive means. These activities do not necessarily have to occur in a single cell.

the injection casting and trimming processes. Byproducts (2) are the graphite crucible, the heel, and the quartz molds after trimming. The crucible and molds will be disposed as waste. The heel could remain in the crucible until the operator decides to remove it. Or, the heel may be removed after a campaign and stored in a buffer until it is recycled into the injection casting equipment. During the normal operation, scrap or the leftover alloy from the mold trimming process is recycled back into the melting and casting equipment (3). The final products (4) are the metal fuel slugs. These would be transferred from the cell to subsequent processing for full fuel element assembly. Finally, some quality control analysis could serve as an ancillary activity (5). This activity may be necessary in order to determine if the product satisfies other physical requirements, such as straightness and diameter. Some destructive assay (DA) may also be required. DA would likely be performed on the fabricated slugs in order to test SNM content. Ideally, the ingots of U and TRU (with Zr added) would form a homogenous metal solution in the melter. Therefore, the slugs would be expected to have a consistent SNM composition, and DA would test for this. Considering only these minimum five activities, modeling any process in the system can become exceedingly complex.

4. DES model

This is the first build for a full system pyroprocessing model intended to quantify safeguardability for different facility designs and material throughput goals. The model is developed with Python. It offers a modular environment which is conducive to the use of discrete event simulation and the batch nature of pyroprocessing. The basic code architecture allows an efficient model platform for the full pyr-oprocessing facility. This Python code can perform many processes and operate systems simultaneously. Additionally, this model is open source, with the eventual intent that other users can design and model safeguardability of other nuclear handling facilities.¹

4.1. Model space

The design of the fuel fabrication system is shown in Fig. 4. It is currently assumed that metal fuel slugs are manufactured by an injection casting system based on the history and expected future use of this technology as discussed in Section 2.1. The 'baseline design' is shown in (a) Design A, and the 'equipment design' is shown in (b) Design B. These designs align with the discussion of the minimum activities needed to complete the task shown in Fig. 3. Material flows are indicated by the arrows. Maintenance is also included. Chemical analysis and waste streams are currently neglected. The vertices are: (1) storage buffer, (2) melter, (3) trimmer, (4) product storage, and (5) recycle storage. These would be 'base elements' of the fuel fabrication subsystem, as discussed in Section 3.1. State changes occur at these vertices. The solid lines indicate the path of the state variable; i.e., these are the edges through

¹ https://github.com/lee7632/Fuel-fabrication-process-code-development.



Fig. 4. DES modeling framework for fuel fabrication. The 'baseline design' is shown in (a), and the 'equipment design' is shown in (b). The state variable is the 'true weight' of the material that will be processed in the system. As metioned above, the vertices are: (1) storage buffer, (2) melter, (3) trimmer, (4) product storage, and (5) recycle storage. The path of the state variable is indicated by the solid lines, and state variables do not change at the vertices. There are key measurement points numbered 0, 1, 2, and 3, and the edges represent state transitions from vertex to vertex. Maintenance is not defined as a vertex, and equipment transfer to it is indicated by a dotted line. In this configuration, each vertex is a material balance area.

which the state variable transitions from vertex to vertex. There are no changes to the state variable on the edges. The KMPs are numbered 0, 1, 2, and 3. Maintenance is not a vertex because there is no state variable transition. The dotted line indicates equipment transfer. Based on Fig. 4, and the discussion in Section 3.3, DA would not be performed until after the product storage vertex. Therefore, DA is neglected at this phase of the model build.

4.2. Assumptions

Without a commercial pyroprocessing facility built yet and the proprietary issues surrounding engineering-scale facilities, as well as the widely known difficulties with regards to scaling from laboratory experiments, obtaining input parameters has been difficult over the years of this model development. Citations have been provided in this section for some of the input parameters, and reasonable assumptions have been made for the rest. This has been based on prior experience from the research collaboration between the Korean Atomic Energy Research Institute and UC-Berkeley, Department of Nuclear Engineering, where the HRS methodology was initially formulated. Further discussion of this collaboration is contained in Borrelli (2014a,b).

KAERI was constructing the Pyroprocess Integrated Inactive Demonstration (PRIDE) facility, a cold-test, engineering-scale, mock-up facility designed and operated by KAERI to support pyroprocessing subsystems demonstration and equipment development (Kim et al., 2010a; Kim et al., 2010b, 2011; You et al., 2011). Therefore, modeling the PRIDE system also required a similar approach. There were many discussions and preliminary work on how a facility could be constructed while also maintaining strong safeguards; i.e., safeguardability, as part of this collaboration, which partially led to the development of this model and the approach applied here (Hwang, 2009; Kim, 2009; 2010; Borrelli et al., 2010; Chang, 2011). These assumptions for input parameters are reasonable because actual operational targets, such as designing a safeguardable facility that will process a specific amount; e.g., 800 MTHM per year, are not needed currently. The main focus and motivation is to test the safeguardability of different designs while observing how much material can be processed per operational period. This discussion is continued in Section 6.2 following the presentation of the results and subsequent discussion.

4.3. Safeguardability criteria

The reasoning in studying the Type I error as a safeguardability metric is that when there is some event, whether it arises from safeguards, safety, or security, there will be a mass balance conducted at least on some subsystem in the facility, if not the entire facility. Therefore, the associated statistical measures are common across all regimes, which is part of the synergistic approach initially conceptualized for safeguardability. However, a mass balance is not only performed due to anomalies in safety, safeguards, or security. It can also be performed after routine maintenance. For example, the crucible in the injection casting machine may be replaced regularly after a set number of campaigns. A facility mass balance may be conducted after a full campaign, or at regularly scheduled intervals in the operational period. These are mass balances over normal operating conditions and would be established most likely by the operator as part of the licensing process, and, presumably, based on IAEA guidelines. This optimization of designing the facility to maximize throughput, while also integrating safeguards, safety, and security measures appropriately into the design is the essential basis for safeguardability.

If an alarm arises, the subsystem will have to cease operations, if not the entire facility. The alarm is an indication of a potential diversion event. It is not known ahead of time whether the alarm is indicative of a statistical anomaly, which can be resolved upon further inspection; i.e., a false alarm. If it is assumed that an inspection would ensue to resolve a potential diversion and that some part of the facility is shut down, this will cost time and resources, as well as affecting the operational goals of the facility. Therefore, if a particular facility design elicited a high number of false alarms, this would be detrimental to all the stakeholders involved. This will carry a high cost in terms of resources needed for inspections and materials accounting, as well as the loss of productivity. There will also be an intangible detriment in that a high number of potential diversion events would raise concerns that the State may have malicious intent in terms of the use of this facility. This could cause concern in the international community and perhaps result in political reprisal, such as imposed sanctions. Therefore, a primary criterion for this proposed safeguardability metric would be that the more safeguardable facility design elicits the lowest number of false alarms while maintaining a reasonably high detection probability.

4.4. Systems operation

One campaign is defined as the processing of one batch. That is, the transition of the state variable from the storage buffer to the product storage. Material flow is sequential. Because there are no experimental studies on the commercial scale, some values were assumed, and others were based on prior study. Material flow is simulated for a prescribed 250 day facility operation period, which is about a 0.70 capacity factor (KAERI, 2008). Facility operation is continuous for the operational period except for equipment failure and maintenance, or facility inspection and mass balance. The edge transfer time refers to transition of the state variable from the storage buffer to KMP0, from KMP0 to the melter, etc., as shown in Fig. 4. Inspection times for both, the end of campaign and after equipment failure, are assumed to be 4 h. Additional operational data is contained in Table 1.

In a real facility, material would arrive to the fuel fabrication process from multiple sources. TRU metal arrives from the cadmium distillation process. Uranium metal arrives to a storage buffer after a salt distillation process, which follows electrorefining. The fuel fabrication process would commence when a sufficient quantity is accumulated in the storage buffer. It is assumed that there is a sufficient amount of feedstock in the storage buffer at TIME = 0 for the fuel fabrication process.

4.5. Inventory difference

The inventory difference for this system is due to the heel in the crucible. There are variables for true ID, expected ID, and measured ID. In this study, the actual values of the three variables are used although

Table 1

Input values for the simulations.

Input variable	Value	
Batch size	20 kg	
Operational time	250 days	
Melter failure rate	$1/30 day^{-1}$	
Expected material left in the crucible	250 grams	
True material left in the crucible	0-500 grams, randomly distributed	
Measurement time at a KMP	30 min	
KMP transfer time	30 min	
Storage buffer batch preparation time	1 h	
Melter operation time	8 h	
Trimming operation time	3 h	
Product storage preparation time	2 h	
Maintenance time	4 h	
Recycle storage time	1 h	
Maintenance transfer time	1 h	
Melter cleaning time	2 h	
End of campaign inspection	4 h	
Failure inspection	4 h	

a measurement error is included. During operation, the heel is not removed at the end of each campaign because this causes frequent stoppages. Developing an accurate system of materials control and accountability is perhaps the fundamental tenet of a safeguardable nuclear materials handling facility. For a non-nuclear weapons State, materials accounting is required for IAEA design information verification and related treaty obligations.

A mass balance (inspection) is conducted at the end of each campaign. This takes 4 h. A false alarm is triggered when the measured ID is greater than 2 kg. This threshold is selected as a nominal value below the typical IAEA goal of 2.4 kg due to a lack of any safeguards goals for pyroprocessing facilities.

4.6. State variables

From the DES perspective, the state variable is defined as the 'true weight' of the material that will be processed in the system. In reality, the true weight is never known in the facility. In general, data recorded at KMPs; e.g., weight, neutron count, etc., are compared to expected results based on historical data cohorts. In additional to the state variable of the true weight, for this model, there are also 'expected weight' and 'measured weight' variables.² These are the means for estimating the true weight. The 'expected weight' is defined as the batch quantity expected to transition through each vertex. This is based on historical data cohorts, experimental studies, pilot studies, etc. Determination of 'measured weight' at each KMP is the true weight \pm measurement error. In Eq. (2), each of the quantities that comprise the ID has a 'random error of the measurement' associated with it, and these errors are assumed to be independently and normally distributed (Avenhaus, 1977). Therefore, the uncertainty in measurement is sampled from a normal distribution about a user prescribed mean of 0.10 kg. Measurement time is 30 min. In reality, this is the only known value of the batch in the system.

4.7. Vertices

4.7.1. Storage buffer

The fuel composition is prescribed, by weight per cent. It is 65U-20TRU-5REFP-10Zr, REFP = rare earth fission products (Borrelli, 2013). Based on the flowsheet in Fig. 1, prior to fuel fabrication, U is obtained from electrorefining, where U metal is collected on a solid cathode, typically graphite, and TRU is obtained from electrowinning and is collected on a liquid cadmium cathode. Then, these materials will be processed further into metal ingots and stored separately in buffers. The ingots would be subsequently transferred to the fuel fabrication system.

Currently, the model assumes a storage buffer vertex that already contains the ingots of U and TRU metal. It is assumed that when the ingots are placed into the crucible and heated, sufficient time has elapsed such that the composition is homogeneously distributed. The batch size is 20 kg (Kim, 2010; Borrelli, 2013), where the subcriticality limit is 25 kg (Kim et al., 2010a; Gao et al., 2011). The expected weight at this vertex is then 20 kg. Because no processing occurs, the true weight is also 20 kg. There is a 1 h 'batch preparation time.' The correct amount of material for a 20 kg batch is then assumed to be transferred from the storage buffer to the melter in this current model.

4.7.2. Melter

Operation time for the melter is 8 h (Battles et al., 1992). For this stage of the model development, the true amount of material held up in the crucible per campaign; i.e., the heel, is assumed to be a random

 $^{^2}$ The use of 'expected' here is not the statistical quantity; i.e., expected value of a random variable. Here, an 'expected quantity' is defined as a amount of material that is anticipated to exist at a KMP in the model.

variable. The injection casting equipment melts the metal ingots, then the quartz molds are inserted, and the resulting vacuum induces injection of the melt into the molds. Upon removal, some of the melt remains as the heel. This could be due to the melt dripping off the outside of the molds, or perhaps one or more of the molds were not completely filled. Either of these events, however, is of a random nature. When the next campaign starts, the heel is melted along with the new ingots that have been placed into the crucible. The amount of material that remains as the heel is overall more than that from the prior campaign, but the amount that is left from the current campaign is again random and could be more or less than the prior campaign. Therefore, the material left in the crucible per campaign is sampled from a continuous uniform distribution. This is used for many problems where there is a lack of data describing the phenomenon of interest. Typically, laboratory experiments would be performed to quantify the heel, and these data would be fit to a known distribution. Then, the mean and variance could be used in the model. Since these data are not currently available, the true amount of material left in the crucible is conservatively assumed to be a continuous uniform distribution between 0 g and 500 g, based on prior study (Borrelli, 2013). The expected process loss is prescribed at 250 g. Scrap is currently neglected. Therefore, the expected weight is 19.75 kg. Failure testing occurs halfway into operation. This is discussed at length subsequently.

4.7.3. Trimmer

Operation time for the trimmer is 3 h. There are currently no failures or process losses. Therefore, the expected weight is also 19.75 kg, and the true weight is the same as determined in the melting process.

4.7.4. Product storage

No processing occurs here. The weights are the same. There is a 2 h 'product storage time.'

4.8. Melter failure

Any piece of equipment in an industrial facility will have several failure modes associated with it, depending on the complexity of the equipment. Analysis of these failure modes is essential for preparing a probabilistic risk assessment for the entire facility. A pyroprocessing facility exhibits additional complexity because proliferation risk must be characterized as well. While fully assessing equipment risk is beyond the scope of the current paper, equipment failure can be nominally modeled for this system.

There are numerous failure modes in the injection casting system, in both the melter and the trimmer. Failures of the trimming equipment are neglected. For the melter, frequent and expected failure modes include crucible or quartz mold cracking. The alloy may not be completely melted due to a heater failure. There may be a failure with the injection system where the alloy may not completely fill the molds. The loss of the inert atmosphere could result in a fire. It can be reasonably assumed that any of these failures results in a complete shutdown of the injection casting equipment. Therefore, a single, general failure of the melter is assumed, and this results in a system shutdown and necessitates removal of the failed equipment and installation of a new melter.

Upon a melter failure, after the batch is measured at KMP3 and transferred to the recycle storage, the facility inspection is conducted to calculate ID. This is where a false alarm could occur. If a failure occurs during the first processing campaign, the ID is due to the random amount of heel present in the crucible. For subsequent campaigns, the ID is due to the random amount left due to the current campaign and the quantity accumulated from prior campaigns.

The cumulative distribution function based on the Weibull distribution is used to model the stochastic failure rate of the melter (McCool, 2012). The Weibull distribution is a widely accepted and applied model for failure analysis especially in cases where information about failures or related failure modes is largely unknown. The 'unreliability' of a system element can be defined under Weibull as:

$$Q(t) = 1 - e^{-(\frac{t}{\eta})^{p}},$$
(3)

where: $t = facility operation time [T], \eta = mean time to failure [T⁻¹],$ and β = shape parameter [-]. In the facility, as operation time increases, the probability of melter failure will increase. By definition, Eq. (3) then gives the probability of failure over the operation time T in the facility as $P(T \le t)$. The unreliability function based on Weibull is very useful because it is rather generalized and can be applied to a wide variety of problems. Typically, the shape parameter is determined based on historical operational data. From a mathematical perspective, it should be relatively intuitive that variation of the shape parameter will significantly affect the character of the distribution. This is the strength of the Weibull distribution; fitting failure data by adjusting the shape parameter will yield information about the nature of failure. For example, with $\beta < 1$, this implies failure rate that decreases with time. Therefore, this equipment is still in the early life stage. However, here, with the lack of operational expertise, it is assumed that $\beta = 1$; i.e., 'general' failures. Any of the failures described above cease activity and require maintenance within the system. Therefore, Eq. (3) reduces to the exponential distribution, and the reciprocal of the mean time to failure (η^{-1}) equals the constant failure rate (λ). A melter failure rate of once per month is assumed.

A Monte Carlo routine based on Q(t) was then developed to this end to model the failure of the melter. Upon failure, the batch is moved to recycle storage from the melter. The equipment is then 'cleaned;' i.e., the heel is moved to recycle storage with a 2 h cleaning time. During maintenance, the defective equipment is removed, and a new equipment is installed. The total amount of material is then transferred from recycle storage to the melter, and operation resumes.

4.9. Features of the code

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The code focuses on maintaining a hierarchical decomposition of the facility components. This design logic goes well with batch processes since only the state variable is passed from vertex to vertex. In this regard, each node in Fig. 4 is represented by its own class in Python. Each of these objects accepts the batch (which is its own object), acts on it accordingly, and then passes it to the next vertex class.

The vertices in the system model act as the bottom-most children of the hierarchy. They are grouped together according to proximity as shown in Fig. 4, and each group is assigned a managing object that can call on any of its children at any given moment for pertinent information; i.e., the measured weight, the expected weight, etc. That information is then passed on to the supervisor who uses the information to make facility-wide calculations and decisions such as when an alarm should be triggered. However, the supervisor does not call on the managers to collect this information until it is needed, minimizing the computation time by avoiding unnecessarily frequent updates.

Although many programming languages are robust enough, Python is favored for its flexibility in importing objects and accessing components. An entire object can be imported to a different object, or one can bring in only a few variables or methods from that object. These objects are passed internally by reference, minimizing overhead costs when manager and supervisor nodes call their children nodes. This structure can be readily expanded in order to model the full system shown in Fig. 1 in a similar manner.

4.10. Simulations

First, the input/output directories of the full system were created. The system input parameters in these directories included relevant operational data. Then, the simulation was run for the operational period of 250 days. At the end of each campaign, the full material balance over the facility was performed, and in each case, the measured

inventory difference was checked against the expected inventory difference as a semi-empirical Shewhart's test (Massart et al., 2003). If this difference was above the prescribed threshold, an alarm was raised. The system output data obtained from the simulation were recorded in the output directories. Execution scripts were built to automate simulation of the operational period for a user prescribed number of times. The simulated false alarm probability was computed based on actual false alarms over potential opportunities for a false alarm. Simulated melter failure rate was calculated by dividing the number of failures by operation time.

To assess safeguardability on a pyroprocessing facility, it is imperative to test various facility designs. Material throughput for two different facility designs were simulated based on Fig. 4: the 'baseline design (Design A)' and the 'equipment design (Design B).' Design B was with KMP1 removal. From a qualitative perspective, Design A was intended to exhibit stronger safeguardability because each vertex is its own MBA, while for Design B, the removal of KMP1 was intended to maximize material throughput. Optimization of each is the basis for a highly safeguardable facility. Operation periods were simulated for 1000 times, 2000 times, and 3000 times, and the average output values with standard deviations were calculated for both designs.

5. Results and discussion

5.1. System output

It was determined that 1000 simulations were large enough to achieve convergence in the output data. Results are presented as the average values with standard deviations over the 3000 simulations. Fig. 5 shows the melter failure probability for both designs. The simulated melter failure probabilities shown in Fig. 5 for Design A and Design B are essentially equal at 0.150 \pm 0.013. This shows that the subsequent results are not a function of melter failure, and therefore, safeguardability is not a function of the choice of equipment and only based on material flow and design. Therefore, from this result, the code is producing results consistent with the physical conditions established in this study.

The average completed fuel fabrication campaigns are shown in Fig. 6. The average number of campaigns of Design A is calculated as 229 \pm 4.2, and that of Design B is 229 \pm 4.1. This indicates that the proposed designs do not affect operational goals. The false alarm probability of Design A and that of Design B are also effectively similar, as shown in Fig. 7. The false alarm probability of Design A is given as 0.019 \pm 0.007 and that of Design B is 0.019 \pm 0.008. This is considerably less than the typical IAEA recommended goal of 0.05. After the 250 day operation, the amounts of processed material for Design A







Fig. 6. Simulated number of completed campaigns. The average number of campaigns of Design A is 229 \pm 4.2, and that of Design B is 229 \pm 4.1. These proposed designs do not affect operational goals, but these results also indicate that the designs are essentially equivalent.



Fig. 7. Simulated false alarm probability. The false alarm probability of Design A is 0.019 \pm 0.007, and that of Design B is 0.019 \pm 0.008. Again, these values are less than the typical IAEA recommended goal of 0.05. A low false alarm probability with a reasonably high detection probability is a proposed criteria for safeguardability assessment and indicative of a strong, safeguardable design.



Fig. 8. Simulated amount of processed material at the end of the operational period. The amount of processed material for Design A is 4568 ± 84.2 kg and for Design B, is 4570 ± 83.0 kg. There are currently no operational goals for the pyroprocessing facility, but this will have to be optimized with safeguardability.



Fig. 9. Simulated inventory difference. The inventory difference for Design A is 0.868 ± 1.152 kg, and for Design B, it is 0.940 ± 1.189 kg. Both of these designs offer strong safeguardability. The ID is well below the 8 kg for a significant quantity for plutonium for both, and the SEIDs for both are below the 2.4 kg based on suggested IAEA goals.

and Design B are 4568 $\pm\,$ 84.2 kg and 4570 $\pm\,$ 83.0 kg, respectively, shown in Fig. 8.

5.2. Inventory difference

The inventory differences for Design A and Design B are shown in Fig. 9. The simulated ID of Design A is 0.868 \pm 1.152 kg, and that of Design B is 0.940 \pm 1.189 kg. This indicates that both Design A and Design B are relatively safeguardable designs. The ID for each design is well below 1 SQ of 8 kg for plutonium, and the simulated SEIDs are below the 2.4 kg limit previously discussed.

To further examine the implications of SEID on safeguardability, Eq. (1) is applied. Here, for α , the simulated false alarm probability of 0.019 ± 0.008 is substituted. Because it is essentially equal, the simulated false alarm probability with the higher standard deviation is used as a conservative estimate. Detection probabilities $(1 - \beta)$ of 0.90 and 0.95 were selected. Appropriate design approaches can render decisions by the State to initiate a diversion attempt to be strategically poor because the detection probability is reflective of a State decision. A detection probability of 0.90 is considered a reasonable lower bound for study of this system. The SQ is 8 kg for plutonium. Therefore, the SEID in Eq. (1) (σ) can be obtained directly. These calculations are contained in Table 2, where the IAEA goal of SEID = 2.4 kg is included for reference, as well as the SEID of 2.7 kg for $\alpha = 0.05$ and $(1 - \beta) = 0.90$. Clearly, for the simulated false alarm probability range, the calculated SEIDs shown in Table 2 ranging from 2.03 kg to 2.38 kg fall below the IAEA goal of SEID = 2.4 kg, except in the one instance of 2.49 kg. However, the value of 2.49 kg falls below the calculated limit of 2.7 kg. Even though there are no current IAEA goals for the advanced fuel cycle, the simulation and related calculations are on par with the suggested IAEA goals previously discussed. This shows that the use of the

 Table 2

 Calculated standard errors of the inventory difference using Eq. (1).

False alarm probability (α)	Detection probability $(1 - \beta)$	SEID (kg)
0.05	0.95	2.4
0.05	0.90	2.7
0.011	0.95	2.03
0.019	0.95	2.15
0.027	0.95	2.24
0.011	0.90	2.24
0.019	0.90	2.38
0.027	0.90	2.49

false alarm probability offers merit as a safegurdability assessment metric.

More importantly, the simulated SEIDs of 1.152 kg and 1.189 kg for Design A and Design B respectively, are far below the calculated SEIDs. Both designs are highly safeguardable and therefore could be prohibitive for State-driven attempts at material diversion even at a detection probability of 0.90. Yet at the same time, these facility designs showed that approximately 4500 kg of material could be processed. This model can offer the capabilities of optimizing operational goals with an assessment of design in terms of safeguardability. This is a significant result for safeguardability assessment. Applying the false alarm probability to safeguardability assessment in this way is a valuable, preliminary effort into developing a safeguards- and security-by-design approach for a commercial pyroprocessing facility.

5.3. Functional design components and preliminary safeguardability assessment

Ultimately, the intent is to use this model in order to assess proposed facility designs and offer functional design components to enhance safeguardability. To this end, Design A was expected to be a highly safeguardable design, due to key measurement points after each vertex and a material balance after the product was stored in the final vertex. Design B was expected to exhibit a higher throughput with the removal of KMP1 but potentially be less safeguardable.

Essentially, Design A and Design B processed about the same amount of material over the operational period. In Design A, MBA was established for each process step, and for Design B, the melting and trimming processes were included in a single MBA. Ideally, maximizing material balance calculations will produce a strong, safeguardable facility. With no appreciable changes in the false alarm probability and the quantity of processed material, both Design A and Design B can be applied to this system without sacrificing operational goals. Therefore, these results show that there is almost no difference in terms of safeguardability between Design A and Design B; i.e., these are equivalent designs based on the conditions established for this proposed facility. This is still a meaningful result and a good application of this model. In reality, two proposed designs might look different where one carries a much higher cost. The model can show that the designs are in actuality equivalent and provide a nominal economic tool.

The simulated SEIDs for both designs fell well below the calculated SEIDs even for the lower bound detection probability of 0.90. When instituting safeguards measures in a new facility, the use of the lower detection probability may result in less overall cost. IAEA does not currently have safeguards goals for advanced nuclear fuel handling facilities, and this result could be the basis for new evaluations of safeguards between IAEA and the host State. In essence, this could be similar conceptually to ALARA, where an economic limitation is placed on the quantitative reduction in radiation exposure. Increasing the detection probability in the safeguards system from 0.90 to 0.95 may be cost prohibitive and potentially not necessary if SEID simulations can be shown to fall below projections obtained from Eq. (1). Clearly, this is also based on a simulated low false alarm probability as was the case in this study.

6. Future work

The results in this study lead to substantial upcoming work. Nearterm activities will focus on three overall features: (1) measurement and accounting, (2) building in practicality, and (3) integrating the chemistry and physics that govern these processes through mathematical modeling. Currently, the model has not been developed to the point of being usable as a tool for major design approaches for the fully pyroprocessing facility. However, these results are promising in the development of a robust manner in which safeguardability can be assessed within the context of facility design in its current form. Upgrades to the model will focus on a more accurate simulation of the safeguards system and NMA, and operational considerations, which affect safeguardability assessment.

6.1. Measurement and accounting

Activities at the KMPs require further development. This includes the removal of different KMPs, investigating changes in parameters such as the uncertainty of the KMP measurement, the ID inspection at each KMP, and changes in the weight threshold on operational goals. Currently only a weight measurement is simulated at the KMP. If the U and TRU ingots could be melted to produce a homogenous mixture. then it may be possible to use neutron counting after this occurs. This could be upon transfer of the injected molds to the trimmer or after slug trimming. This would be at KMP1 and KMP2 in Fig. 4. In terms of configuration of KMPs in the system; i.e., examining the possible formations of MBAs, observing how system parameters are affected will yield further insight into safeguardability. Whether it is more prudent to minimize the number of KMPs but not necessarily the number of material balance calculations will also be considered. There may be centrally located assay station(s) in order to conduct the measurements. Therefore, it may be possible to enhance operational goals while maintaining strong safeguards.

As part of an NMA system, DA should also be considered. For fuel fabrication, if there is a storage buffer of fabricated slugs, as presented in the current model, where the next stage would be fuel rod assembly, it is reasonable that DA could be performed at this point in the system, where slugs would be presumably chosen at random for assay. DA would be needed to address inhomogeneity of processed materials. Therefore, DA would not cause an operational disruption because the slugs are already stored in the buffer. Additional analysis is needed to determine if the destroyed material is a diversion risk or how much of a risk it is in comparison to other potential diversion pathways in the facility. The NMA system will also have to include accounting for the SNM content in tested material. The final state of the tested material would need to be considered. An operator would want to process as much material as possible and might want to recycle the material back into the melter, rather than outright disposal, but the composition of the melt is prescribed. New procedures would then be needed to address recycle in this manner. The material could still be stored and monitored relatively long-term in a separate, dedicated buffer.

6.2. Practical use of the model

Every effort was made to build a practical model, compiled over several years of study, but there could be more robust input data. Currently, assumed parameters were used, as previously discussed in Section 4, in order to test the model, analyze its performance, and determine directions for the next phase of development. It was established that the model described the physical conditions established for this study, which is important, and, that the results showed the proposed designs under these conditions were equivalent, which partially supports the hypothesis set at the start of this study. Process loss in the trimmer was neglected. The physical material in this process will be fine particulates of metal. Quantifying the amount of this material as well as determining how much material can be cleaned will be challenging. If a suitable model can be developed, or more reliable data can be obtained to include process loss in the trimmer, then the model should again be applied to assess Design A and Design B in terms of safeguardability.

Historical operational data is currently lacking. However, injecting casting, as an industrial process, has been used for decades. Applying operational data from an analogous process to the injection casting of the U and TRU to this pyroprocessing system model would be fairly useful, from a risk assessment perspective, in terms of failure modes and associated failure rates. Recent dissemination of this work for the first

time (Borrelli and Tolman, 2016) has generated interest in further discussions on this work and could help address this issue. Engaging with other experts in this field has been an ongoing process, and additional solicitation of expert judgement would be beneficial. Failure rates for both the melter and the trimmer are needed, as well as processing times and determination of held up material for both. More accurate processing times will elicit a clearer conclusion in terms of operational goals. In reality, there are multiple failure modes for the equipment, and an envelope of the most common modes should be developed. A parallel study is focused on developing a high-level HAZOP analysis for the pyroprocessing facility in order to better understand operational considerations and equipment failure modes. Therefore, with more robust input data and improved engineering design, as discussed in Section 6.3, the safeguardability of a facility design with operational goals can be optimized, and the outcomes put forth under HRS can be achieved.

6.3. Engineering design

Results from this study were not exactly as expected. Our hypothesis asked whether the false alarm probability can be used as a metric to evaluate system designs in terms of safeguardability. Because there has not been any studies formulated in this way, there is not really any additional guidance on how to proceed. The results show that the proposed designs themselves are equivalent, but there needs to be more insight into actually quantifying safeguardability in a meaningful way that is readily acceptable. The engineering design aspect of this study needed to be stronger, and in the next build of the code, more demonstrably different designs will be considered.

6.4. Complementary approaches

The next phase of model development beyond bulk material flow, as presented here, will be to integrate the chemical and physical processes governing the fuel fabrication subsystem; i.e., applying the bottom-up approach to the system model. DES is a useful modeling structure to this end because mathematical models that describe these processes can be built into the appropriate vertices. For example, with injection casting, the melting process is modeled as the classical Stefan problem found in heat transfer. With these upcoming accomplishments, the model can be expanded for the full pyroprocessing system.

Finally, when this model achieves a reasonable level of maturity, it can be validated against similar models in the literature; e.g., most notably, the model developed by Cipiti et al. (2012), but other published work as well. Validation will aid in expanding this DES model significantly and provide meaningful insight into safeguardability assessment.

7. Summary remarks

The design of a safeguardable facility in the advanced fuel cycle will involve optimization of operational goals with accurate NMA. This paper presented the first built material throughput model for the fuel fabrication in a commercial pyroprocessing facility by applying discrete event simulation principles. The goal was to determine how established safeguards metrics, namely, the false alarm probability, can be used for quantitative safeguardability assessment. An initial criterion was proposed that a safeguardable facility would elicit a lower number probability of false alarms while maintaining a reasonably high detection probability when comparing different facility designs. False alarms in the facility occur due to safeguardability assessment can yield important design information.

The material throughput model simulated fuel fabrication campaigns over a 250 day operational period for two different designs, one to maximize safeguards, the other to maximize material throughput. The main implications from the simulations are:

- Results described the physical conditions established for this study, and the model is performing as expected.
- Major system output parameters are not demonstrably different over each design. Therefore, operational goals are not affected, and the designs are essentially equivalent in terms of safeguardability.
- The simulated standard error of the inventory difference obtained for each design fell well below that calculated from the standard, mathematical relationship used for safeguards. This suggests the system could detect a diversion attempt reliably.
- The simulated standard error of the inventory difference is sufficiently low as to potentially lower the current IAEA goal for detection probability, thus offering a less costly approach to establishing the safeguards system in the facility. It would not be prudent at this time to establish a criteria for safeguardability assessment based on the SEID because there are no current IAEA goals for the advanced fuel cycle. As this model matures, new criteria may come to light within this context.

Near-term work will focus on addressing modeling limitations such as obtaining input data, studying failure modes for the equipment, and integrating the chemical and physical processes into the model. Further DES modeling in this way is applicable to a pyroprocessing facility due to the batch nature of subsystems processing, including transfers between subsystems, and salt recycle. Additionally, once facility data can be obtained; e.g., equipment reliability, maintenance times, etc., DES can be used to identify locations where 'bottlenecks' will occur and material throughput is held up. This will further inform facility design by suggesting hot cell configurations where bottlenecks can be minimized, while enhancing safeguardability. With no current goals for the Type I error probability, there is wide latitude in the development of possible design strategies for a design-driven, safeguardable model for a pyroprocessing facility.

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