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Modeling, Analysis, and Optimization of Complex Nuclear Processes and Facilities via Computational Methods: The HALEU Process Case Study

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Abstract

Improving and adapting industrial systems to timely meet changing programmatic and market demands is an important goal to achieve, including when operating and maintaining complex nuclear processes and facilities. However, changes to these complex systems are costly, particularly when they are already in place and bounded to stringent requirements and constraints such as when handling radioactive material and contaminated equipment. These conditions often exist when treating spent nuclear fuel remotely within shielded nuclear radiation chambers, commonly referred as hot cells, to condition nuclear material and/or fabricate products for utilization in other nuclear enterprises such as in the manufacture of advanced nuclear fuel. The illustrative case considered here is the production of high assay low enriched uranium (HALEU) products supporting the deployment of advanced nuclear reactors. For the HALEU program, resources invested were and are being systematically analyzed so that these investments are maximized in a facility that is nearly 60 years old. A methodology that has effectively enabled optimized and improvements in the Spent Fuel Treatment (SFT) program, and consequently the HALEU program, involves discrete event simulation as addressed in this article. The quantification of multiple productivity metrics, including material processing rates, cycle times, bottlenecks, number of material transfers as well as equipment, workstation, and material handling utilization, has resulted in a myriad of diverse discoveries and data-informed decisions regarding process layout and constituent, labor levels and schedules, selection of new process units, storage needs, and other critical process configurations. This article describes such a computational capability being applied for decision-making, illustrates its application to an actual process and program, provides illustrative results, and argues how computational methods for the modeling, analysis, and optimization of complex processes and facilities does lead to informed decisions derived from data and not only from intuition.

Keywords: nuclear process modeling, analysis and optimization, high assay low enriched uranium (HALEU), process productivity optimization, nuclear processing systems, advanced nuclear reactors.

1. Introduction

Computer simulation is an effective tool for designing, analyzing, and optimizing the design and operation of engineered systems, including manufacturing processes. Computer simulation, which includes mathematical modelling, is utilized to estimate and predict the behaviour of systems under specified conditions. In this way, it enables the systematic evaluation of proposed options without committing capital and operational resources or disrupting the actual system at hand. Multiple and diverse elements (e.g., activities, resources, operational methods and technologies, as well as control procedures) associated with systems under examination can be readily changed, rearranged, and then evaluated in a simulated environment to discover ways to improve diverse qualities including efficiency, operability, productivity, sustainability, resiliency, safety, and security.

The analysis of real-world systems continues to be a challenging endeavour due to the ever-growing levels in complexity, uncertainty, and volatility. For example, the handling and treatment of radioactive material impose stringent requirements for remote operation, safety, and physical space, leading to systems composed of multiple elements interrelated in complex arrangements. Furthermore, the inclusion of new missions and programs for the treatment and utilization of nuclear material has often led to the growing need to modify and modernize nuclear facilities. Not only the selection, configuration, and integration

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of new technologies have become more complicated, but also it is challenging to quantify how much improvement is gained by implementing proposed operational changes.

In principle, operational analysis and optimization of systems may be achieved without using systematic techniques. However, operational process states and changes may be far more difficult to characterize, correctly interpret operational behaviors, and respond to in systems composed of numerous steps involving a finite number of resources including material movement constraints. Ad-hoc and trial-and-error methods as well as engineering judgement may be used to assess the benefits of proposed modifications. However, these approaches often result in costly, time consuming, and disruptive undertakings. On the other hand, computer simulation is being utilized by the research and industrial community as a powerful, cost-effective decision-making tool during the design, implementation, and operation of actual or proposed installations, including nuclear facilities (Banks, Carson, Nelson and Nicol, 2014).

As part of its effort to support the development of new nuclear fuel technology (e.g., HALEU) and to improve the treatment and/or manufacturing of advanced nuclear materials, the U.S. Department of Energy (DOE) has made and continues to make significant capital and labor investments in the development of computational capabilities as well as in the design and evaluation of new equipment and labor resources in support of the actual facilities located at the Materials and Fuels Complex (MFC) of the Idaho National Laboratory (INL), including the Fuel Conditioning Facility (FCF). These facilities are equipped with labor-intensive material-handling equipment, specialized processes, and flexible unit operations supporting diverse programs, such as the High Assay Low Enriched Uranium (HALEU) program. As a significant number of process units are already installed and those being considered for update and/or inclusion are unique to the nuclear fuel conditioning goals at hand, multiple challenges and opportunities emerge when simulating, analyzing, and optimizing potential process configurations and networks of equipment proposed for achieving optimality of work conducted with respect to diverse metrics including productivity, sustainability, flexibility, cost-effectiveness, and safety. Resources and operations are gradually analyzed and accordingly upgraded to meet potentially time-varying production targets. Modification and upgrades are being accomplished via a combination of additional equipment installations and process improvement projects.

Using an actual illustrative application, this article discusses the utilization of computational methods, such as discrete event simulation (DES), for: i) the discovery of insights into current and proposed operations in the process systems under consideration, ii) the quantification of important productivity metrics, as well as iii) the evaluation of proposed changes in operations, including rearrangements in process layout configurations, new equipment and workstations, and labor schedules. The discrete event model of the actual facility here illustrated was verified and validated by comparing computed productivity estimates against actual observations. Numerous analyses and recommendations for improvement, with some of them briefly discussed in this article, demonstrate the practical benefits of employing this sort of decision-making tools for achieving significant improvements in terms of production rates increase, resource (equipment and labor) utilization feasibility, and cycle time reduction, among other criteria. Use of the decision-making capability and methods here discussed can be applied to other processes and facilities.

1.1. Contributions

This article addresses a rigorous approach for analyzing and optimizing the operations conducted at actual nuclear facilities in response to actual DOE programs, focusing in this article on those related to the High Assay Low Enriched Uranium (HALEU) program. To this end, this article describes the operational analysis performed on a nuclear fuel treatment facility and the benefits obtained from simulation experiments. The nuclear facility considered here is FCF located at MFC of INL (Stevenson, 1997). Processes conducted at this facility involve the electrometallurgical treatment (EMT) of nuclear fuel, which involves multiple batch operations conducted in remote, isolated hot cells (Goff, Benedict, Johnson, Mariani, Simpson and Westphal, 2000). The complexity of the processing and material handling operations present at this facility is typical of nuclear facilities and makes it important to employ computational methods to quantify performance measures and suggest optimal improvements.

1.2. Related work

A survey of the literature on the formal application of computational methods, and DES in particular, in support of system evaluation studies in nuclear facilities revealed multiple instances. Due to page limitations, few of them are briefly introduced next. For example, Houshyar and Imel (1996) reports the modeling of the fuel handling strategies used to process nuclear fuel assemblies. This work illustrated the power of DES as a managerial tool to study different processing options. Similarly, Garcia, Houshyar and Imel (1995) reports the development of a model intended to use on-line information to identify, based on current operational state, the best strategy for fuel handling and conditioning. The advantage of this model was its capacity to correct deviations (due to unpredictable down times and delays) from specified fuel transfer schedules. Garcia and Houshyar (1998) discusses the use of DES techniques to analyze fuel transfer strategies expected to improve safety, productivity, and cost reduction. In continuation of these efforts, operation analysis and improvement of a spent nuclear fuel handling and treatment facility using DES is reported in (Garcia, 2000). Similarly, DES was utilized to conduct a preliminary evaluation of the Melt-Drain-Evaporate-Calcine

(MEDEC) (Toews, Herrmann, Sell, Rigg and Pahl, 2002), (Garcia, Herrmann and et. al, 2003). A DES-based model, named PyroFlow, is reported in (Lee, Kim, Kim and Lee, 2011) that simulates the dynamic material flow of a pyroprocess. Bottleneck analyses were carried out using PyroFlow, concluding, among other findings, that selected operation strategies influence its productivity. Similarly, a DES strategy is reported in (Lee, Ko, Choi, Kim, Lee, Im, Hur, Choi, Park and Kim, 2014) to construct an integrated operation model that analyses an oxide reduction process, showing that material flow could be tracked under a DES modeling environment. Related to it, a DES strategy is reported in (Lee, Im and Park, 2016) to create an integrated operation model for which simulation showed that dynamic material flow could be accomplished to provide significant insights into the process operation as well as calculations associated with mass balance. Using the Versatile Test Reactor (VTR) program as a case study, DES models, along with nuclear physics model outputs, of a nuclear fuel fabrication process are used in (Bourque, Clarno and Leibowicz, 2022) to determine the optimal number of staff that ensures that fuel production goals are met, that operations comply with effective dose limit regulations, and that overall project costs are acceptable. Predicting nuclear power plant operator performance using DES is addressed in (Yow, Walters, Plott, Laughery and Persensky, 2005). Similar to the work here reported, a DES approach is described in (Lee, Kim and Park, 2009) for an operation analysis of a headend process facility, with this process being the first part of the pyroprocess. The application of DES to determine if nuclear materials accounting can potentially serve as a metric for safeguardability in nuclear facilities is discussed in (Lee, Tolman and Borrelli, 2017). Similarly, Garcia, Simpson, Lin, Carlson and Yoo (2017) uses DES to evaluate the application of process monitoring for anomaly detection in nuclear material processing systems via system-centric interpretation of data collected from distributed sensors of varying reliability.

The rest of the paper is organized as follows. Section 2 provides a background for the study addressed here including computational techniques and benefits from simulation. Section 3 summarizes key aspects associated with the problem formulation at hand, including motivation, goals, elements supporting operations research (OR) capabilities, and potential applications. A process overview of the actual nuclear process and facility selected for discussion is provided in Section 4. The developed computational capability is discussed in Section 5 including methodology, developed facility operations model, and associated modeling constructs. The use of computational methods for decision-making is illustrated via two what-if analyses in Section 6. Section 7 concludes this article.

2. Preliminaries

2.1. Discrete event simulation

Discrete-event simulation (DES) is an effective computational method often utilized to model, analyze, and optimize real world systems that can be decomposed into a set of logically and functionally separate processes and whose dynamics progress through time based on well-defined recipes and as a (discrete) time sequence of events. Each event, occurring at a specific process at a particular instant in time, is assigned a logical time, and marks a change of the state in the system (Robinson, 2004). Characterized from having discrete-event driven dynamics, no change in the system occurs within consecutive events, hence the simulation time jumps and progresses directly to the occurrence time of the next event, a notion called next-event time progression. The occurrence of an event can be an outcome passed to one or more processes, with the outcome potentially resulting in the generation of new events to be processed at some specified future logical time. Textbook treatments of discrete event systems can be found in (Cassandras and Lafortune, 2008) and (Law, 2014).

2.2. Benefits of Simulation

Multiple computational methods employed for operations research (OR), such as DES, have provided a large variety of operational benefits for designing proposed processes and facilities. To illustrate, personnel in the MFC production facilities division at INL have acknowledged the significant value of and multiple benefits obtained from developed facility operations models (FOMs) and their experience, along with historical operational performance, supports the models' findings and recommendations). Broadly speaking, benefits from using computational methods may be grouped into three main areas as follows.

- System Understanding: FOMs can assist in collecting insights into the dynamics of proposed processes and their associated facilities. Operation dependencies and bottlenecks can be uncovered and the impact and limitation that material handling may have on productivity can also be quantified. Similarly, productivity dependencies on process layouts and on supporting operations can be better understood. These unveiled discoveries and acquired understanding can support the identification and implementation of effective and feasible solutions to remove operational deficiencies and improve productivity.

- System-centric Strategy: FOMs can assist in directing R&D and engineering efforts towards activities and solutions anticipated to deliver the greatest gains to achieve identified goals as measured by metrics such as productivity, efficiency, sustainability, and resiliency. Opposite to a bottom-up strategy, FOMs can also direct efforts toward first focusing on overall system aspects and then zooming in where needed.

- System Optimization: FOMs can assist in identifying operational strategies for getting the most out of equipment, processes, workstations, and resources. Diverse elements conforming particular endeavours can be optimized including physical layout, equipment capacity, operational modes, as well as labor and maintenance schedules.

- System Risk Assessment: FOMs can assist in minimizing and/or managing risk. A FOM implemented during the initial design phases and enhanced through the design and implementation phases of the process and/or facility at hand can support a rigorous approach towards assuring that the process or/and facility can meet production goals at acceptable risk levels. From these risk analyses, problem areas can be identified, including changes expected to deliver the most improvements. Even before a given equipment or unit operation is installed and/or the facility is constructed, a FOM can be used to assess whether identified systems will operate as intended, significantly reducing the risk of project failures.

3. Problem Formulation

3.1. Motivation

The processing of nuclear fuel, particularly radioactive (spent) fuel, often requires nuclear facilities with high levels of operational complexity, involving the compound interaction of disparate operations within multiple dimensions including resource allocation, workload distribution, material control traffic, labor restriction, as well as equipment layout, operation, and scheduling. This complexity increases exponentially when nuclear facilities, such as FCF located at MFC of INL, are repurposed to support "production" and multi-missions objectives after having been constructed to support R&D and often single mission objectives. Throughput goals at actual facilities, processes, and "services" may have to be ramped up by several orders of magnitude.

In order to address the numerous challenges arising in support of the EBR-II Spent Fuel Treatment (SFT) program and in particular for the High Assay Low Enriched Uranium (HALEU) program, diverse system-centric computational capabilities were developed for modeling, simulating, analyzing, and monitoring intended processes and their facilities as well as for determining advances that may be needed for optimizing operations, increasing throughput, pursuing simplicity, enhancing resiliency, and enabling transparency and efficiency of operations. Within these on-going efforts, a facility operations model (FOM) of the HALEU process and its hosting facility (i.e., FCF) has been developed and continues to be updated as new strategies are implemented and demonstrated. Integrating labor, production, and material handling operations, this FOM relies on diverse data including facility layout, process time estimates, permissible buffer locations, equipment capabilities, and material handling constraints, as well as assumed resources and operation event sequences. Payoffs come in the form of a decision-making tool that can be used to quantify, compare, and optimize different operational strategies proposed for achieving the productivity target at hand and compute life-cycle cost estimates.

3.2. Goals for Facility Operations Modeling

The fundamental goal for investing in facility operations modeling was and continues to be to timely understand, predict, and alter system behavior in a manner to cost-effectively meet given program requirements under established constraints. The possibility to experiment with all sort of operational scenarios, conduct comparison studies, as well as predict and quantify system productivity responses under different situations continues to be assessed as beneficial at INL. In this regard, operations research (OR) studies being conducted at INL can be grouped into five main categories as described next:

- Capacity Analysis: The main goals here are to estimate whether given throughput is feasible, quantify facility capacity based on installed or proposed equipment and operational practices, evaluate process flow and work distribution among workstations, and quantify processing and material handling equipment utilization.

- Constraint Analysis: The main goals here are to identify process bottlenecks, weak links, and inefficient operations, assess whether production rates are sustainable under proposed technologies, estimate impacts of equipment up-time and downtime, and provide operational recommendations. The assumption of increasing system productivity by increasing a single machine throughput is usually valid for simple manufacturing lines. However, when a machine is a component in a more complex arrangement where other machines, resources, and buffers of limited sizes exist, increasing a machine processing rate capacity may not necessarily improve overall system throughout. Given that material handling plays a significant role in HALEU as implemented at FCF, the availability of FOMs has been proven to be instrumental for constraint analysis.

- What-ifs Analysis: The main goals here are to: i) estimate operational metrics (e.g., throughput, cycle/wait time, resource utilization) under various conditions; ii) understand the implication of new systems or operational upgrades; iii) observe impact of process layout, workload distribution, in-cell inventory, equipment capacity, material handling resources, and labor schedule; iv) quantify processing and material handling equipment utilization; and v) identify unproductive ventures and direct attention to areas yielding operability and productivity gains.

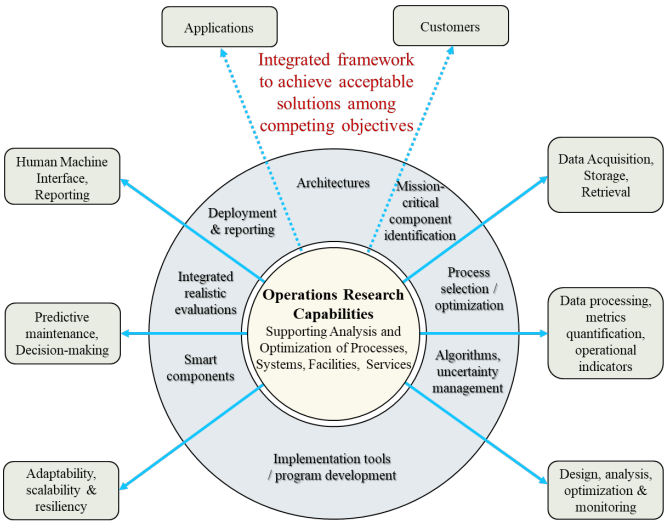

Figure 1: Operations research elements supporting the analysis and optimization of processes, systems, facilities, and services.

- System Optimization Analysis: The main goals here are to optimize labor and maintenance schedules, physical layouts, processes, and inventories, as well as to evaluate statistical variations.
- Operations Monitoring, Tracking, and Prediction: The main goals here are to monitor and track the movement of materials and execution of unit operations in a user-friendly manner as well as to readily devise and evaluate future conditions and solutions.

3.3. Operations Research (OR) Elements

In order to support the analysis and optimization of systems using OR techniques, several of its key elements require continued development and improvement including architectures, discrete event modeling and simulation (M&S), algorithms, and distributed process monitoring intelligence. Figure 1 depicts some of these key elements of a simulation-centric approach. Beginning at the top and progressing clockwise, this figure suggests that a robust computational architecture should be first formulated before constructing the intended M&S capability. Then, to manage model complexity and obtain valuable returns from simulations, mission-critical components should be identified, as well as those processes that may be in need of optimization. As manufacturing processes typically exhibit stochasticity in their inputs and outputs as well as in the availability of resources, for example, algorithms for uncertainty quantification should be synthesized. With these elements in hand, it is necessary to select the computational tools for implementing FOMs. After its construction, realistic evaluations should be designed not only to verify and validate FOMs but also to report calculations useful for decision-making.

3.4. Applications

The following list exemplifies the application of computational methods relevant to INL nuclear facilities. Similarly, several programs have successfully utilized FOMs at INL including those listed in Table 1.

- *Fuel Conditioning Facility (FCF) Operations Model.* It accommodates multiple unit operations including nuclear material receiving and shipping, nuclear fuel chopping, nuclear fuel electrorefining, salt distillation, material consolidation, isotopic dilution, reguli recasting, material sampling, and many more, in addition to material handling and labor resources.
- *Hot Fuel Examination Facility (HFEF) Operations Model.* It accommodates multiple unit operations including metal and ceramic waste processing, in addition to material handling and labor resources.
- *Analytical Lab Operations Model.* It accommodates multiple process analysis stations including those workstations and services for the analysis of samples.
- *Operations Monitoring and Tracking.* It accommodates: i) automatically feeding given FOM with data stream collected from a related facility and using it as a visualization and analysis tool to best understand the facility's production state and conditions; and ii) using FOM as a predictive tool to assess future conditions or evaluate what-if scenarios such as what would happen if certain actions are taken or certain events (e.g., equipment failure) occur.

Before focusing from hereafter on HALEU, Fig. 2 provides a screenshot of the DES constructed for evaluating the use of processing monitoring to detect facility misuse and/or material diversion in spent nuclear treatment facilities. Assuming pyroprocessing, the FOM constructed models three primary operations: oxide reduction (OR), electrorefining (ER), and electrowinning (EW). In addition, the model includes cathode processing (via two cathode processors (CP)), which is considered to be a secondary operation. These operations generate multi-modal sensor data that is sent on to a set of safeguards computational observers located at the Process Monitoring Module via the data acquisition system (DAS) block. The red blocks and red text in the green blocks denote multiple distributed sensors. More information about this DES-supported effort can be found at (Garcia et al., 2017).

4. Process Overview

4.1. HALEU Process Description

Most advanced nuclear reactor concepts being proposed by the nuclear commercial sector require uranium fuel enriched between 5% and 19.75% (< 20 wt% ^{235}U) for startup core. Consequently, future demands for HALEU may potentially be very significant, while recognizing that there

Program	POP	Summary
Spent Fuel Treatment	1995–Present	Introduction of operations research (OR) at INL to identify optimal operational solutions and achieve diverse productivity goals.
Melt-Drain-Evaporate-(MEDE)-Carbonate (MEDEC)	2001–2003, 2023–Present	Studies to support a conceptual design and cost analysis of the MEDE/MEDEC process to treat and dispose Fermi-1 sodium-bounded spent nuclear fuel.
Acc. Driver-Only Campaign	2014–2015	Multiple studies conducted to identify optimal operational solutions to achieve diverse productivity goals.
Process monitoring safeguards	2014–2017	Rigorous methodology developed to assess intrinsic safeguards observability property of a process/facility given selected sensor configuration and implement operations accountancy via an optimal network of distributed multi-modal sensors. Minimal information needed for guaranteeing process detectability and diagnosibility, hence reducing cost and operability intrusiveness and improving the tamper-resistance characteristic of the safeguards monitoring system.
High Essay Low Enriched Uranium	2019–Present	Multiple studies being conducted analyzing diverse options and scenarios.

Table 1: INL programs using facility operations models

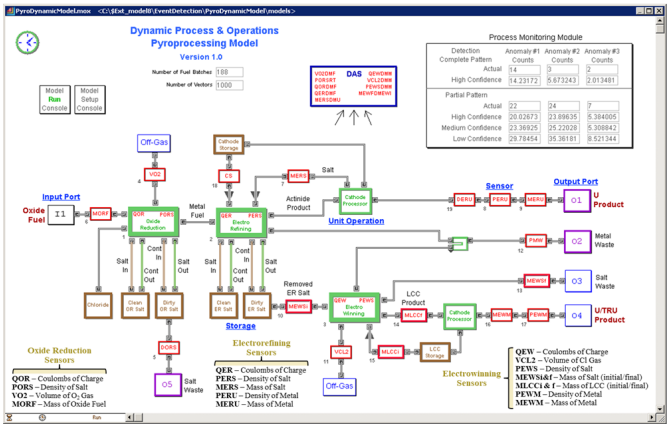

Figure 2: Operations model developed to examine the use of process monitoring for safeguards purposes.

are national missions anticipated to require a reliable supply of HALEU. Advanced reactors utilizing metal fuel and fast spectrum, for example, are well suited to utilize the HALEU recovered from the treatment of the EBR-II driver fuel elements. Likewise, those designing fuel fabrication facilities which have appropriate controls (i.e. containment / gloveboxes) to accommodate proper radiological controls to address any residual contamination that may be associated with the recycled material will be well positioned for direct use of the material. This is the case with Oklo, (e.g., see press release (INL Communication, 2020)). In view that one of the top HALEU options under development relies on electrochemical processing, INL has successfully demonstrated the ability to utilize aqueous chemistry techniques involving nitric acid dissolution and solvent extraction on the HALEU metal recovered from EBR-II to do additional contaminant removal and conversion of the metal to an oxide to accommodate those advanced reactor designs utilizing thermal spectrum, such as many of the concepts planning to utilize TRISO fuel (Patel, 2021).

The target enrichment level of the final uranium ingots is $19.5 - 19.75$ wt% ^{235}U, with these nuclear materials being referred to as high assay low enriched uranium (HALEU) (Fredrickson, Patterson, Vaden, Galbreth, Yoo, Price, Flynn and Searle, 2022). However, there are currently no commercial facilities based in the United States that have the capability to produce this material. As a result, the nuclear industry requested support from the Department of Energy (DOE) to meet this need. One approach being considered by DOE is to recover highly enriched uranium from used nuclear fuels and downblend it to enrichment less than 20% ^{235}U. Being the concentration of the fissile isotope U-235 between 5 and 20 percent of the mass of the fuel, HALEU material is higher than the 3 to 5 percent U-235 concentration, or "assay," of Low-Enriched Uranium (LEU) that fuels the existing fleet of light water reactors.

It is useful to note that DOE's past research related to liquid metal fast breeder reactors resulted in the irradiation of more than 3 metric tons (MTs) of nuclear fuel composed of highly enriched metallic uranium, which resides at INL. The majority of this fuel was irradiated in the Experimental Breeder Reactor II (EBR-II) over the course of 30 years of operation. This sodium cooled fast reactor utilized a core comprised of highly enriched, sodium-bonded, metallic fuel to drive the reactor. This inventory of used nuclear fuel is currently being conditioned using an electrometallurgical treatment (EMT) process (interchangeably also called pyroprocessing) in the Fuel Conditioning Facility (FCF) at the Materials and Fuels Complex (MFC). As part of this treatment process, the highly enriched component of this used fuel is separated, recovered, down-blended to < 20 wt% ^{235}U, and stored as a metallic uranium ingot. The metallic uranium recovered as a component of this process has been proposed as a potential source for producing of HALEU material.

4.2. Process layout and material streams

As typical in manufacturing, spent nuclear fuel treatment processes involves the presence of several material streams. The modeling of the most relevant material streams should be considered whenever constructing a FOM related to the process at hand as each of these streams will compete and seize resources available, hence impacting productivity. Fig. 3 illustrates the layout of the nuclear facility (i.e., FCF) where the manufacturing process (i.e., HALEU recovery) being addressed in this article is being

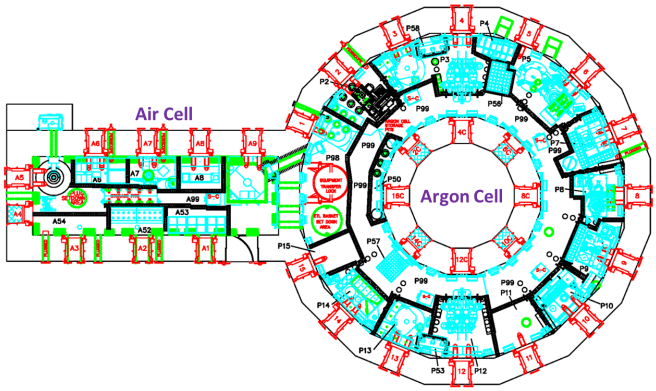

Figure 3: Illustration of nuclear facility where HALEU is conducted.

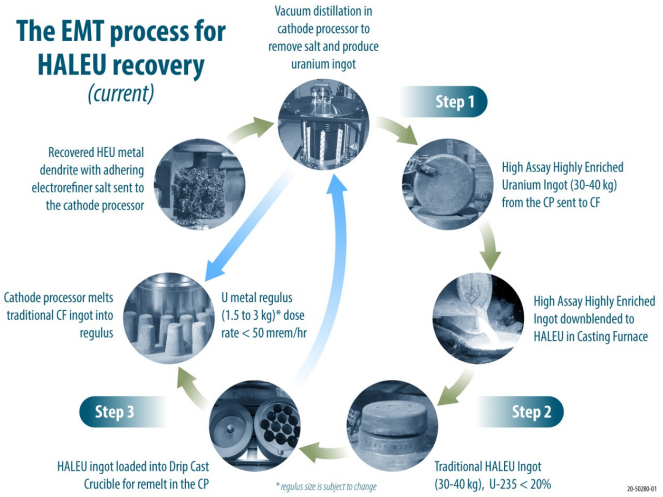

Figure 4: Current material flow of EMT process for HALEU recovery.

conducted. Similarly, Fig. 4 illustrates the current material flow for the HALEU process. In particular, spent nuclear fuel elements are introduced into FCF, handled and processed inside hot cells and removed from the facility as three main (direct) products: HALEU product, metal waste, and salt waste. Indirect waste streams (not shown in these figures), such as un-reusable containers, also exit FCF but are not considered in this study. Six (6) main types of materials involved in HALEU are briefly described next. For more detailed description, please see, for example, (Fredrickson et al., 2022).

1. Spent nuclear fuel elements: This material stream encompasses spent fuel elements resulting from the operation of a nuclear system(s) (e.g., EBR-II) that are brought into the facility under consideration (e.g., FCF) and inspected and sorted out for further processing throughout the operation (e.g., HALEU) at hand. Presently, EBR-II spent fuel inventories reside at four locations, namely: Idaho Nuclear Technology and Engineering Center (INTEC) in water storage pools, Radiological Scrap and Waste Facility (RSWF) in underground silos, and lesser inventories within the FCF and Hot Fuel Examination Facility (HFEF) hot cells (Fredrickson et al., 2022).

2. Chopped nuclear fuel elements: This material stream encompasses nuclear fuel elements that passed their inspection prior to treatment and are then chopped to make them amenable for EMT processing.

3. Uranium product: This stream encompasses those materials resulting from sequentially conducting EMT processing, salt-distillation processing, and uranium casting processing of chopped nuclear fuel elements.

4. HALEU product: This material stream encompasses those products resulting from uranium recasting toward manufacturing metallic Uranium regulus.

5. Metal and Salt Waste: This material stream encompasses metal and salt waste resulting from conducting the several steps constituting the HALEU process such as metal from cladding hulls coming out from nuclear fuel elements as well as spent salt coming out from the electro-refiners and salt distillation furnaces (e.g., CP, MFF #1, and MFF #2).

6. By-products: This material stream encompasses those products resulting from diverse processes. Two key ones are described next for illustration purposes. First, the graphite crucibles used in the high temperature applications associated with the EMT process as well as those used in uranium (re)casting are coated at FCF with zirconia or yttria based solutions in an attempt to prevent interaction of the uranium with the graphite. This interaction can cause the uranium to adhere to the graphite, making it difficult to remove from the crucible. While the coating is successful at facilitating the release of the uranium metal from the crucible, there is some amount of reaction that occurs between the coating and the uranium metal, producing a by-product called “dross”. Second, the uranium re-casting process used to produce HALEU regulus generates another by-product, namely, the heel that remains referred to as slag. While similar to the ingot in its form, it consists primarily of oxides that have formed with the uranium metal and fission products during the EMT process. Due to the high melting temperature of these oxides, they remain in the upper crucible as the uranium metal melts and flows into the lower crucible. More info on this stream can be found in (Price, 2020).

4.3. Hot Cells

To prevent inadvertent criticality and track special nuclear material closely and safely, hazards control regulations are enforced in nuclear facilities. These regulations comprise the limits, boundaries, and conditions established by nuclear criticality safety analyses and the spe-

cific rules under which activities involving radioactive material are conducted. Thus, material handling (a non-value added activity) is of paramount importance in typical nuclear processes as those being conducted at FCF. Consequently, significant efforts should be allocated to model it with sufficient fidelity considering its dynamic constraints. While the current material flow of the EMT process for HALEU recovery follows the production flow illustrated in (Fig. 4), its movement within FCF is much more complex and constrained.

In particular, nuclear facilities often include several hot cells to provide a means for safely working with irradiated nuclear materials that undergo constant radioactive decay. These hot cells are often divided into zones. To illustrate, there are two hot cells in FCF, namely, the air-cell (air atmosphere) and the argon-cell (argon atmosphere) as visualized in Fig. 3. Air-cell operations include entry/exit of material, disassembly of spent fuel assemblies, and interim storage of fuel elements and uranium product, including HALEU material. Disassembly of nuclear assemblies, if conducted, results in metal scrap and spent fuel elements. The fuel elements are then transferred to the argon-cell where the remaining operations are conducted. The argon-cell is annular in form and constructed in the shape of a 16-sided regular polygon with high-density reinforced concrete walls. As seen from Fig. 3, the air-cell is connected to the argon-cell via one of these sides. Each of the other 15 outer sides is provided with a shielded window or other viewing mechanism. Specifically, the argon-cell is further divided into the following sixteen (16) zones listed clockwise: P98, P99, P51, P2, P3, P4, P5, P7, P8, P9, P10, P55, P12, P13, P14, and P15 as illustrated in Fig. 3. These hot cells and their corresponding zones were modeled within the developed simulation capability.

4.4. Receiving and Shipping Units

Nuclear facilities often include several receiving and shipping units, where nuclear materials are typically received and shipped out, respectively, in shielded casks specially designed to safely handle radioactive nuclear material. For example, FCF includes a shielded cask used to transfer spent nuclear fuels into FCF called HFEF-5. This shielded cask and other devices were also modeled.

4.5. Material Handling Units

As processes conducted on nuclear material occur in hot cells, it is often the case that material handling equipment are used to manipulate material, including for moving them among workstations, transferring material from one container to another, conditioning crucibles, assembling and disassembling process equipment, storing and retrieving material, and receiving and shipping material. To illustrate, material handling available at FCF include cranes and electro-mechanical manipulators (EMM).

4.6. Preparation and Processing Units

Nuclear material is often prepared and processed in nuclear facilities to produce derivatives in support of multiple nuclear programs. In the case of HALEU, the treatment of spent nuclear fuel treatment process conducted in the argon-cell primarily relies on three types of machines: element choppers (EC), electrorefiners (ER), and induction furnaces, including the Cathode Processor (CP), the Casting Furnace (CF), and the Multi-Function Furnaces (MFFs). Nuclear fuel elements from spent fuel assemblies are chopped at the EC to a length specified to support EMT processing. At the ER, chopped nuclear fuel elements are dissolved and treated, which results in recovery of uranium and separation of fission products and transuranic elements (Ackerman, 1991). The CP and MFFs support separation of adhering electrolytes from the products collected through the electrorefining process. The CF and MFFs support sampling and metal waste consolidation, while the CP and MFFs support HALEU reguli recasting.

The size and radiological dose rate associated with the uranium ingot traditionally recovered from the treatment of EBR-II fuel at FCF made it challenging to work with in many proposed re-use scenarios as those defined for HALEU. It was thus assessed that the large 20–40 kg HALEU ingots needed to be recasted into smaller sized ingots better suited for fuel fabrication. In response to these challenges, a new method for re-casting the traditional ingot using a two-part graphite crucible has been implemented. The two-part or multi-tier graphite crucible or arrangement, shown in Fig. 5, is referred to as the Drip Cast Crucible (DCC) system, with the top and bottom component called DCCT and DCCB, respectively. Once the uranium recovered during the treatment process has been cast at CF into the traditional ingot shape and analyzed to confirm its composition, the 30-40 kg HALEU ingot is placed within the top crucible DCCT and melted at a specialized furnace (e.g., CP and MFFs). The molten uranium is gravity cast into the cascading, multi-pocket, lower crucible producing multiple, reduced size, lower dose, HALEU ingots known as “reguli” that are typically 3 or 7 kg, with photos of them provided in Fig. 6.

4.7. Storage and Packaging Systems

Nuclear facilities typical furnish a diverse portfolio of storage options including containers, baskets, magazines, racks, and pits. All of them, small and large, need to be carefully selected and operated based on different criteria including criticality safety. For example, the approach for storage of the material generated during the production of HALEU material is to utilize a standard type of containers called Uranium product storage (UPS). This is because criticality safety analysis shows that storage outside of the argon-cell will have a relatively low quantity limit that will most likely be exceeded by any containers with larger capacity. Similarly, it is expected that the dross produced

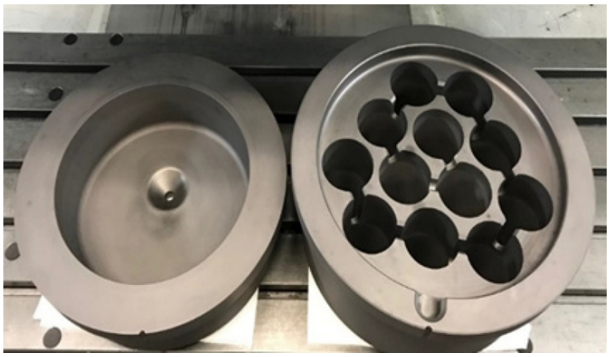

Figure 5: Drip Cast Crucible (DCC) system, with the top component called DCCT and the bottom called DCCB.

Figure 6: Reguli after removal from crucible.

during processing of EBR-II material will be co-mingled with HALEU slag due to its lower fissile loading. Four UPS containers are typically packaged in a fuel storage can and welded into an outer waste can. Because the locations where storage are located within the hot cells and how material streams are packaged for their eventual removal from a given nuclear facility do have an impact on productivity, it is imperative that these storage and packaging systems are modeled with adequate granularity.

5. Developed Computational Capability

5.1. Methodology

A key strategy applied for the analysis and optimization of those complex nuclear processes and facilities located at INL was, and continues to be, to construct FOMs based on the technology of DES. As an example of a FOM that has been successfully employed by operators, systems engineers, and decision makers of actual production facilities, the following description relates to the FOM developed for FCF named the FCF Operations Model (FOM).

In particular, FOM characterizes and simulates the main processing and material handling activities that support the EBR-II SFT program, including the HALEU program. The model is used to verify that the process layout,

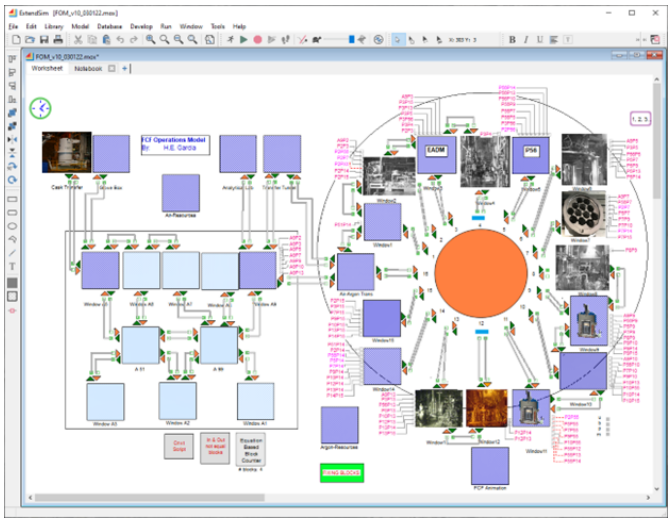

Figure 7: Screenshot of highest level of FCF Operations Model.

material processing and handling, storage area sizes, and other elements are adequate to meet HALEU throughput goals. Where inadequacies are discovered, the HALEU process may be modified and FOM is run to assess the effectiveness of the modification. This process is interactive and may repeat until it is demonstrated that HALEU throughput goals are met, for example. FOM also provides a means to study and optimize operations in FCF.

FOM is divided into a hierarchical set of operations patterned after a given detailed process flow sheet. FOM models processing and material handling actions to the level of individual activities or steps that take time and use a given set of resources. Activities include operations such as moving a fuel assembly from a cask to a storage rack location; cutting the top end off a fuel assembly; running a piece of processing equipment through a single unit operation; welding the lid on a container; moving a cask cart from one workstation to another; opening a transfer lock; loading one type of material into a piece of process equipment; and so on. Resources in need for modeling include floor space, transfer ports/locks, process equipment, material handling equipment, containers, storage racks, consumables, and operators.

5.2. FCF Operations Model (FOM)

FOM was developed using the simulation software called ExtendSim for discrete event, continuous, discrete rate, and agent-based simulations (ImagineThat, 1987-2022). This M&S tool was selected because it not only is easy to use and provides multiple advanced modeling blocks and features for simulating all sort of components and functionalities but also is constructed in an open architecture that allows users to inspect and change blocks' codes towards creating new blocks. FOM consists of four interconnected capabilities, namely, "DES model", "Configuration Setup & Output Database", "Notebook", and "Animation and Graphic User Interface (GUI)" briefly described next.

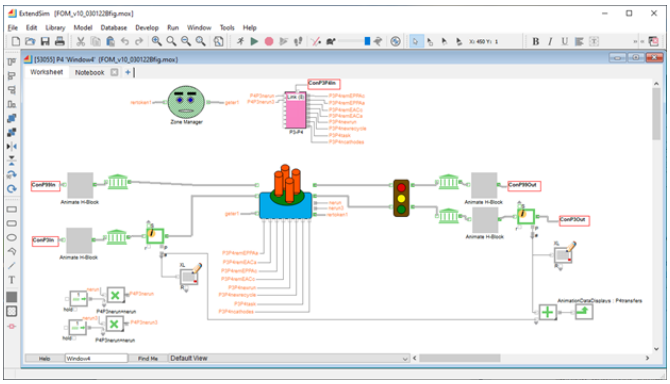

Figure 8: FOM: Hierarchical block showing a workstation/zone (i.e., P4) hosting processing operations only (i.e., electrorefiner ER-4).

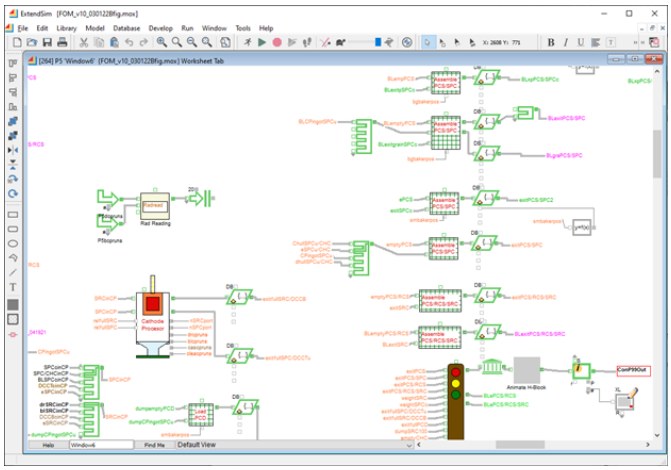

Figure 9: FOM: Hierarchical block showing a workstation/zone (i.e., P5, P6) hosting both processing (i.e., CP) and material handling (e.g., assembling of diverse containers) operations.

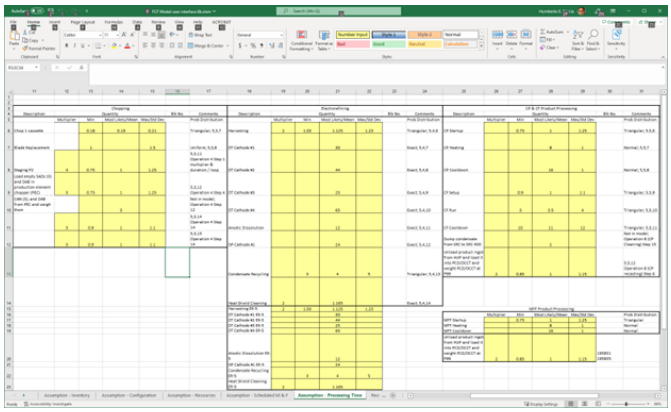

Figure 10: FOM capability: Config. Setup & Output Database.

5.2.1. Discrete Event Simulation Model

This capability of FOM contains the computational machinery hosting all modelling constructs and libraries developed and embodies the computational engine that computes all productivity estimates identified for analysis and optimization. Numerous constructs and/or modeling blocks were created using either libraries provided by the commercial M& S environment used or constructed in-house to accommodate specific M&S functionalities. Figure 7 provides a screenshot of the highest level of FOM, which resembles the layout for FCF illustrated in Fig. 3.

Following an object-oriented architecture, FOM is organized in multiple hierarchical blocks of diverse depths. In this way, a given hierarchical block may subsequently open several hierarchical constructs until reaching a final hierarchical block where only atomic blocks resides. The highest level of hierarchical blocks characterize workstations or zones were operations/tasks are conducted. In FOM, the argon-cell, for example, is further divided into sixteen (16) hierarchical blocks as shown in Fig. 7, each representing an actual zone defined within FCF as those mentioned at end of section 4.3. Depending on what operations are conducted there, hierarchical blocks may host processing operation only or alternatively both processing and material handling operations.

To illustrate, Fig. 8 provides a screenshot of an illustrative workstation conducting processing operations only, where the whole zone is occupied by a single processing equipment (in this case, electrorefiner Mk-IV ER, also called here ER-4 for simplicity). Similarly, Fig. 9 provides a screenshot of an illustrative workstation hosting both processing and material handling operations. To illustrate the level of sophistication embodied in it, few salient characteristics of FOM are provided next.

- *Flexible and modular implementation*
- *In-detail characterization of facility operations*: $>$ 150 container types; $>$ 110 material types; $>$ 150 parent operations.
- *Dynamic simulations*: discrete event modeling rather than database (static) implementation; transient and steady state responses; material handling dynamics modeled as a function of time-varying hot cell states.

5.2.2. Configuration Setup and Output Database

This capability of FOM significantly facilitates entering and retrieval of parameters defining scenarios of interest. It is organized into two sets of tabs, namely, “assumption” tabs including five sub-tabs: Inventory, Configuration, Resources, Scheduled Maintenance and Failure Rates, and Processing Time, as well as “Results” tabs including two sub-tabs: “Throughput” and “Resource Utilization”. Fig. 10 provides a screenshot of a portion of this database.

5.2.3. Notebook

This capability of FOM facilitates the examination of key operational settings (e.g., container loading, equipment availability and assignment, number of operators, labor schedule) and productivity estimates (e.g., zone and resource utilization, throughput values) associated with the what-if scenario under investigation. Fig. 11 provides a screenshot of this FOM capability.

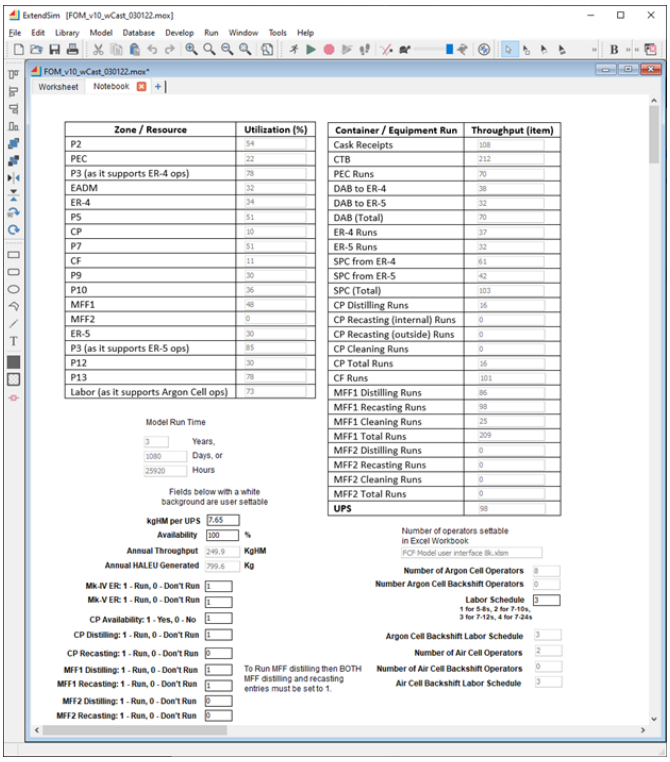

Figure 11: FOM capability: Notebook.

5.2.4. Animation and Graphic User Interface (A-GUI)

This capability of FOM supports the animation of key operations within FCF including material preparation, conditioning, and processing tasks as well as material handling and movement of nuclear material as they are concurrently executed at different workstations. It also displays key productivity metrics related to HALEU process under the particular what-if scenario under examination. Fig. 12 provides a screenshot of this FOM capability as it pertains for a given what-if scenario, showing main processing workstations (i.e., Element Chopping, Electrorefining [two units], Cathode Processing, Casting Furnace, and Multi-Function Furnaces [two units]) as well as supportive operations (i.e., Receiving/Shipping, Fuel Inspection and Loading of Cassettes, and Crucible Conditioning). It also animates material movements and equipment on-off states and reports productivity metrics such as total and annual throughput and batches completed, receipts and shipments, task cycle times (TCT), zone utilization (ZU), task utilization (TU), equipment utilization (EU), equipment runs, number of containers moved on each key material stream as well as the number of material transfers involving diverse interim storage locations (i.e., P56, P14, P15).

The developed computational capability involves the integration of seven distinct types of modeling constructs, namely: i) material receiving and shipping, ii) material processing, iii) material support, iv) labor, v) material handling and movement, vi) material storage, and vii) control and communication. Brief descriptions on each of these types of modeling constructs are provided next.

5.3. Material Receiving and Shipping Modeling Constructs

FOM models and tracks more than 110 types of material received, processed, and shipped out from FCF. For reasons of brevity, the material types of interest will only be introduced. In doing so and considering that nuclear materials are moved in specific canisters, their corresponding containers are briefly mentioned. Fig. 12 facilitates visualizing material flow throughout the HALEU process.

- Received material: spent nuclear fuel and depleted uranium (DU) received in casks and containers, respectively, in addition to receiving consumable containers such as empty Uranium Product Storage (UPS) containers. Not addressed further in this article, it is here noted that in situ downblending adding DU diluent may occur at three distinct locations: electrorefining, salt distillation, and/or uranium casting.

- Processed material:

  i) nuclear fuel pins/elements in baskets (i.e., Fuel Bottle Baskets, FBB) containing several (i.e., eight) inner containers (i.e., Fuel Bottle Containers) transferred from "air-cell" to the argon-cell "Fuel Inspection and Loading Cassette" (ILC) station;

  ii) inspected fuel pins in baskets (i.e., Cassette Transfer Baskets, CTB) containing several cassettes loaded with acceptable fuel pins transferred from ILC station to "Element Chopping (EC)" station;

  iii) chopped fuel pins in baskets (i.e., Driver Anode Baskets, DAB) transferred from EC station to "Electrorefining (ER)" stations (conducted at ER-4 and/or ER-5);

  iv) electrorefined material in crucibles (i.e., Solid Product Collectors, SPC) loaded into outer containers (i.e., Process Crucible Transport/Storage Containers) transferred from ER stations to "Salt Separation (SS)" stations (conducted at Cathode Processor, CP, and/or Multi-Function Furnaces, MFF);

  v) salt-removed material in containers (i.e., CAC) transferred from SS stations to "Casting" station (conducted at Casting Furnace, CF);

  vi) casted material in containers (i.e., Drip Cast Crucibles, DCC) transferred from Casting station to "Recasting" stations (conducted at CP and MFFs);

- Shipped material: HALEU product (i.e., metallic Uranium regulus) transferred from recasting stations in containers (i.e., UPS) and packaged (four of them) in a fuel storage can at air-cell and welded into an outer can, which are in turn loaded into a shielded cask (e.g., HFEF-5 cask).

There are also multiple waste (e.g., salt, metal, dross) flows, which are not addressed further in this article.

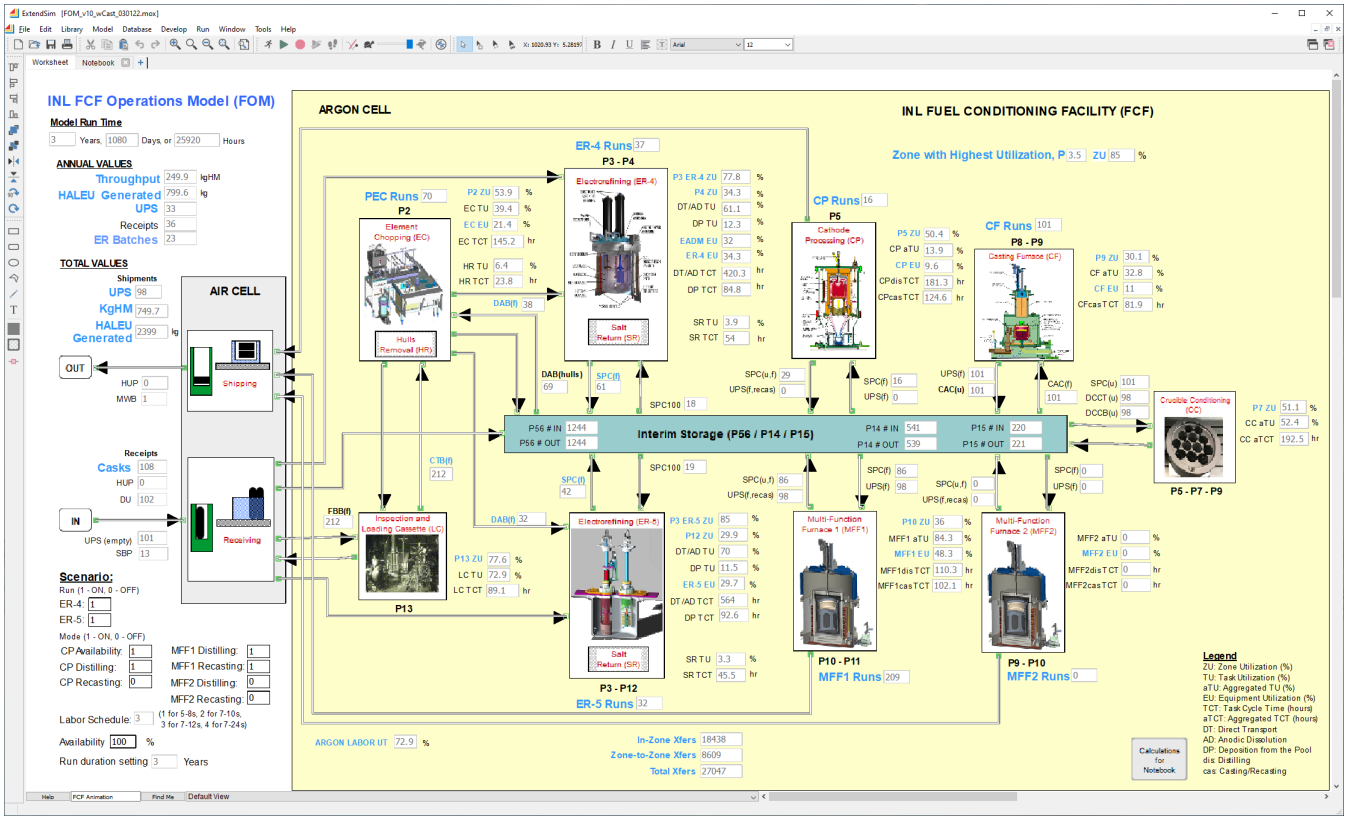

Figure 12: FCF Operations Model (FOM) capability: Animation Graphic User Interface

5.4. Material Processing Modeling Constructs

Five distinct material processing workstations are modeled as illustrated in Fig. 12.

- *Element Choppers (EC)*: element chopping (EC) is used to expose the bond-sodium and fuel alloy for the subsequent electrorefining operation. EC is an electromechanical shear. De-wired fuel elements loaded into cassettes are in turn loaded into EC and chopped, with fuel segments falling directly from EC into the DAB. Additional information on EC can be found in (Yoo, Fredrickson, Galbreth, Patterson and Vaden, 2021) and (Fredrickson et al., 2022).

- *Mk-IV, Mk-V Electrorefiners (ER-4 and ER-5)*: electrorefining (ER) is used to separate actinides from fission products and other constituents in the nuclear fuel and produce products suitable for manufacturing advanced nuclear fuel (e.g., HALEU) or for disposition. Mk-IV and Mk-V ERs are uranium electrorefiners based on molten salt electrochemistry. In the case of Mk-IV ER, for example, impure uranium is anodically dissolved into the molten salt and purified uranium is cathodically deposited from the molten salt. Metals in the spent fuel that are more electronegative (more noble) than uranium remain in the anode basket, while those more electropositive (less noble) than uranium accumulate in the molten salt as metal chlorides. Additional information on ER can be found in (Mariani, Benedict, Lell, Turski and Fujita, 1996) and (Fredrickson et al., 2022).

- *Cathode Processor (CP)*: cathode processing (CP) is used to distil the salt from the actinide product resulting from electrorefining. After removal from ER, actinide product is loaded into the CP (or a MFF), where a high temperature distillation sequence results in separation of the salt and melting of the metal into a high-density ingot. Additional information on CP can be found in (Brunsvold, Roach and Westphal, 2000) and (Westphal, Vaden, Hua, Willit and Laug, 2002).

- *Casting Furnace (CF)*: uranium casting is used to down-blend and sample the uranium product. After salt distillation is completed, the uranium ingot produced in CP or MFF is advanced to CF. At CF, the uranium is remelted and samples are drawn directly from the molten uranium into quartz tubes. These samples are sent to an analytical lab for chemical and isotopic analyses to assess the chemical and isotopic compositions of the ingots regarding a host of elements, verify purity and uranium enrichment level of the uranium product, and assure that the produced ingots meet specifications. Additional information on CF can be found in (Fredrickson et al., 2022).

Figure 13: New multi-function furnace (MFF).

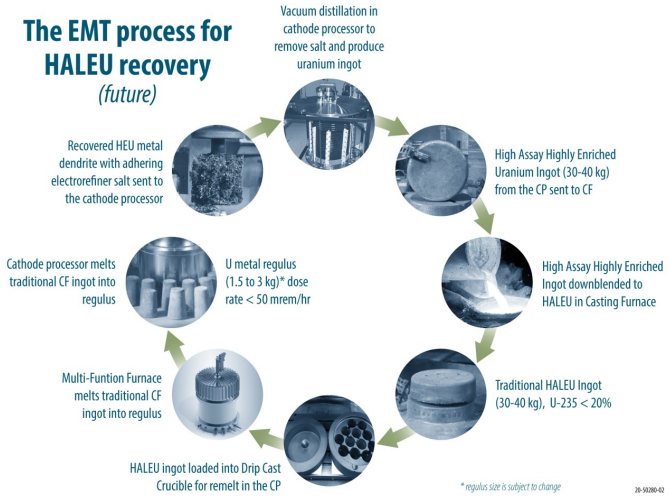

Figure 14: Future material flow of EMT process for HALEU recovery.

- *Multi-function Furnaces (MFF)*: heating and melting metals/materials at high temperatures is used to support several processes including salt distillation from dendrites and hulls, dendrite/hulls consolidation, sampling of molten Uranium and steel alloy, and reguli recasting. Consequently, this high temperature vacuum atmosphere furnace functionality provides redundancy in salt distillation and uranium casting activities. Figure 13 shows a picture of this induction furnace. Likewise, Fig. 14 illustrates the material flow of the EMT process for HALEU recovery anticipated when the MFF is installed at FCF.

5.5. Material Support Modeling Constructs

Nuclear facilities are often equipped with specialized equipment for material support. In FCF, one of this type of equipment is the Electrode Assembly Disassembly Machine (EADM), employed to assemble and disassemble the anode and cathode electrode assemblies utilized with the Mk-IV ER. There are also preparation stations to conduct a myriad of nontrivial tasks such as the inspection of nuclear fuel as well as the conditioning of crucibles as shown in Fig. 12. To illustrate the former, fuel bottles withdrawn from the transfer cask at the FCF air-cell are transferred to the "Inspection and Loading Cassette" station in the argon-cell where the following procedure is applied to each bottle. The cap is removed and tested for water. If no water is detected, the bottle is cut open. If water is detected, the bottle is first dried prior to being cut open. Each fuel element is removed and inspected. After removing spacer wires, de-wired fuel elements suitable for treatment are loaded into cassettes holding a number of elements (typically five elements), ready for chopping at the chopper station. Corroded fuel elements and fuel rubble are returned to bottles for alternative treatment.

5.6. Labor Modeling Constructs

Operations conducted at hot cells are often labor intensive. Consequently, the particular labor schedule employed highly limit the number of operations that can be completed in a given time period and largely determine achievable throughput. For example, operating under a 5/8 labor schedule can be expected to return small throughput values due to being a very restrictive labor schedule rarely employed in production facilities. In order to model labor resources, two pools of operators were created in FOM, namely, one for air-cell operators, one for argon-cell operators, with their availability for cell operations depending on the selected labor schedule, each including labor unavailable periods to accommodate shift changes and necessary breaks. Labor modeling constructs allow selection of labor schedule and composition as follows:

- Any type of labor schedule (e.g., 5/8, 7/10, 7/12, 7/24, hybrid, with the latter denoting strategies in which certain workstations are operated at a given labor schedule, while others at another).
- Air- and argon-cell operators as well as specialized subgroups of operators authorized to support certain tasks, workstations, and/or equipment based on training qualifications and time availability.

5.7. Material Handling and Movement Modeling Constructs

Material handling represents an important but very limiting component, frequently accounting for most of the production activity. For example, the material handling equipment installed at FCF Argon-cell consists of the following units, with a corresponding electro-mechanical manipulator (EMM) and a crane at the Air-cell:

- Electro-mechanical Manipulators (EMM) (four EMMs)
- Cranes (i.e., two cranes)
- Balances (i.e., four units)

EMM operability constraints present at FCF introduce severe operational dependencies among processes, limiting the number of operations that can be conducted concurrently. Within FCF argon-cell, operations requiring EMM must be conducted within workstations separated by at least two zones in order for them to occur concurrently. While operations may be "logically independent," the limited availability of resources makes many of them "operationally dependent." These resource-originated dependencies often force operations to pause, introducing non-value-added wait times, with its reduction being a primary goal in high production facilities. Idle time between subsequence operations is probably the most critical contributor in this problem category. Simulation results reveal that long wait times are common throughout the HALEU process. It is also important to notice that productivity is not necessarily improved by increasing the number of operators available per shift but instead by increasing the number of hours operators are available. Moving of material within FCF hot cells is also restricted to follow certain paths and use specified transfer ports as follows:

- Transfer Ports (e.g., Cask Hatch, Cask Transfer Port)
- Transfer Hatches (e.g., Small Transfer Lock, Equipment Transfer Lock, Rabbit)
- Tunnels (e.g., Cask Tunnel, Transfer Tunnel)

Given the significant complexity described above, commensurate care was directed to model material handling operations with sufficient level of fidelity. In this regard, the time that would take a material to be moved from one location to another was not modeled by assuming that it follows a given probabilistic distribution. This simplistic but often misleading approach would have been incorrect as the time a material transfer takes depends not only on the current state of the facility and the starting and end locations for the given material transfer but also on the availability of material handling equipment and other supporting equipment (e.g., material balances). Consequently, after it receives a request for material transfer, the material handling module runs an optimization algorithm to identify best route to complete the requested transfer given the current states of the cells, indicating which:

- i) path to follow within the given cells
- ii) EMM or EMMs to use, potentially including the need of using multiple EMMs
- iii) material balance to use to assure that the material to be moved into a new station/zone does not violate critical and any other safety constraints.

After such decisions are computed, the material transfer is executed when identified resources (e.g., material handling equipment, balance, and labor) become available. With this level of modeling sophistication, the HALEU project can accurately assess the implication of moving equipment from one location to another or identify best locations to install new equipment, for example, in addition to more realistically quantifying the impact of material handling in a facility with little automation. In addition to the material handling resources mentioned above for moving material, there are other resources (e.g., trucks, fork lifts, tractor trailer transport) employed for similar function. However, they are not addressed in this article due to length limitations.

5.8. Material Storage Modeling Constructs

In many manufacturing applications, and more prevalent in batch (as opposed to continuous) processes as is the case with the HALEU process, buffers are a crucial component for interfacing and coordinating the operations of multiple unit operations. It is one of the areas that may be threatened by competing mission work existing within facilities. For example, traffic in a given area of a facility may pick up significantly as processing rate ramps up. Storage racks may play an important role in processing operations by providing a buffer storage location for material as it awaits entry into the process under consideration. Thus, buffers are typically used to adapt the production process in the presence of variations and uncertainty with the goal of ensuring that production continues to operate adequately under the presence of unanticipated factors (e.g., failure of given equipment, changes in labor availability). They can also assist in matching diverse speeds and availability times among downstream devices. Several types of buffer-type components are included at FCF and modeled by FOM including storage racks (e.g., P55, P56), storage pits (e.g., P51), floor positions (e.g., P14, P15) and table positions (e.g., P5, P9).

5.9. Control and Communication Modeling Constructs

The control logic constructs constitute the "brain" that manages the initiation, execution, and termination of all activities modeled within FOM. For FCF, this operations execution involves both the air- and argon-cells, with each further divided into multiple zones. For example, zones defined for FCF argon-cell includes the following sixteen listed clockwise: P98, P99, P51, P2, P3, P4, P5, P7, P8, P9, P10, P55, P12, P13, P14, and P15 as illustrated in Fig. 3 and Fig. 12. It is useful to group them into four categories based on their functions: "material transfer zones" (e.g., P98, P99, and P51), "material storage zones" (e.g., P56), "material handling zones" (e.g., P3, P13), and "material processing zones" (e.g., P2, P5, P7, P9, P10, P55, P14, and P15). The first two types can be viewed as "service" zones as their functions are to serve the remaining two "client" types. As a subclass of the "material processing zones", there are also "only process equipment zones" (e.g., P4, P8, P12), where large equipment are installed, using the all space available as illustrated in Fig. 8.

With the above server-client zone classification, it is understood that client zones essentially drive the manu-

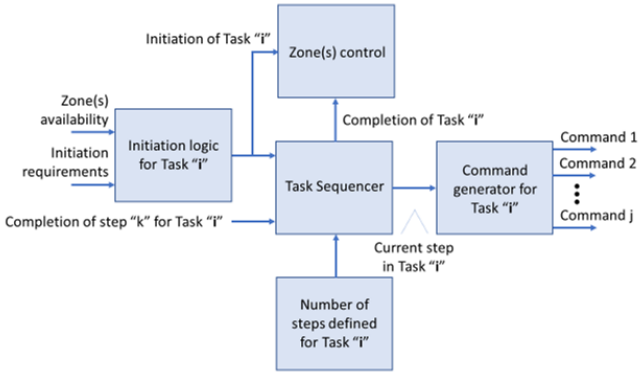

Figure 15: Control logic construct incorporated within FOM.

facturing process (e.g., HALEU) at hand, with each managing a number of tasks. To maintain operational regulations, only one single task can operate at a zone during a given time period. It was then necessary to devise a control strategy that consider the status of other tasks and the hot cells at large to ensure that the maximum number of tasks can be performed concurrently within a given cell(s) in a harmonious manner without resulting in deadlocks, for example. To this end, the first step was to place a control logic construct at each client zone. Each "Zone Control Logic" then includes a "Task Manager" for each task defined on it. This "Task Manager" was synthesized as illustrated in Fig. 15.

The operation of a "Task Manager" is as follows. The initiation logic component assesses whether the particular task can be initiated based on whether the zone or zones required for its completion is/are available and whether the initiation requirements are met. These initiation requirements may involve all sorts of conditions including availability of specific material in containers (e.g., HALEU material in UPS), process crucibles (e.g., DCCT), and states of other tasks. When all conditions are met, the given task is allowed to initiate, starting from step 1 and incrementally counting up until reaching the number of steps defined for this task. A signal is also sent to the "Zone(s) control", which makes the given zone(s) only available to this task. Based on which step the task is in, a corresponding command is sent out. A command may trigger diverse actions such as initiating a transfer of a container/crucible located in a given zone or equipment to another zone or equipment, from example. When a given step is completed, an acknowledgment of its completion is sent to the "Task Sequencer', which then increments the step of the task to its next value. When the last step defined for the task is reached, a signal is sent to the "zone control", who then makes the zone(s) available for other tasks. The control strategy so synthesized is independent of the process being modeled and has been successfully employed in multiple FOMs including those developed for INL SFT, HALEU and MEDE programs (e.g., see Fredrickson et al. (2022), Regalbuto (2020), and Preusser and et. al (2023)).

Table 2: Induction furnace capabilities located in FCF.

Operation	**Cathode Processor**	**Casting Furnace**	**Multi-Function Furnaces**
Salt distillation from dendrites	Yes	No	Yes
Salt distillation from hulls	Yes	No	Yes
Dendrite consolidation	Yes	No	Yes
Hulls consolidation	No	Yes	Yes
Molten Uranium sampling	No	Yes	Yes
Molten steel alloy sampling	No	No	Yes
Reguli recasting	Yes	No	Yes

5.10. Modeling Parameters for What-if Selection

Numerous what-if scenarios can be simulated and analyzed by changing a large number of parameters. While listing here all possibilities (e.g., time needed to complete a given atomic task, inventory of available crucibles/containers, material loading size in crucibles, equipment configuration) is beyond the scope of this article, the typical parameters selected to create a given scenario are as follows, set using the Notebook capability shown in Fig. 11.

- Simulation time.
- Labor schedule and composition.
- ER availability.
- Furnace availability and utilization. In selecting this parameter, FOM constrains selections to a manner that meets furnace capabilities as summarized in Table 2 derived from (Fredrickson et al., 2022).

5.11. Model Validation

Model validation and tuning based on actual observations is an important activity that should be periodically conducted to assure that the particular FOM adequately characterizes the facility, resources, and process at hand. In the case of FOM, for example, throughput estimates were periodically compared with actual values during different projects, resulting in a modeling error of 3.5% consistently observed. The process of model validation rarely involves going through databases describing particular steps and details within each main task. Instead, it often involves having system engineers provide estimates on how much it may take to complete key relevant tasks, from beginning to end. Estimates for task cycle times (TCTs) should include time spent on preparation,

equipment running, post-preparation, and material handling activities. For example, FOM estimates that it takes about 45 hrs (or almost 2 days) to complete the task of "inspecting and loading 60 cassettes" under a 7/24 labor schedule from beginning to end. Similarly, TCT estimates computed by FOM for other tasks that do not involve new equipment (e.g., ER-5 and MFF) are as follows:

- Element Chopping (EC) TCT: 87 hrs (i.e., 3.6 days) to chop three subassemblies worth of elements (corresponding to 3 loaded CTB [Cassette Transfer Basket], each with 20 cassettes for a total of 60 cassettes) at EC and produce one DAB (w/ 3 S/A) ready for electrorefining operations.
- ER-4 Direct Transport (DT)/Anodic Dissolution (AD) TCT: 192 hrs to process an ER batch of 3 S/A loaded in a DAB and produce and load in SPCs all dendrite materials collected from running ER-4 several times under multiple DT and AD runs.
- ER-4 Deposition-from-the-Pool (DP) TCT: 46 hrs to produce and load in SPCs dendrite materials collected from running ER-4 under a DP run.
- CP salt distillation TCT: 87 hrs to process at CP one SPC loaded with ER dendrite material, including preparation, CP assembling, running, disassembling, as well as post-handling of CP ingot material.
- CF uranium casting TCT: 52 hrs to cast at CF one CAC loaded with a CP ingot and produce casted material, including preparation, CF running, and post-handling of CF casted material.
- CP uranium recasting TCT: 61 hrs to process at CP one Drip Cast Crucible-Top (DCCT) loaded with CF casted material and produce HALEU regulus, including preparation, CP assembling, running, and disassembling, as well as post-handling of regulus.

The above TCT estimates were computed by FOM assuming a 7/24 labor schedule. These estimates may accordingly increase as labor schedule decreases (because there may be more "idle moments" when labor is not available to conduct work). Regardless, system engineers may provide their TCT estimates observed under any labor schedule of their preference (e.g., 7/12). TCT for the same tasks can then be computed by FOM at their selected labor schedule. After investigating potential reasons for discrepancies between computed productivity estimates and collected productivity observations, the FOM at hand may be accordingly modified so that system engineers' observations and model's estimates for each TCT are sufficiently close. The process for model validation and tuning may involve requesting from system engineers associated with the process under consideration their estimates for each of selected TCTs under a given labor scenario, assuming no significant equipment failure. Even when actual productivity observations "available" might have been collected in conditions that are not necessarily steady-state but rather under diverse disturbances such as downtimes, these actual observations can still be utilized by "preparing" the given FOM so estimations and observations are compared in similar settings and correctly used to tune the model.

It is important to point out that as operations become more familiar to those conducting them, efficiencies should be expected to be gained and the time to perform discrete task within the process should be reduced. Based on this understanding, it is key to periodically revisit the time assigned for completion of tasks within the FOM and adjust them accordingly. The FOM was developed to incorporate this type of periodic feedback to improve the accuracy of the modeled results. For this and other validation objectives, it is critical that staff and systems engineers maintain clear records, in a digital, trackable form, that is available to FOM analysts for comparison purposes.

6. Computational Methods for Decision-Making: Examples

This section briefly reviews two analysis exercises, namely, one analyzing a single scenario and another comparing two distinct scenarios, with all results computed assuming 100% facility availability for simplicity.

6.1. Analysis of a single scenario

Single scenario analysis is quite straight forward and useful. They are conducted for evaluating a given scenario via the computation of bottom-line productivity metrics such as throughput, workstation and equipment utilization, and task-cycle time (TCT). They are also useful for supporting data-informed discussions among stakeholders (including project management, customers, system engineers, and operators) on the process under examination by effectively visualizing the estimated results and derived assessments using FOM.

To illustrate, let's assume that there is an interest to assess the productivity characteristics of the scenario specified in Table 3. Productivity estimates obtained under this scenario are provided in Table 4, while Fig. 16 provides a screenshot of the corresponding FOM Notebook.

Table 3: Analysis of a single scenario: Assumptions.

Parameter	**Value**
ER-4	Yes
ER-5	No
MFF	one available for salt distillation ONLY
CP	for uranium recasting ONLY of CF ingot, producing HALEU reguli
Labor Schedule	7/24

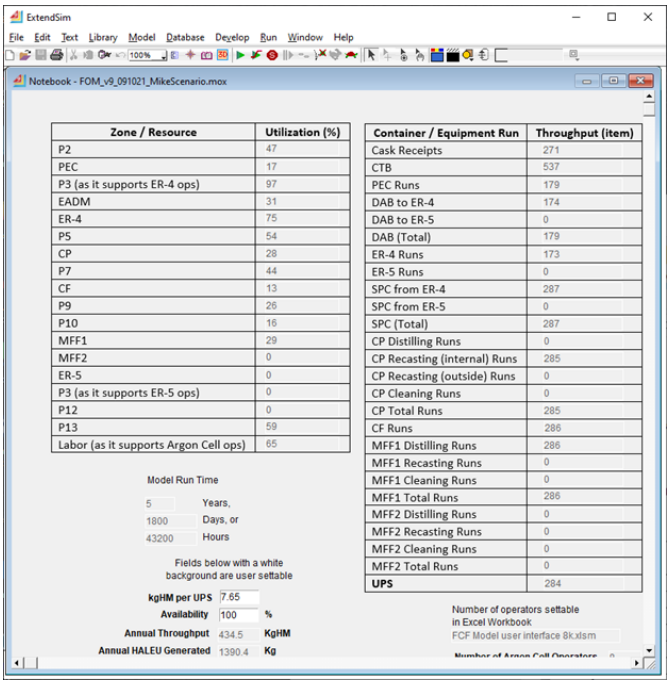

Figure 16: Results reported by FOM-Notebook for single scenario.

Table 4: Results from single scenario after 5 years of operation.

Metric	Estimation
Annual throughput	435 KgHM
Annual HALEU generated	1390 kg
Estimated time to complete 158 cask receipts	2.9 years
Estimated time to complete 105 treatment batches	3 years
Bottleneck	P3

In addition to providing estimates of all sort of productivity metrics, the computational capabilities (e.g., Notebook and GUI) associated with a given FOM may assist in the discovery and reporting of dependencies not easily recognizable. For example, let's assume that the interest is to determine how long it may take to process 105 batches through ER-4, or equivalently send 105 "DAB to ER-4". Similarly, the interest may be to determine how long it may take to reach 158 "Cask Receipts". However, the values for them reported by the Notebook shown in Fig. 16 are 174 and 271, respectively. The reason for the difference is that these estimates of "DAB to ER-4" and "Cask Receipt" reported there are computed after five years of processing material as shown at the bottom top left of this FOM-Notebook under the label: Model Run Time: 5 years. Notice also that the value in this Notebook for full DABs ready for processing (i.e., "DAB (Total)") is 179. Given that there is an inventory of DABs equal to 6 and considering that the bottleneck is P3 in the HALEU process, then there is an accumulation of full DABs (=5) produced by the "Fuel Inspection and Loading Cassettes" and the "Chopping" steps that are waiting to be treated at ER-4. Except for those values reported under the labels "Annual" in the FOM-Notebook, most productivity estimates are computed after five years of operation.

With the understanding of a 5 year simulation, the predicted time to complete 158 cask receipts and 105 treatment batches were computed as 2.9 yrs ($= \mathbf{158}/271 \times 5$) and 3 yrs ($= \mathbf{105}/173 \times 5$), respectively. Because FOM operates in a greedy mode, processing as much material as possible as they become available, the proper way is not to input 2.9 years, and see what FOM returns. One could run FOM for only 3 years and evaluate whether it returns a value around 105 treatment batches. A benefit of doing a 5 year simulation instead is that one could obtain productivity values when FCF has reached a steady state of operation (a typical desired condition for productivity analysis), hence returning "average/sustainable" values. Otherwise, if FOM is set to run for 3 years, the treatment batches estimated is for a scenario where FCF starts with zero inventory. To illustrate, Table 5 reports results assuming that FCF starts with no material inventory. Notice that the number of treatment batches estimated in this simulation is 103, just a bit less than the 105 previously estimated for three years operation using the explained calculation strategy based on a 5 year simulation instead.

Table 5: Results from single scenario after 3 years of operation.

Metric	Estimation
Total throughput	1285 kgHM
Total HALEU generated	4113 kg
Total no. of cask receipts	167
Total no. of treatment batches	103
Bottleneck	P3

6.2. Comparison of multiple scenarios

Comparing two or more scenarios is quite useful in order to assess and determine those operational changes that may deliver the most gain. To illustrate, the two (Alpha-1 and Bravo-1) scenarios reported in Table 6 are considered next. The main objective was to evaluate whether adding a second ER for conducting electro-refining on spent nuclear fuel may provide value under a 7/12 labor schedule.

Table 6: Comparison of two scenarios: Assumptions.

Parameter	Scenario Alpha-1	Scenario Bravo-1
ER-4	Yes	Same
ER-5	No	Yes
MFF	for salt distillation ONLY (one unit)	Same
CP	for Uranium recasting ONLY of CF ingots, producing HALEU reguli	Same
Labor Schedule	7/12	Same

Results obtained under both scenarios are reported in Table 7, being them interpreted as average productivity values obtained after reaching steady-state, achieved after three years of operation. To illustrate, an annual productivity of 277.9 kgHM obtained under Alpha-1 scenario means that FCF should be able to sustain this productivity level if continually operated under this scenario. Consequently, the implicit assumption is that FCF, starting with no inventory, is not emptied between subsequent years but keeps building up inventory as it is operated, while subjected to FCF storage capacity limitation.

Table 7: Comparison of two scenarios (three year simulation).

Metric	**Scenario Alpha-1**	**Scenario Bravo-1**
Annual Throughput	277.9 kgHM	234.6 kgHM
Annual HALEU generated	889.4 kg	750.7 kg
Total no. of ER-4 runs	68	15
Total no. of ER-5 runs	0	54
Total no. of ER batches	68	69
Total no. of SPC	113	97
Total no. of MFF-1 runs	112	96
Total no. of UPS shipped out	109	92
Bottleneck	P3 at 91%	P3 at 87%

The annual HALEU throughput obtained under Alpha-1 scenario is higher that than obtained under Bravo-1 scenario (i.e., 889.4 kg vs. 750.7 kg). This suggests that there is no benefit but rather be counterproductive to bring ER-5 to operation under a 7/12 labor schedule. This interesting discovery may be explained as follows. FOM does not prefer using one ER over another; instead, it decides which ER to run based on their availability at a given moment of need. Under this strategy, it happens that FOM runs more batches through ER-5 (=54) than through ER-4 (=15) under Bravo-1 scenario, for a total of 69 ER runs. When ER-5 is unavailable under Alpha-1 scenario, FOM runs a total of 68 runs (through ER-4). Consequently, there is no benefit of adding ER-5 in terms of increasing ER runs. Even though the number of ER batches completed are essentially the same under both scenarios, the number of salt distillation runs (at MFF-1) is significantly different (i.e., 112 and 96 under Alpha-1 and Bravo-1, respectively). Similarly, the number of crucibles (i.e., SPC) going for salt distillation is higher under Alpha-1 scenario (i.e., 113) than under Bravo-1 scenario (i.e., 97). These results suggest that the preparation and movement of batches through salt distillation is being held and has become more inefficient under Bravo-1 scenario, potentially because of the increased material handling traffic occurring around ER-5 (P12), which may hinder salt distillation operations at MFF-1 (P11) and others. While the production of HALEU material may be held/constrained by the limited capacity to process ER batches under Alpha-1 scenario, it may be held/constrained by operations occurring "after" electrorefining under Bravo-1 scenario; thus, the location of the bottleneck for the HALEU process seems to have been moved to downstream under Bravo-1 scenario.

6.3. Variation from previous comparison

A comparison among scenarios may often lead to the interest of running derivative variations to dig into it and gain additional insights. Following from the previous section, the variation described here is one where there is no uranium recasting into regulus as indicated in Table 8. Under this scenario, the CF parent ingot would be the final product form, and packaged in the traditional UPS, 4 UPS's to an HFEF-5 can, and when full, the HFEF-5 shielded cask is removed from FCF. Results obtained under this variation are reported in Table 9.

Table 8: Comparison of two derivative scenarios: Assumptions.

Parameter	**Scenario Alpha-2**	**Scenario Bravo-2**
ER-4	Yes	Same
ER-5	No	Yes
MFF	for salt distillation ONLY (one unit)	Same
CP	for salt distillation as well. CF ingot final HALEU form, no recast into regulus	Same
Labor Schedule	7/12	Same

Table 9: Comparison of two derivative scenarios (3 yrs simulation).

Metric	**Scenario Alpha-2**	**Scenario Bravo-2**
Annual Throughput	290.7 kgHM	257.5 kgHM
Annual HALEU generated	930.2 kg	824.1 kg
Total no. if ER-4 runs	70	32
Total no. of ER-5 runs	0	38
Total no. of ER batches	70	70
Total no. of SPC	116	103
Total no. of CP runs	0	0
Total no. of MFF-1 runs	115	102
Total no. of UPS shipped out	114	101
Bottleneck	P3 at 87%	P3 at 83%

The annual HALEU throughput obtained under Alpha-2 scenario is (still) higher (i.e., 13%) than that obtained under Bravo-2 scenario (i.e., 930 kg vs. 824 kg) as expected. Furthermore, the values obtained under this Alpha-2 scenario is only slightly higher than those previously obtained (930 kg. versus 889 kg, hence a 5% gain) suggesting that electrorefining is the bottleneck when only ER-4 is in operation and under a 7/12 labor schedule. Notice though that the productivity estimates obtained under this version of Bravo-2 scenario is higher than those previously obtained (i.e., 824 kg vs. 751 kg, a 10% gain) potentially due to the reduction of operations downstream from electrorefining by removing uranium recasting. Notice also the high utilization values at P3 (i.e., 87% and 83%) under Alpha-2 and Bravo-2 scenarios, respectively. This fact does then limit the productivity gain that could be obtained from the addition of ER-5 to the HALEU process.

Under this version of Bravo-2 scenario, FOM runs batches through the ERs more evenly (i.e., 32 and 38 via ER-4 and ER-5, respectively) for a total of 70 ER runs. When ER-5 is unavailable under Alpha-2 scenario, FOM also completes

a total of 70 ER runs (through ER-4). Consequently, there may be no benefit from adding ER-5 in terms of increasing ER runs completed under a 7/12 labor schedule. Even though the number of ER batches completed are exactly the same under both scenarios, the number of salt distillation runs (at MFF-1) is significantly different (i.e., 115 and 102 under Alpha-2 and Bravo-2, respectively). Related, the number of SPC for salt distillation is higher under Alpha-2 scenario (i.e., 116) than that under Bravo-2 scenario (i.e., 103). As before, these results suggest that the preparation and movement of batches through salt distillation is being held and has become more inefficient under Bravo-2 scenario, potentially because of the increased material handling traffic occurring around ER-5 (zone P12), which may hinder salt distillation operations at MFF-1 (zone P11). While the production of HALEU material may be restricted by the limited capacity to process ER batches under Alpha-2 scenario, downstream operations from electrorefining may be hindered by material handling operations occurring "at" ER-4 electrorefining under Bravo-2 scenario. Notice that all salt distillation is arbitrarily and coincidentally being conducted at MFF-1, even though the CP is also available to do so. This result suggests that all salt distillation needs for the HALEU process when operating at a 7/12 labor schedule can be comfortably taken care of by one machine (i.e., either CP or MMF-1, with FOM arbitrarily selecting MMF-1 for this purpose). This result also supports the conjecture that electrorefining, particularly the operations supporting electrorefining at P3, may be the bottleneck for the HALEU process when operating at a 7/12 labor schedule.

To further support the above conjecture, Bravo-3 scenario was also run under a 7/24 labor schedule. The results are reported in Table 10. The results obtained are as expected. In particular, a considerable productivity gain of 95% (i.e., from 824.1 kg to 1607.5 kg) is estimated, with both CP and MMF-1 now joining forces to take care of the significantly-increased production of material coming out from both ERs, although still mostly being processed at MFF-1 (i.e., 21 and 177 distillation runs through CP and MFF-1, respectively). Notice also that FOM arbitrarily runs batches through the ERs quite evenly (i.e., 67 vs. 66 via ER-4 and ER-5, respectively) for a total of 133 ER runs. There is essentially no bottleneck either within the HALEU process. Given the low utilization values estimated at those zones associated with salt distillation, it is expected that a commensurate level of productivity (with significant productivity gain) may also be achieved if the supportive operations related to electrorefining (e.g., P3) are operated at 7/24 labor schedule. Thus, among others, a potential strategy to justify the inclusion of ER-5 to the HALEU process may be to operate P3 at a 7/24 labor schedule. These results and conclusions match those often speculated by FCF systems engineers and management suggesting that a very limited back-shift crew could provide significant throughput benefits by relieving some of the bottleneck areas. The insights gained from the model help to further validate those intuitions from experts.

Table 10: Additional Bravo-3 Scenario 7/24 (three year simulation).

Metric	**Estimation**
Annual throughput	502.3 kgHM
Annual HALEU generated	1607.5 kg
Total no. of ER-4 Runs	67
Total no. of ER-5 Runs	66
Total no. of ER Batches	133
Total no. of CP runs	21
Total no. of MFF-1 runs	177
Total no. of UPS shipped out	197
Bottleneck	None

Clarifications:

- Before starting a simulation, assumptions for the scenario under examination are entered. FOM, with no initial inventory, is then run for a given time period (e.g., three-year) to compute sustainable productivity values and identify bottlenecks more accurately.
- If the goal is to compute productive estimates when a particular equipment (e.g., ER-5) becomes operational at a given time under a Bravo-1 (or Bravo-2) scenario, for example, FOM could be run first under Alpha-1 (or Alpha-2) scenario (i.e., no ER-5) for one year only and then extract productivity values. Then, the average productivity values estimated under Bravo-1 (or Bravo-2) scenario can be added to subsequent years when ER-5 enters in operation (assuming that FCF starts a given year from the inventory left from the previous year).
- If the facility under consideration is always started with no inventory at the beginning of each year of resumed operation, then FOM should be run for one year only to compute productivity estimates.
- FOM includes elements described by probability functions, hence stochasticity is present in it. Consequently, it is customary to run a sufficient number of times the scenarios under comparison to provide error bars for discussion. However, the examples presented here do not include uncertainty estimates because the employed strategy discussed here is to run a given scenario long enough as to produce average values acceptable for comparison.

6.4. Lessons learned

As indicated in Section 3.4, INL initiated efforts for actively utilizing computational methods to assess processes and facilities from a productivity perspective since 1998.

From that time, OR capabilities have been restored and expanded in multiple occasions and are available at MFC for the systematic design, analysis, optimization, and monitoring of operations and maintenance (O&M) processes conducted at actual and proposed nuclear facilities. This impactful endeavor includes the development of a DES model that represents the production activities occurring inside FCF in support of treating the sodium bonded fuels from EBR-II and other nuclear reactors. The treatment of the EBR-II used fuel inventory has been one the largest environmental liabilities within the Department of Energy's Office of Nuclear Energy and FOM has taken on increasing importance as the deadlines established between the Department and State of Idaho in the 1995 Idaho Settlement Agreement draw nearer.

In support of it, an extensive upgrade of FOM has been recently completed not only to equip it with the latest computational advancements in modeling and simulation (M&S) but also to incorporate the production of HALEU material as part of the ongoing treatment operation at FCF. HALEU is a key component to advancing new nuclear reactor technology and the OR capability reported here is helping to develop, following a rigorous approach, the strategy for supplying this critical material. The vision, leadership, and teamwork displayed when initially engaging in the development of FOM and other OR capabilities (e.g., modeling of the Hot Fuel Examination Facility and the Analytical Lab) more than 25 years ago, and the value from using these computational tools today as means to analyze and optimize production scenarios related to fulfilling the Departments obligations, may be viewed as a testament to the quality and thoroughness of the innovating solutions here addressed. By applying state-of-the-art M&S concepts, modern decision-making tools have been created, which have the ability to expand well beyond conventional DES models and OR capabilities in general. Accurately modeling the process steps necessary to treat sodium bonded fuels, a distinctive analytical platform was developed that not only replicates the activities occurring within FCF, but also has the capability to be expanded to other facilities and missions currently at and/or envisioned for MFC, and thus helping to deliver the next generation of nuclear fuel cycle solutions.

Even though INL, in particular MFC, are heavily focused on conducting research and development activities, and to a lesser extent production based undertakings, these computational capabilities have assisted INL management convey its message on the most efficient means possible to approach the EBR-II and other reactor inventory. For example, INL management has used FOM to communicate and illustrate to various stakeholders the benefits of expanded operations (i.e., the change in operating shifts from 4 x 10 to 7x12 and 7x24) as well as of redundant capabilities (i.e., installation of the multi-function furnace to eliminate the single point failure). Use of the FOM as a communication tool to various stakeholders and sponsors has been effective and INL plans to continue to utilize it in the future. It is the hope of the authors that by presenting on and communicating the benefits of FOM, we might see expanded use of this type of modeling in other areas across INL and perhaps the DOE complex. Thus, OR activities described in this article may be viewed as a testament of applying rigorous theories toward practical applications of significant importance.

7. Conclusion

The efficient and reliable execution of activities conducted in nuclear facilities is an important component for achieving sustainable radioactive waste management and production of nuclear material. To this end, Idaho National Laboratory (INL) has invested in the development of diverse facility operations models using discrete event simulation techniques to assist in the improvement of current and proposed nuclear fuel treatment operations conducted at the Materials and Fuel Complex (MFC) of INL. In this regard, the FOMs developed have provided a powerful decision-making tool to identify which operational changes can significantly improve efficiency, reliability, and productivity. Using computational methods, what-if scenarios are developed to compare several operational strategies. These computational capabilities have provided numerous types of suggestions, from increasing the process batch size of certain subsystems (e.g., CP–CF subsystem) and installing equipment/workstations at optimal locations, to adding new equipment using more efficient modes (e.g., electrorefining, salt distillation, uranium recasting) and operating with more effective labor schedules. By implementing operational recommendations, achieving the desired productivity goals have become feasible. This article can be considered as a case study of using computational methods for operational improvement of facility operations. It demonstrates the potential of discrete event simulation methodology, facility operations modelling, and computational methods as decision-making tools to model, analyze, and optimize the operational performance of complex processes, facilities, and services.

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