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Final Electrochemical Safeguards Model for the MPACT 2020 Milestone

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ABSTRACT

The Material Protection, Accounting, and Control Technologies (MPACT) program is working toward a 2020 demonstration of Safeguards and Security by Design for advanced fuel cycle facilities. This milestone ties together modeling and experimental work and will initially demonstrate the concept for electrochemical processing facilities. The safeguards modeling tool used is the Separation and Safeguards Performance Model (SSPM). This report outlines the baseline model design that will be used for the 2020 milestone analysis, which was updated to represent a new baseline flowsheet developed for the MPACT program. The model was also used to generate simulation data for other labs to use as part of their safeguards analysis. Finally, this report describes how the 2020 milestone will be met.

ACKNOWLEDGEMENTS

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ACRONYMS AND DEFINITIONS

Abbreviation	Definition
AMFP	Active Metal Fission Products
CuSum	Cumulative Sum
DA	Destructive Analysis
ER	Electrorefiner
FP	Fission Products
ID	Inventory Difference
LCC	Liquid Cadmium Cathode
MBA	Material Balance Area
MC&A	Material Control & Accountability
MPACT	Material Protection, Accounting, and Control Technologies
MT	Metric Tons
MWF	Metal Waste Form
NDA	Non-Destructive Analysis
NRC	Nuclear Regulatory Commission
OR	Oxide Reduction
PUREX	Plutonium and Uranium Extraction
RE	Rare Earth
SEID	Standard Error of the Inventory Difference
SITMUF	Standardized Independent Transformed Material Unaccounted For
SNF	Spent Nuclear Fuel
SSBD	Safeguards and Security by Design
SSPM	Separation and Safeguards Performance Model
TRU	Transuranics
UREX	Uranium Extraction
U/TRU	Uranium/Transuranics

1. INTRODUCTION

The Materials Protection, Accounting, and Control Technologies (MPACT) program is working toward a demonstration of a Virtual Facility Distributed Test Bed for Safeguards and Security by Design in 2020. The Virtual Test Bed focuses on tying together new measurement technologies, data from experimental test beds, and modeling capabilities across the laboratory complex. These capabilities are used to develop and analyze safeguards and security approaches. The goal is to develop a capability for complete Safeguards and Security by Design (SSBD) for future fuel cycle facilities. The 2020 milestone will demonstrate the concept for a generic electrochemical reprocessing facility.

The Separation and Safeguards Performance Model (SSPM) is one of the systems-level modeling capabilities used for the overall design of a materials accountancy strategy. However, the modeling results are only as good at the data fed into the model, so the analysis work is strongly dependent on modeling and experimental work in the rest of the MPACT program which provides more detail on the facility, measurement technologies, and overall safeguards approaches. A key aspect of this work has been the integration and coordination of data with other laboratories.

In FY19, the model was updated to be consistent with a baseline flowsheet, developed by Argonne National Laboratory [1]. A few modifications were required to make this change, and there will be some minor implications on the safeguards analysis. In addition, simulation data was generated for Los Alamos National Laboratory to assist in the Advanced Integration tasks [2,3]. That work takes a deeper dive into the performance of key MPACT technologies given the materials and environments they will face in a commercial electrochemical facility. In turn, the advanced integration work can then provide input to the SSPM such as expected measurement uncertainties.

In FY20, the final safeguards analysis will be completed based on the best information that is available about the measurement technology performance. The safeguards design will be presented along with its performance under diversion scenarios. The goal of this past year's work was to prepare the model for the final analyses.

2. BACKGROUND

2.1. MPACT 2020 Milestone

The MPACT campaign's Virtual Facility Distributed Test Bed concept is shown in Figure 1 [4,5,6]. There are three key systems level modeling capabilities that are used for safeguards and security analysis. Starting at the bottom and moving up, the flowsheet modeling work defines the process parameters and feeds into the above modeling capabilities. The safeguards model is built using the flowsheet and is used to design and analyze the safeguards measurements and overall safeguards system. Key metrics include overall measurement uncertainty and probability of detection of diversion or misuse. A 3D security model is used to layout the plant and design and analyze a physical protection system.

While the modeling capabilities allow for analysis of safeguards and security designs for new facilities, the models have been informed by a significant amount of experimental work as well as higher fidelity modeling capabilities. These high-fidelity capabilities are shown on the left of the figure and include the wealth of past and current work in the MPACT program on new measurement technologies, experimental data from test beds at the various national laboratories, measurements models, statistical methods, unit operation models, radiation signatures, and consequence modeling.

The overall purpose of the 2020 Milestone is to tie together all these capabilities more to provide a one-stop shop for SSBD. For example, if a future reprocessing facility were to be built and had unique features, the modeling capabilities would work together to help the vendor optimize the facility, safeguards, and security system design. If specific materials accountancy challenges are identified, one of the laboratory test beds may be used to develop a measurement system that will work under the expected operating conditions. The latest developments in measurements, sensors, and data analytics would be applied to provide designs that meet regulatory requirements in a cost-effective manner.

The focus of the safeguards modeling (described in this report) in FY19 has been to update the model to be consistent with the baseline flowsheet. This work has focused on preparing the model for the more detailed analyses that will be done in 2020 to meet the milestone. Data outputs for other laboratories have also been generated.

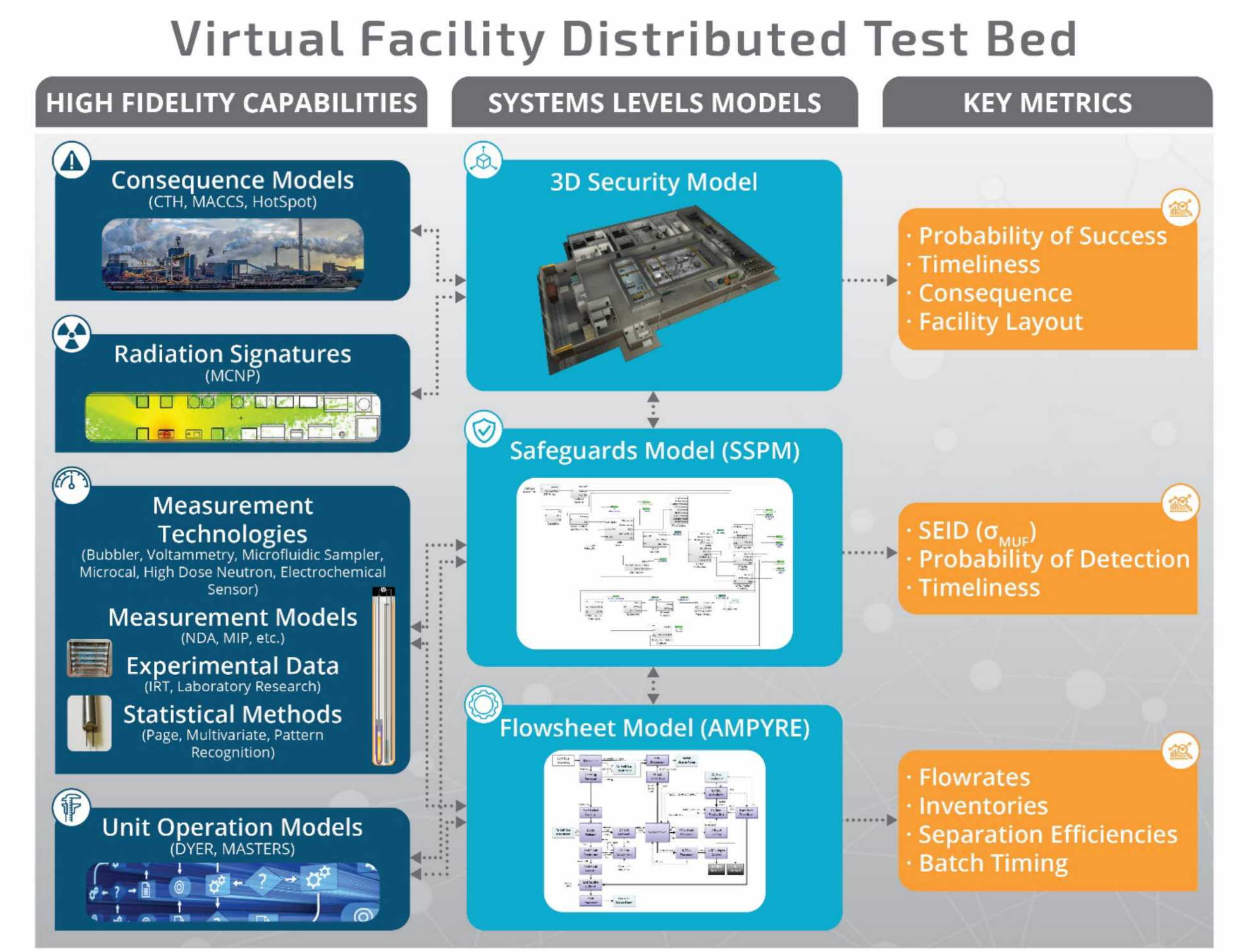

Figure 1. Virtual Facility Distributed Test Bed

2.2. SSPM Background

The SSPM was designed for systems-level analysis of the safeguards design for reprocessing facilities. However, the modeling capabilities have been extended to include other facilities as well. Currently, various versions of PUREX, UREX+, and electrochemical reprocessing facilities exist along with fuel fabrication, enrichment, and molten salt reactor facilities.

The electrochemical SSPM model has been developed over the past 5 years [7,8]. In that time, the modeling detail has improved significantly, preliminary safeguards approaches have been tested (virtually), and a number of safeguards by design recommendations have been generated. That being said, there are still many safeguards challenges with electrochemical facilities, and more experimental work is required.

Figure 2 shows the original baseline flowsheet (before modification in FY19). In the original flowsheet, the spent fuel pins, including cladding, were shredded and sent on to oxide reduction (OR or electrolytic reduction). The cladding would stay in the basket and ultimately go to the Metal Processing operation to produce a metal waste form. The updated flowsheet performs decladding first to reduce the amount of material going into the process.

The original flowsheet also used the same salt for the OR and electrorefining (ER) vessels, so no salt distillation step was required between processes. This also meant that the salt contained all fission products. The new flowsheet assumes the use of two different salts for the OR and ER vessels, so an additional salt distillation step was required. An active metal fission product (AMFP) process was also added to separately remove the AMFPs from the OR salt.

Further discussion on the updated model is provided in section 3.

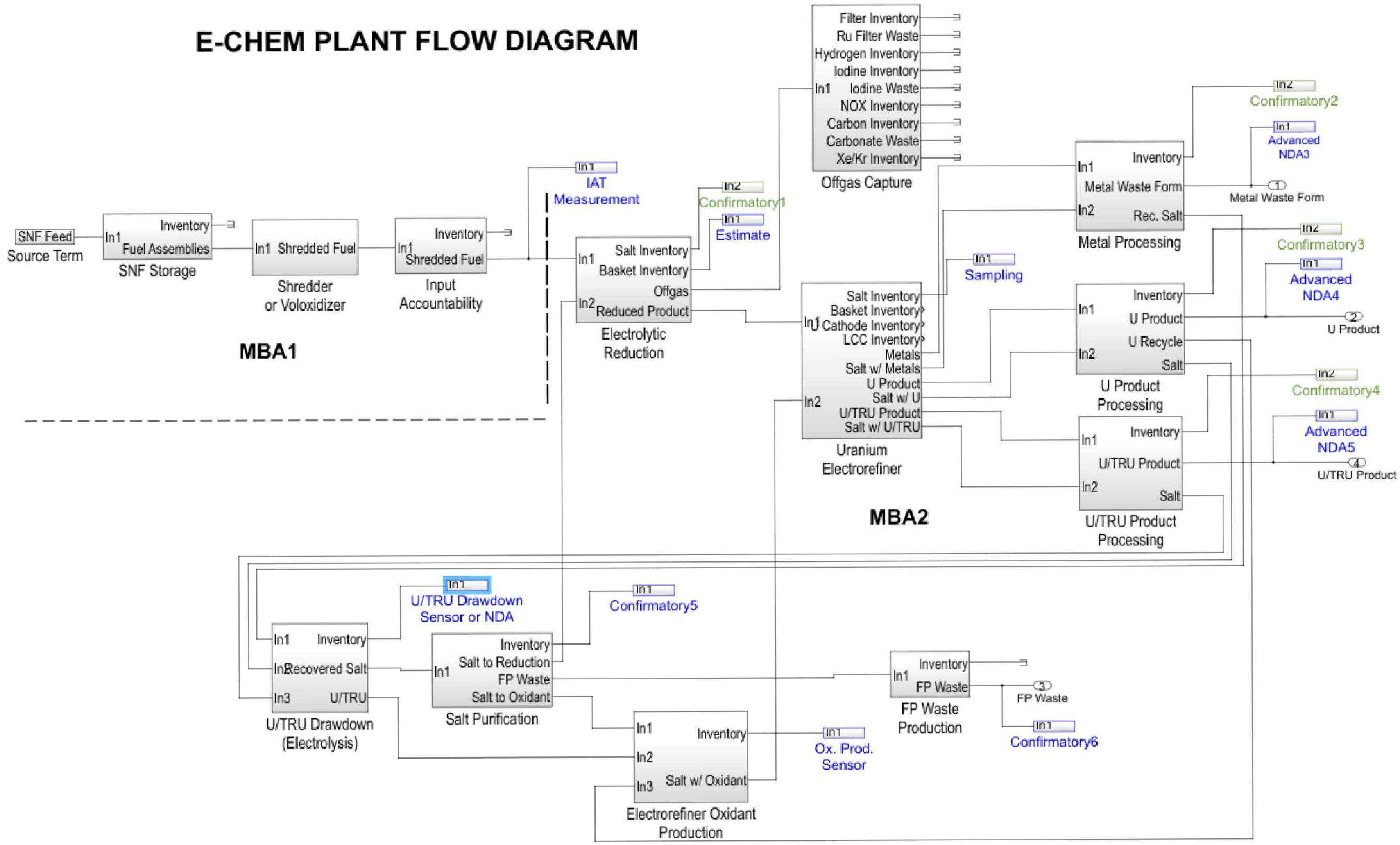

Figure 2. Electrochemical Flowsheet [7]

2.3. Updated Baseline Flowsheet

The flowsheet upon which the model is based represents a pilot-scale facility capable of processing 100 metric tons (MT) of spent light water reactor (LWR) fuel per year. The baseline flowsheet is described in reference 1. This flowsheet changed slightly from the previous flowsheet used for the MPACT studies, but the changes represent the current thinking on how an electrochemical facility would operate. Figure 3 shows the overall flowsheet.

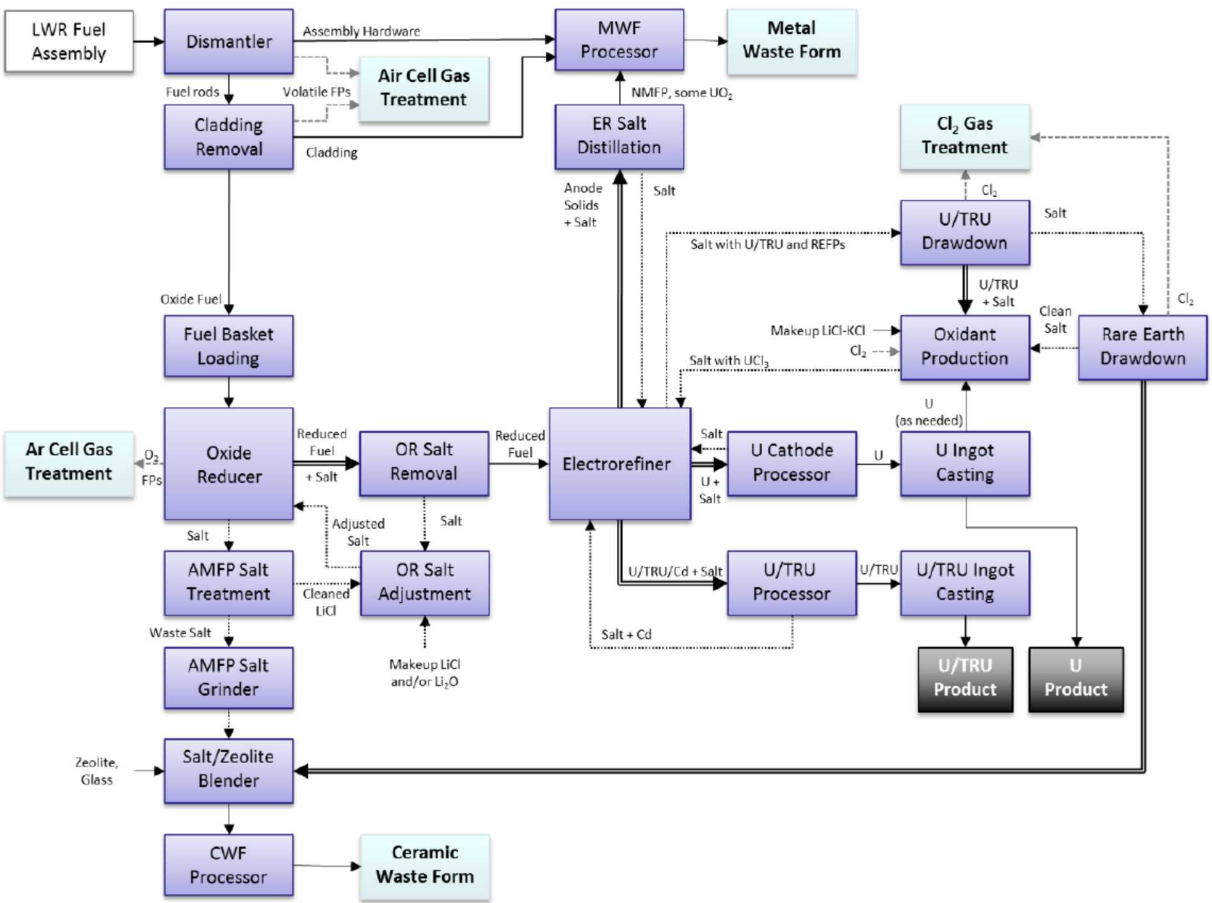

Figure 3. Baseline Flowsheet [1]

The baseline flowsheet starts with spent LWR fuel, dismantles the assemblies, and strips the cladding from the fuel. The fuel would typically be shredded or grinded before loading into porous baskets. All front end operations can occur in a hot cell with an air atmosphere, but then the baskets are transferred into an argon hot cell for the remaining electrorefining processes.

The fuel baskets are loaded into the OR which converts most of the oxide fuel into metallic species. After removal, the OR salt is distilled off the reduced product and returned to the OR vessel. The OR salt will acquire a majority of the AMFPs, so a salt treatment step is required to remove those materials, blend them with zeolite, and place into a ceramic waste form.

The reduced fuel baskets get transferred to the ER next. The ER vessel contains two cathodes which work simultaneously to remove a uranium (U) and uranium-transuranic (U/TRU) product. The salt from these products is distilled off and returned to the ER vessel or recycled through the U/TRU drawdown process. The U and U/TRU products are cast into ingots and placed into storage or used for the production of metallic fuel for fast reactors.

Residual noble metals and other left-over material in the baskets are transferred to the ER salt distillation step to first remove residual salt, and then transferred to the metallic waste form (MWF) processor along with the cladding and assembly hardware. These materials are melted together to form the MWF.

Finally, the rare earth (RE) fission products are acquired in the ER salt, and this material needs to be removed during operation. The U/TRU drawdown process first removes U/TRU material and recycles it back to oxidant production. Then the RE fission products are drawn down and combined with the AMFP waste. The left-over salt and U/TRU from drawdown are used to produce an oxidant which is recycled to the ER to maintain operations.

The updated flowsheet had a few key changes from the previous flowsheet. Cladding removal was added instead of sending the cladding through the process. The OR and ER salts are now assumed to be different, requiring the need for the OR salt distillation step. Finally, the AM and RE fission products are combined into one ceramic waste form. It is important to note that this flowsheet is one option that may be considered for electrochemical operations. Other options will have various tradeoffs associated with them. The safeguards implications of the design options will be an important topic for the 2020 milestone.

3. MODEL DEVELOPMENT

The original Echem safeguards model had the same throughput as the new baseline flowsheet, so the model changes were straight-forward. The finalized safeguards model in Simulink based on the new flowsheet is shown in Figure 4.

The unit operations in the upper left corner through Basket Loading & Input Accountancy would be contained in the air hot cell and would make up Material Balance Area (MBA) 1. The rest of the processes as shown would be contained in the argon cell and would make up MBA 2. The Simulink model follows the overall baseline flowsheet with one minor exception—it assumes that the distilled salt recovered from metals, U, and U/TRU product processing will all go to the drawdown process before being recycled back to the ER vessel. This is shown as the three salt streams which feed into the U/TRU drawdown processin Figure 4. Otherwise, the process steps are identical.

There are a number of assumptions in the model that have not been validated yet due to lack of experimental data. These include separation fractions for each element at all process steps, assumptions of reduction percentages, off-gas release, and extraction rates. Currently these values are set with optimistic values that would be expected through proper engineering design, and experimental data will be added when it becomes available in the future.

The safeguards statistical tests in the model have remained unchanged from previous work, other than small updates due to additional inventory measurement points. The bulk balance was updated to reflect the additional unit operations and changes to existing blocks.

Figures 5 and 6 show the inventories of U and Pu in the unit operations as a function of time for a normal run (no diversion modeled) over 2000 hours. The U inventories show mostly steady operation (Figure 5), but there is variability in the ER vessel due to the fact that the U/TRU ratios change at the beginning of the run. Control functions are used in the model to help control the output to maintain a somewhat steady mode of operation. The content of U in the U/TRU product drops slightly during the run due to this affect. This in turn leads to some variation in U/TRU drawdown and the oxidant production step. Past work has shown that it is useful to have this type of variability in the model so that safeguards systems can be designed to be robust to these fluctuations.

The Pu content (shown in Figure 6) changes more substantially since the ER salt contains zero Pu at startup. There is a buildup of material through the run that appears to reach steady-state near 1500 hours. Again, this behavior is expected, but the only departure from reality is that the first few batches of U/TRU ingots would likely have too low Pu content for fuel use.

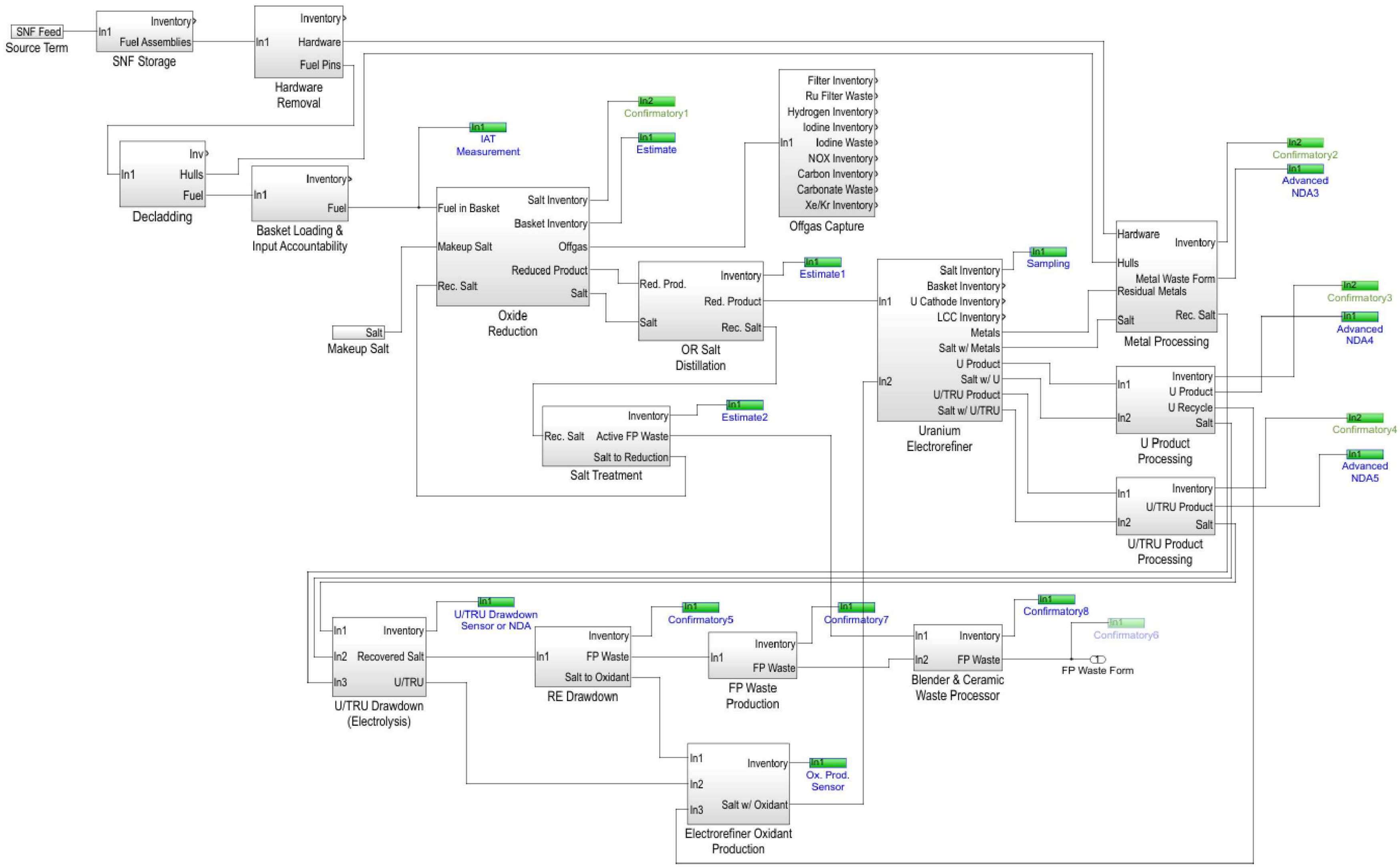

Figure 4. Echem Safeguards Model in Simulink

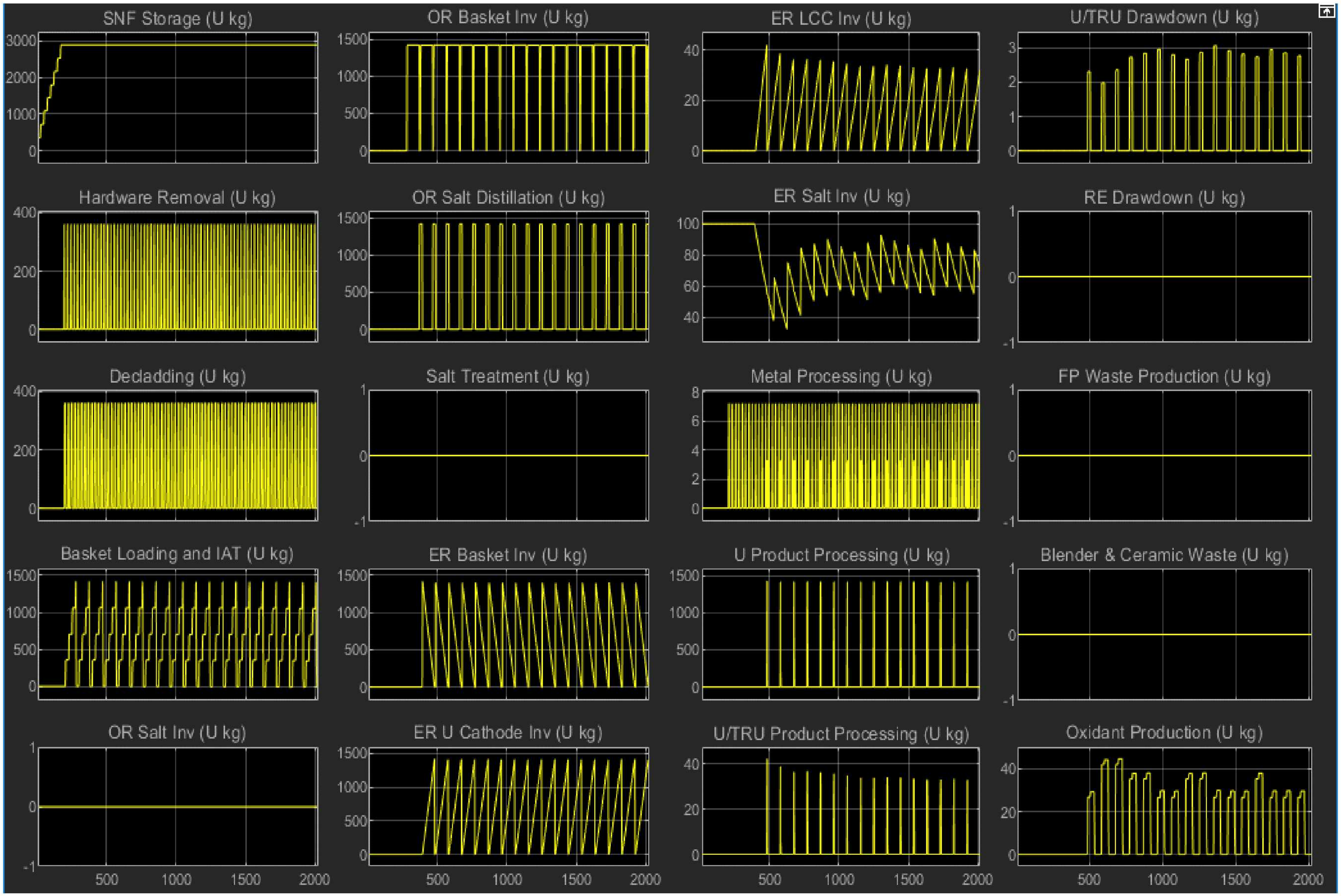

Figure 5. Echem safeguards model in Simulink showing U inventories for a normal run.

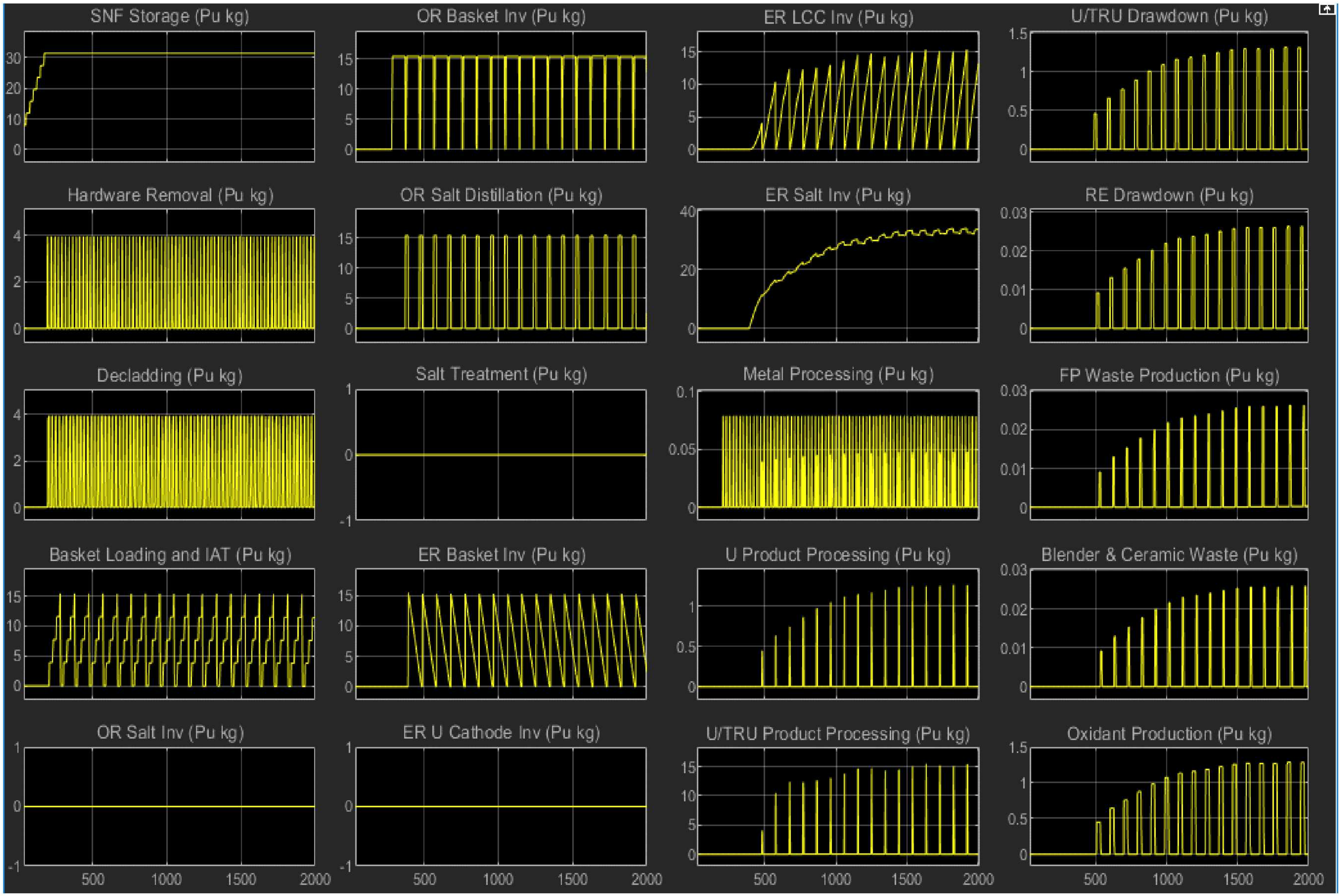

Figure 6. Echem safeguards model in Simulink showing Pu inventories for a normal run

3.1. Materials Accountancy System

The measurement blocks in the SSPM have not changed appreciably since the last model version. Some additional inventory measurements/estimates were assumed due to the added unit operations in the updated flowsheet, and these were properly added to the material balance and error propagation calculations.

The details of the measurement blocks will not be described here since the FY20 work will go into much more detail on that. Future work will focus on a full safeguards analysis, a more finalize materials accountancy design, and thorough discussion of safeguards measurements and timing sequences.

However, it was useful to make sure the material balance was set up correctly in the updated model. Figures 7 and 8 show the U and Pu inventory difference (ID) and cumulative sum (CuSum) ID during the example 2000 hour run. The yellow line represents the individual ID calculated every 672 hours (every 4 weeks). The blue line represents the CuSum. Note that the quantities of U (Figure 7, given as kg) are large due to the high throughput of U for a reprocessing facility. The quantities of Pu (Figure 8, given as kg) are smaller due to the lower throughput. Given the throughputs of material and assumed measurement uncertainties, these example ID values are within the expected range. Note that different runs will lead to different results due to the randomness of measurements in the SSPM.

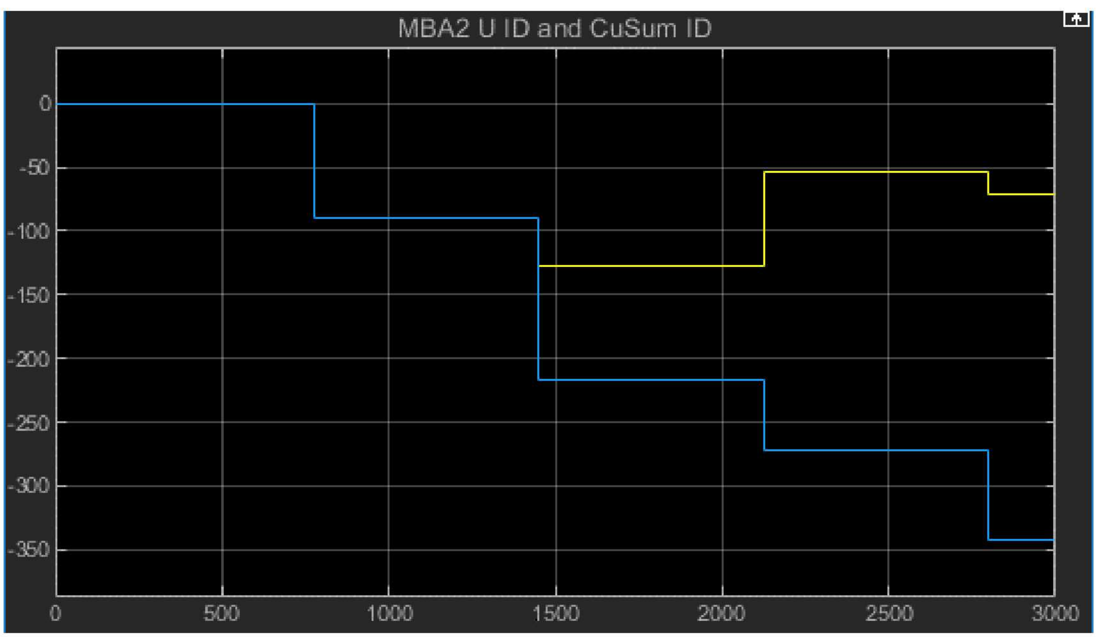

Figure 7. Example U Inventory Difference (yellow) and Cumulative Sum of the Inventory Difference (blue) for a normal run (y-axis unit is kg, x-axis unit is hours)

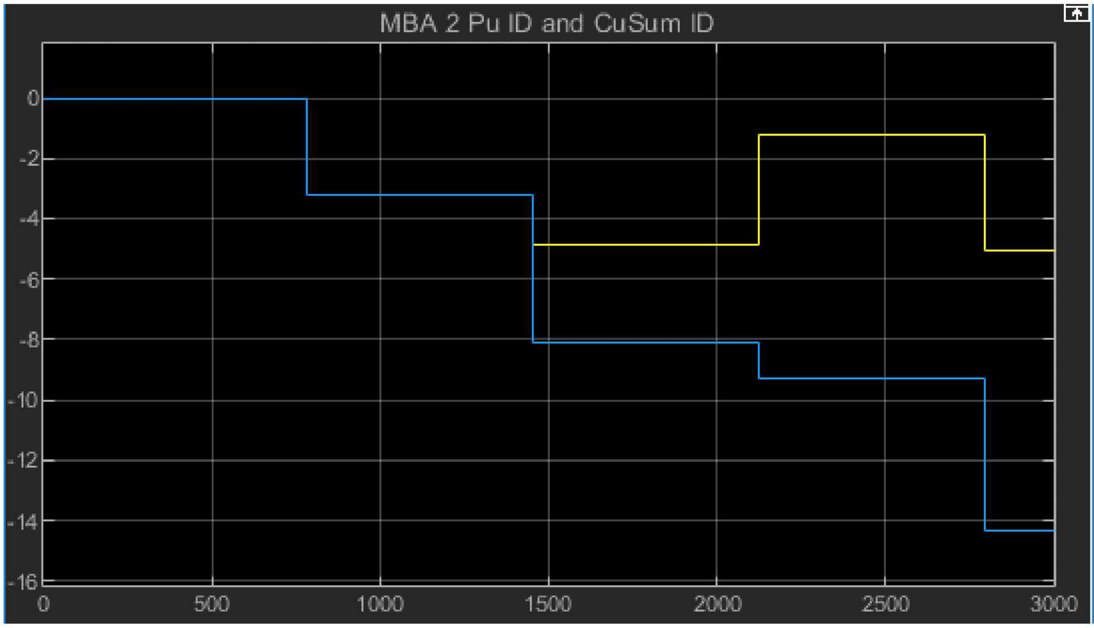

Figure 8. Example Pu Inventory Difference (yellow) and Cumulative Sum of the Inventory Difference (blue) for a normal run (y-axis unit is kg, x-axis unit is hours)

The overall Standard Error of the Inventory Difference (SEID) is a useful safeguards parameter since it indicates how well the materials accountancy system is performing. The SEID represents the overall error (at one standard deviation) for the ID calculation. Figure 9 shows the Pu SEID for MBA 2. Again, given the assumed measurement uncertainties, a steady-state Pu SEID around 4 kg would be expected.

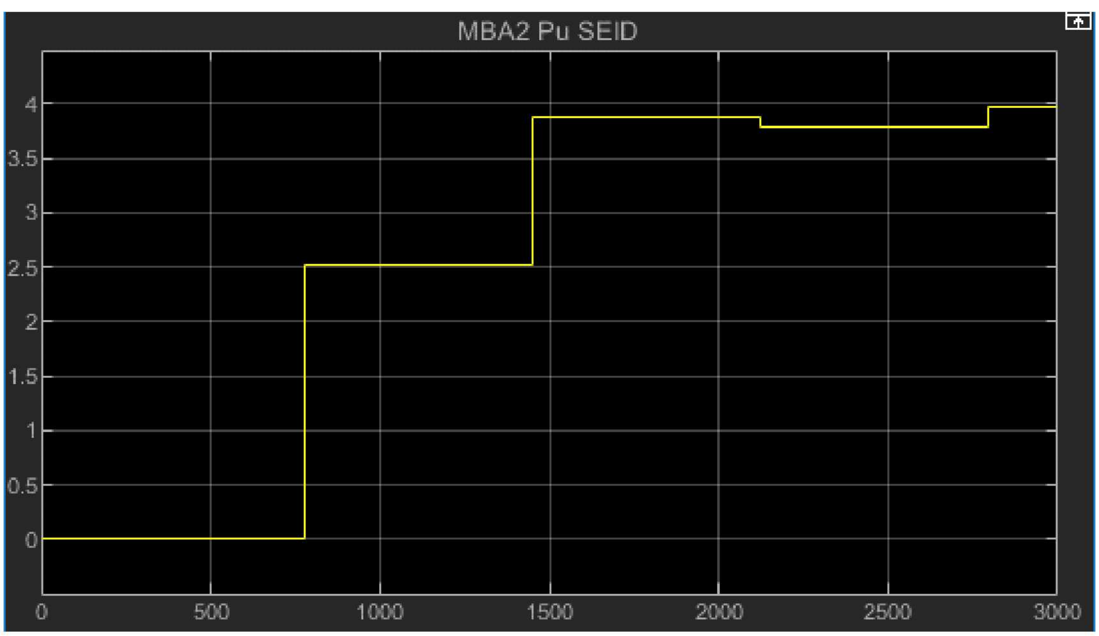

Figure 9. MBA 2 Pu SEID (Standard Error)

A 4 kg SEID means that the overall measurement error is equal to one half of an IAEA significant quantity. Typically a reprocessing plant will want to achieve an SEID lower than this value, but the purpose of the work for this year was simply to update the model. More detail will be spent next year on the specific measurement technologies and their overall performance.

Finally, the main statistical test used in the SSPM is Page's test of SITMUF (Standardized Independent Transformed Material Unaccounted For). The SITMUF calculation uses the SEID and the actual material balance to make a determination if material has been lost. Figure 10 shows the results of the Page's test calculation for this example run with no diversion. The yellow line is the test result for U, and the magenta line is the test result for Pu. The blue line is the threshold condition—an alarm would be indicated anytime the test results surpass the threshold condition. As would be expected, the Page's test result would not indicate an alarm for this run, providing indication that the test is set up appropriately.

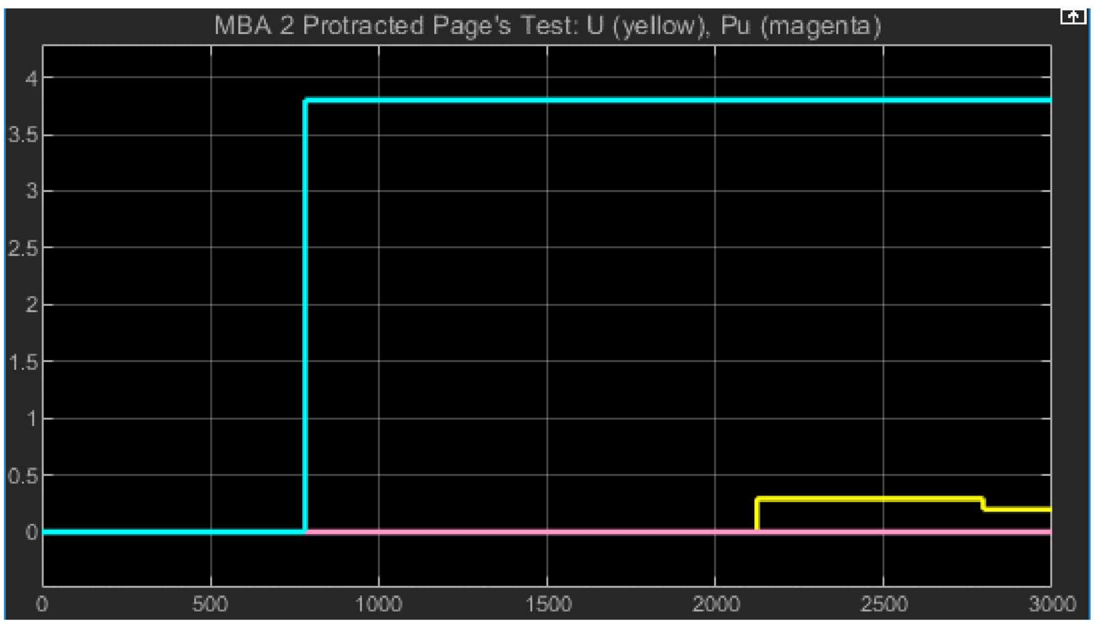

Figure 10. MBA 2 Protracted Page's Test

3.2. GUI Update

The graphical user interface for the Simulink model has been updated due to recent updates to Matlab/Simulink. Matlab has recently provided the ability to package a GUI and model into an application that can be installed and run from a task bar in the Matlab window or a stand-alone executable. This capability makes it easier to share the model with other researchers. The GUI is setup to generate output data for multiple iterations of runs, but can also be used in stand-alone mode to setup the model for individual runs.

The model GUI is shown in Figure 11. From here, the user can input the spent fuel source term and simulation duration—fuel swapping can be turned on to add variability to the throughput. Diversion scenarios can be turned on or off and defined. Finally, the key measurement errors can be defined. This GUI will be updated next year to also provide the ability to perform multiple iterations and parallel processing.

The output control tab in the GUI is shown in Figure 12. This allows the user to choose the type of outputs that will be logged into excel or csv files. Different safeguards metrics and bulk process data can be chosen. The specific elements of interest can also be chosen.

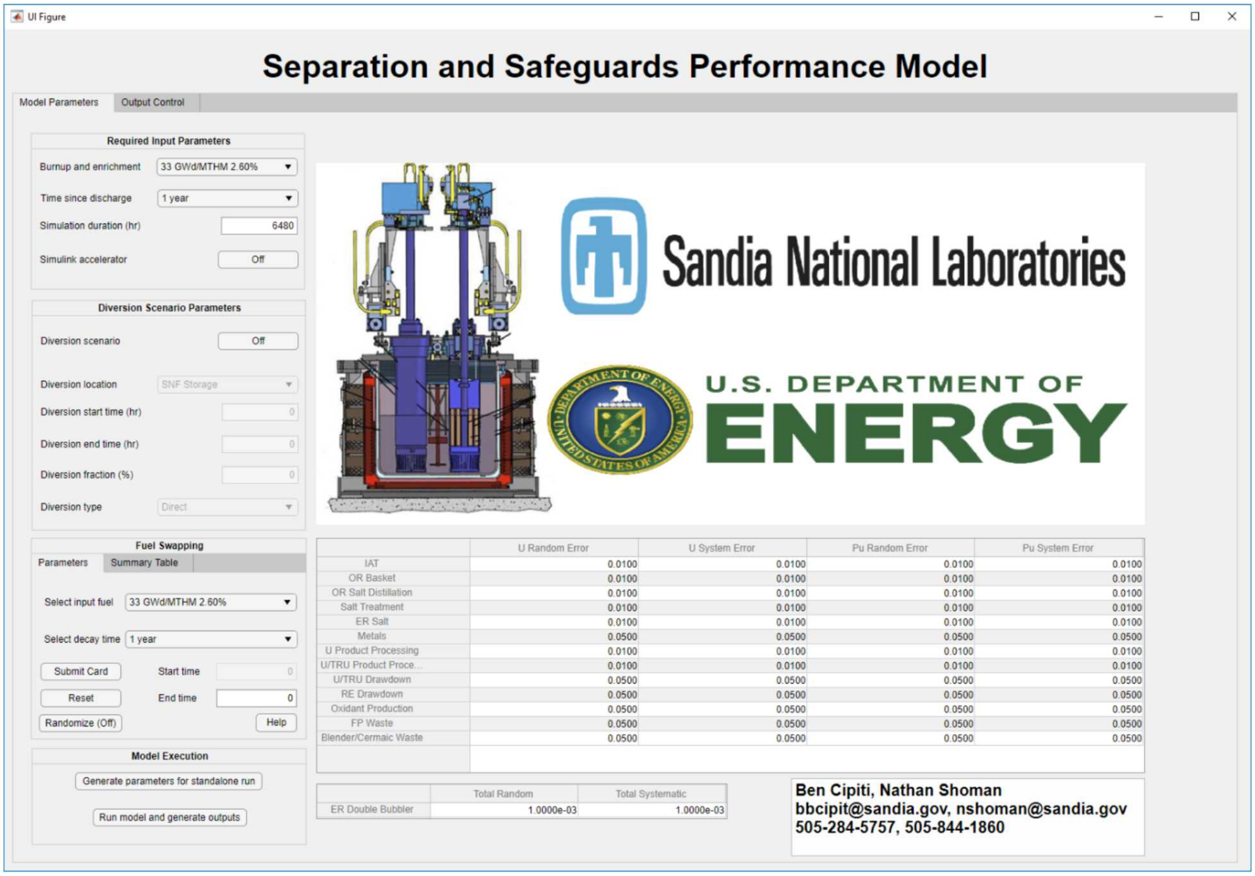

Figure 11. Echem SSPM GUI Parameter Definition

The GUI was developed in order to make the model more accessible for other researchers. Versions of this model have been shared with other researchers for use in evaluating advanced safeguards approaches or to generate simulation data. The GUI also makes it easy to run the large variety of diversion scenarios that will be needed for the 2020 analysis.

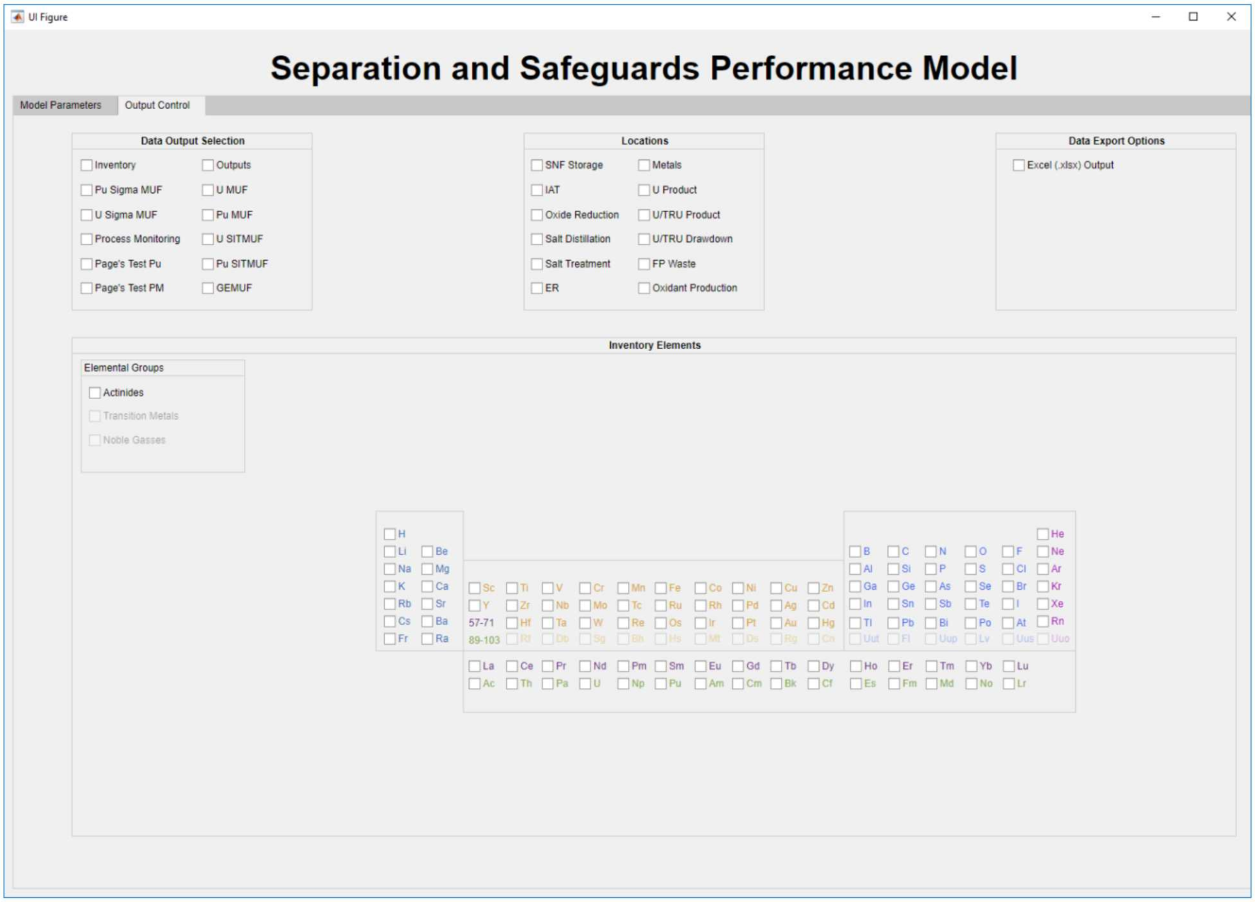

Figure 12. EChem SSPM GUI Output Control

4. SSPM DATA GENERATION

The final safeguards analysis for the 2020 milestone will utilize the SSPM, but the analysis is based on assumptions of the measurement uncertainties at the key measurement points. One of the challenges of measurements for electrochemical plants is that there is limited experimental testing available. The current integrated recycling tests at Idaho National Laboratory have provided much useful information, but in some cases experimental data is not available yet or the conditions may not represent a commercial or pilot scale facility.

To alleviate this gap, Los Alamos National Laboratory has an advanced integration task where they are evaluating expected measurement performance for a number of NDA technologies using SSPM data. The SSPM has been used to generate complete isotopic inventories for the key unit operations, inputs, and outputs. LANL is using that data along with modeling to determine how well gamma or neutron-based measurements can determine actinide inventories. In turn, LANL will provide the expected measurement uncertainties back to the SSPM to improve the analysis.

Data sets were generated for LANL starting in 2018, but these needed to be updated based on the latest baseline flowsheet. The output control portion of the GUI was used to generate an excel table with the full isotopic breakdown of all unit operation inventories, input, and outputs as a function of time. The amount of data is massive, and a 6480 hour run (approximately one year of simulated data) with data logging once per hour led to an excel file over 1 GB. This data file was cut down to only show the last few batches of material toward the end of a run when the model is in a relatively steady-state condition.

The data output is too lengthy to include in this report, but it is available for other researchers as needed.

Much of the SSPM model development and model assumptions has been based on experimental data, extrapolations from aqueous processes, and conversations with other researchers in the MPACT program. Model validation of the SSPM is difficult since electrochemical facilities do not exist, so clearly identifying assumptions and references to past work are important in this work. Next year's work will clearly describe these assumptions and references that tie much of the MPACT program together.

5. MPACT 2020 PATH FORWARD

For the past three years, the MPACT campaign has been preparing for the 2020 milestone, which is about one year away. The purpose of the milestone is to demonstrate how the MPACT capabilities come together to develop complete SSBD for an electrochemical processing facility. While much useful work will come out of this program specifically for electrochemical processing safeguards and security, the milestone is based on one example that can be applied to additional nuclear facilities in the future.

The milestone will be outlined in a special issue of the Journal of Nuclear Materials Management. The special issue will contain approximately eight papers describing the various MPACT capabilities, and this work would not be possible without the coordinated effort of all the researchers in the MPACT program. The following is a tentative breakdown of the expected papers in the special issue, but it is subject to change:

1. *Demonstration of a Virtual Facility Distributed Test Bed Concept to Apply Safeguards and Security by Design for Electrochemical Processing Facilities* – This overview paper will describe the Distributed Test Bed concept and summarize key SSBD conclusions and recommendations. It will reference the additional supporting papers.
2. *Flowsheet and Facility Design to Support SSBD* – Various flowsheet and facility design choices will have an impact on safeguards and security designs. This paper will summarize flowsheet and facility design with attention to safeguards and security tradeoffs of each major design option.
3. *Safeguards and Security Modeling Final Analysis* – Safeguards and security modeling is used to develop and test safeguards and security designs. This paper will summarize the modeling analysis and provide key success metrics. It will reference the measurement technology development work described in additional papers.
4. *Advanced Integration of Electrochemical Safeguards Measurements* – The advanced integration tasks link the measurement technologies with the modeling and analysis work. This paper will summarize the detailed measurement modeling results based on simulated data, and how the results are then used to inform the safeguards analysis.
5. *Electrochemical Safeguards Measurements at Argonne National Laboratory* – The various measurement technologies in development at Argonne will be summarized with a focus on their application in the electrochemical facility.
6. *Electrochemical Safeguards Measurements at Idaho National Laboratory* – The various measurement technologies in development at Idaho will be summarized with a focus on their application in the electrochemical facility.
7. *Electrochemical Safeguards Measurements at Los Alamos National Laboratory* – The various measurement technologies in development at Los Alamos will be summarized with a focus on their application in the electrochemical facility.
8. *University Research to Support Electrochemical SSBD* – Several university projects have provided key R&D to support the MPACT program both on measurement

technologies and new safeguards approaches. This work will be summarized focusing on its inclusion in the overall SSBD effort.

It is hoped that the special issue will provide more visibility for the capabilities that have been developed in MPACT. These capabilities could be better utilized by industry to address safeguards and security issues early in the design phase of a new facility.

6. CONCLUSIONS AND FUTURE WORK

This report described the Safeguards model update to prepare for meeting the MPACT 2020 milestone next year. The baseline electrochemical processing flowsheet was recently updated, and the SSPM was modified to be consistent with that flowsheet. In addition, some small updates to the SSPM GUI were completed. This work is one capability within the DOE NE MPACT program 2020 milestone to develop a Virtual Facility Distributed Test Bed for complete Safeguards and Security by Design.

The SSPM was also used to generate simulation data for other researchers in the MPACT campaign. This data will ultimately strengthen the overall safeguards analysis by developing better assumptions for measurement technologies in key locations.

For FY20, all measurement technology performance data will be incorporated into the SSPM along with the latest safeguards approaches developed by researches in the MPACT campaign. The model will then be used to generate a final analysis on the expected safeguards performance of an electrochemical processing facility. Key metrics like SEID and the probability of detection of a wide variety of diversion scenarios will be generated. Particular attention will focus on Safeguards by Design aspects, and design recommendations for future facilities.

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