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Material Protection, Accounting, and Control Technologies (MPACT)

Modeling and Simulation Roadmap

Prepared as part of the U.S. Department of Energy's Fuel Cycle Technologies Program

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EXECUTIVE SUMMARY

The development of sustainable advanced nuclear fuel cycles is a long-term goal of the Office of Nuclear Energy's (DOE-NE) Fuel Cycle Technologies program. The Material Protection, Accounting, and Control Technologies (MPACT) campaign is supporting research and development (R&D) of advanced instrumentation, analysis tools, and integration methodologies to meet this goal (Miller, 2015). This advanced R&D is intended to facilitate safeguards and security by design of fuel cycle facilities. The lab-scale demonstration of a virtual facility, distributed test bed, that connects the individual tools being developed at National Laboratories and university research establishments, is a key program milestone for 2020. These tools will consist of instrumentation and devices as well as computer software for modeling.

To aid in framing its long-term goal, during FY16, a modeling and simulation roadmap is being developed for three major areas of investigation: (1) radiation transport and sensors, (2) process and chemical models, and (3) shock physics and assessments. For each area, current modeling approaches are described and gaps and needs are identified.

For radiation transport and sensors, much of the basic radiation-transport tool development is complete. Modern Monte Carlo radiation codes are already quite advanced and meet many necessary criteria, but many application gaps remain and nuclear fuel cycle processing codes are particularly undeveloped as applied to nuclear materials accounting and control. A new capability in MCNP is the ability to handle moving radiation sources, this may be particularly useful for a bulk processing facility and is largely untested.

Process models provide a rapid and stronger assessment of upsets, deviations, and diversions for sensor optimization than is currently available for reprocessing. They can enable effective early detection of excursions, rapid evaluation of the causes, and effective timely and appropriate responses. Existing models are being expanded to create direct relationships between radiation signatures of chemical streams and the operations that result in those compositions. Integration of these models between one another and with facility-level models is needed as well.

A range of security assessments and modeling approaches are identified. In the United States, spent nuclear fuel (SNF) is safely and securely stored in spent fuel pools and dry storage casks. This report identifies several current evaluation techniques associated with the security of SNF dry cask storage for consequence modeling, force-on-force modeling, and risk-based scoring. Knowledge gaps include source term estimates and source terms for underground systems.

For all three areas of investigation (radiation transport and sensors, process and chemical models, and shock physics and assessments) modeling techniques are identified and a roadmap is developed for improving codes where needed and applications specific to the MPACT Campaign.

1 RADIATION TRANSPORT AND SENSORS

1.1 INTRODUCTION

During the past several decades modeling and simulation has evolved into an increasingly important design and analysis paradigm. This evolution has transpired in part because of tremendous advances in computer hardware. Performance of the fastest machines has grown exponentially from 10^4 floating point operations (FLOPS) per second on the Los Alamos MANIAC-II (Mathematical Analyzer Numerical Integrator and Computer Model II) in the 1950s to well in excess of 10^{15} floating point operations (petaflops, PFLOPS) per second recently (Top 500 Statistics, 2016). Dependable performance that is a factor-of-10^3 less than that for high-performance computers is available for less than one million dollars, which brings very meaningful computing power to budget-conscious organizations.

Concurrent major advances in software bring ever increasing realism to simulations. Improvements in phenomenological models are translated into computer languages as deeper understanding of phenomena are developed, and as increases in computer memory enable refinements to models. Moreover, new software paradigms facilitate improved execution. For examples, Message Passing Interface (MPI) is a language-independent communications protocol that is used to program parallel computers. MPI is a standardized and portable system that functions on a wide variety of parallel computers.

Together these hardware and software advances provide powerful predictive modeling and simulation capabilities for a wide range of physical and biological applications wherein modeling and simulation has become an essential component of development. Moreover, importantly, the simulation endeavor is cost-effective, inclusive of facilitating extensive parametric and optimization studies that would not be feasible from an experimental or construction standpoint.

The advances of modeling and simulation are particularly applicable to the nuclear industry, inclusive of facility design and spent-fuel handling. Costs associated with constructing and operating nuclear facilities are enormous. The development and utilization of advanced simulation tools to help customize and optimize nuclear facilities are enormous. The development and utilization of advanced simulation tools to help customize and optimize nuclear facility design and operations can potentially translate into major cost savings. With this in mind, a modeling and simulation roadmap has been developed for radiation transport and sensors as they relate to the MPACT charter. Four key characterization topics were considered: (1) codes and their usage, (2) signatures and sensor design/optimization, (3) application to process monitoring, and (4) gaps or needs and interfaces with other codes. This contribution will help to illuminate progress to date, and identify areas of opportunity and need.

1.2 CODES AND THEIR USAGES

Modern radiation-transport codes provide the analyst with very sophisticated modeling capabilities. These codes have evolved to include a variety of physics capabilities, algorithms,

and diagnostics. Several of these codes also have parallel execution capabilities and can be deployed on desktops, clusters, and supercomputers.

The progressive development of increasingly powerful and less expensive computer hardware and multi-processor execution during the past 20 years has caused the Monte Carlo radiation-transport technique to gain increasing favor. The Monte Carlo paradigm is preferred because it reduces or eliminates modeling constraints associated with deterministic diffusion and transport-theory methods. Some key desirable characteristics offered by Monte Carlo include:

- Error estimates (not provided by deterministic methods)
- Detailed geometry (much greater complexity fidelity than deterministic codes)
- Detailed energy treatment (eliminating processing issues for diffusion and transport)
- Detailed radiation diagnostics

In addition, many modern Monte Carlo codes have incorporated features in addition to basic radiation transport, such as:

- Criticality and burnup for isotopic inventories
- Radiation sources, including prompt and delayed radiation
- Detector modeling to help tailor sensor design/optimization

A number of Monte Carlo radiation-transport codes have been developed at U.S. institutions and abroad. Code capabilities vary, and each has its own verification and validation credentials.[1] More prominent codes include:

- MCNP6 (LANL)
- SCALE6.1/KENO (ORNL)
- TART (LLNL)
- COG (LLNL)
- VIM (ANL)
- TRIPOLI (CEA)
- MONACO/MAVRIC (ORNL)
- MONK/MCBEND (UK)
- EGS4 (SLAC)
- FLUKA (CERN)
- GEANT4 (CERN)
- SERPENT (VTT Finland)
- OpenMC (MIT)

A survey of recent MPACT Working Group Meeting agendas shows, the following investigators, applications, and codes being used in current research and development:

- Eric Rauch – Neutron signatures for used nuclear fuel (UNF) storage casks. MCNP6.

[1] Verification tests the degree to which the algorithms in a code function properly. Validation assesses code capability as compared to experimental data.

- David Meier – Multi-Isotope Process (MIP) Monitor/H-Canyon. MCNP6, MATLAB.
- David Ames/Billy Martin/Ben Cipiti – delayed-gamma (DG) NDA alternative means to help for material accountability. TINDER = MCNP6 + CINDER.
- Rachel Slaybaugh – Spent Fuel Storage Facilities Modeling – Monte Carlo + deterministic (ADVANTG) methods (applied theoretical methods development for improved variance reduction.) This work is intended to improve performance of MCNP6.
- Howard Menlove & Daniela Henzlova – neutron detector design for use in a high-radiation environment. MCNP6.
- Mike Simpson – pyrochemical signature-based safeguards neutron detection. MCNPX POLIMI.
- Haori Yang – muon imaging of dry storage casks. GEANT.
- Kelly Jordan – ^{4}He fast-neutron detector development. MCNP-PoliMi.
- Joe Durkee – electrochemical processing (Echem) radiation signatures. MCNP6.

MPACT researchers are not constrained to use any given radiation-transport code. Code selection is done according to their needs and code capabilities. Selections from the list above are described in more detail below.

The UNF storage-cask investigation is using MCNP6 to study neutron emission from dry storage casks. Isotopic inventory and neutron emission spectra data from Next Generation Safeguards Initiative (NGSI) and Oak Ridge databases are used in MCNP models to calculate time-dependent emission from casks to optimize a neutron based detector under development.

The Multi-Isotope Process (MIP) monitor effort is using MCNP6 to help with the detector deployment locations and the effects of shielding and collimation on spectra for the detector rig. MCNP6 can be used with Synth and SuperSynth to establish a source term of a known geometry and develop gamma ray spectra based upon predetermined burnups, cooldown, reactor types and fuel types. Analysis of spectra is performed using Principle Component Analysis (PCA) to identify variations, discrepancies, and anomalies to provide a near-real-time (NRT) monitor of process chemistry changes that can both support facility operations and be potentially correlated with nuclear material diversion. The PCA is supported by MATLAB code supplemented by a Partial Least Squares toolbox.

The Delayed Gamma material accountability effort used MCNP6 and CINDER to study NDA techniques for electrochemical processing. This effort investigated if an NDA measurement using active neutron interrogation and delayed gamma assay could provide an alternative input accountancy measurement for pyroprocessing. Results found that this particular technique would lead to high measurement uncertainties, but the capability may be useful for other applications or other types of NDA measurements.

MCNP6 is being used as a cost-effective means to optimize the design of a neutron detector in a high-radiation environment. Simulations of a neutron and gamma radiation environment are executed to optimize neutron detection efficiency as layers of boron and polyethylene are adjusted.

MCNP-PoliMi is being used aid the design of a ^{4}He neutron detector for used fuel storage monitoring using neutron fingerprinting. Simulations predict the interaction of neutrons with ^{4}He

as part of an effort whose objective is to determine an unknown incident neutron spectrum using a measured spectrum. Development of ^{4}He gas scintillator detector technology is being supported with the intent of designing an efficient, gamma-insensitive neutron spectrometer for UNF monitoring in dry storage casks.

The electrochemical radiation-transport effort entails simulations for a variety of conditions, including pre- and post-dissolution of fuel in an electrorefiner (ER), and after material has been moved from an ER to other processing units in a pyroprocessing facility. For each condition, the isotopic inventory and material densities are required. MCNP6 does not have an electrorefining module by which simulated dissolution isotopic and material-density can be calculated. That capability will require an interface with and use of an electrochemical code.

Several electrochemical codes are being developed, including the following:

- DyER (ANL) – ER dynamic electrorefining operations (MATLAB). DyER (the Dynamic Electrorefiner model) dynamically simulates electrorefining operations in a single vessel with one anode (solid or liquid cadmium) and one or two cathodes (solid or liquid cadmium).
- AMPYRE[2] (ANL) – mass-balance calculations for a pyroprocessing facility (Excel VBA). The Argonne Model for Pyrochemical Recycling performs mass balance calculations for a pyrochemical recycling facility, iterating the processing of multiple batches of material. The code simulates the unit operations of a complete facility from head end operations to convert fuel assemblies to loaded anode baskets, through electrorefining, product processing, salt treatment and recycle, and waste processing operations.
- MASTERS (INL) – first-principles interactive pyroprocessing flowsheet model with unit process operational constraints (MATLAB with Excel User Interface).
- ERAD (Korea) – ER dynamic electrorefining (Fortran). Performs one-dimensional mass transport and separation in electrorefining.

Because the electrochemical codes are new, they will require verification and validation. Links between these codes and MCNP6 (a Fortran code) will have to be developed. DyER and AMPERE, which are being developed under MPACT, are discussed further in the Process Models and Chemistry document.

1.3 SIGNATURES AND SENSOR DESIGN/OPTIMIZATION

As delineated in the preceding section, several MPACT projects are investigating the use of radiation signatures. Neutron radiation signatures are being studied for merit in verification of spent-fuel content in dry-storage casks. Field tests of the MIP monitor are ongoing at the H-Canyon nuclear separation facility on the Savannah River Security Site. The MIP takes advantage of changes in the gamma-ray spectra of the feed, waste and product streams to identify process chemistry changes correlated with normal operations and potentially nuclear material

[2] Pronounced “ampere”

diversion. Radiation maps for electrorefining are being developed to assist with instrumentation design and placement. The use of radiation signatures for electrorefining is being studied as a means of conducting Nondestructive Assay (NDA) based inferences of quantities such as material content. In the following sections, we briefly review the MPACT radiation-signature and sensor initiatives as they relate to modeling and simulation. This will lead us to a discussion of gaps, needs, and interfaces.

1.3.1 Radiation signatures

The signatures for each of these investigations are complex, time-varying, and reflective of underlying processes, materials, and other properties (physical, chemical, etc.). Modern codes – particularly Monte Carlo – provide meaningful insights into radiation behavior, which aids in sensor design and optimization. For MPACT-related studies pertaining to NDA and process monitoring (PM), neutron and gamma radiation are of particular interest.

1.3.2 Used nuclear fuel monitoring using neutron signatures

Storage and protection of used nuclear fuel (UNF) is an important safeguards and security effort. UNF produced at commercial reactor sites is increasing, and as the inventory approaches the limit of on-site wet storage capacity the UNF must be moved to independent spent fuel storage installations (ISFSIs). To achieve the goal of the MPACT campaign, it is important to ensure that SNM in UNF is not stolen or diverted from civilian facilities for other use during the extended storage.

For example, Fig. 1 illustrates the neutron signatures emanating from spent-fuel content in a dry-storage cask (DSC) for two burnups. These signatures are calculated using MCNP6 with models of DSCs and radiation sources using available data (Rauch, 2014). The cask signature is sensitive to a change in cask contents. The technique is a candidate for content verification over the decadal time scale for dry storage.

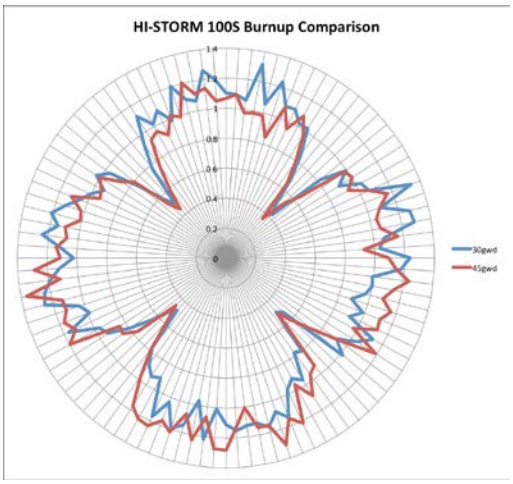


Figure 1. MCNP6 neutron signature emanations from dry-storage cask for two irradiation conditions.

1.3.2.1 Used nuclear fuel storage monitoring using muon radiography (OR Muon Imaging of Casks)

Another study (university based) is examining the feasibility of monitoring DSCs with cosmic ray muon imaging. The objective is to verify the content inside a DSC without opening it. The GEANT4 Monte-Carlo code is used to do the radiation transport. Application-specific image reconstruction algorithms are being developed. A scaled-down muon imaging system is currently under construction. This prototype system consists of muon trackers made of two-dimensional position sensitive plastic scintillator detectors with wavelength shifting (WLS) fiber readout. This system will be first evaluated in a laboratory environment. A field test at the Idaho National Laboratory (INL)'s dry storage cask farm has been scheduled to further investigate impact on imaging performance from radiation background around DSCs.

1.3.2.2 Used nuclear fuel storage monitoring using muon radiography

The LANL muon radiography team is testing cosmic ray muon radiography as a method to image the inside of spent fuel casks (Durham et al., 2016). The intent is to determine whether cosmic ray muon scattering can be used to determine whether spent fuel assemblies are missing from a sealed dry storage cask. Muon tracking detectors were placed on two sides of a partially loaded MC-10 cask at INL, and measured the incoming and outgoing trajectories of individual cosmic ray muons for ~2 weeks. Analysis of the scattering angles of these muons has proved that gross defects in the cask content can be identified in situ, without opening the cask. Additional measurements at INL are underway. This work is funded by the NNSA's Office of Defense Nuclear Nonproliferation R&D.

1.3.2.3 Radiation studies for electrorefining (OR Electrochemical Radiation Signatures Modeling)

For electrochemical radiation studies (Durkee, 2016a), models of ERs are made. In studies to date, models of the INL Mark-IV and ANL Planar Electrode Electrorefiner (PEER) have been created. These models are executed to study radiation behavior. Figure 2 illustrates MCNP6 plots of gamma radiation in a hypothetical pyroprocessing facility before and after electrorefined material movement from an electrorefiner.

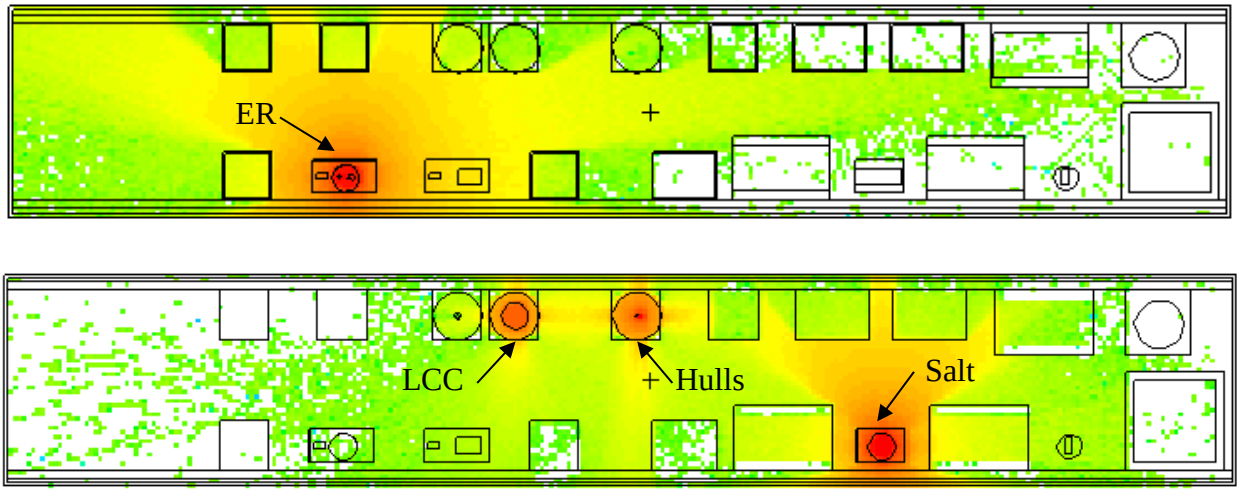


Figure 2. MCNP6 gamma radiation distribution flux within a hypothetical pyroprocessing facility. Upper: Contents in ER. Lower: Contents moved to processing bins.

In these and other applications, the high-fidelity radiation field predictions can be used to help guide sensor development and use as a means of cost-effective optimization for design and monitoring. Simulations can give detailed insights into conditions and behavior for nominal and off-normal conditions. Of particular interest is the ability to model time-varying radiation signals as a means of enhanced PM. An effort to do so using the new MCNP moving-objects feature (Durkee et al., 2016b, 2016c) is just beginning in FY16.

1.3.3 Sensor development

MPACT is supporting several sensor-development projects. These sensors are being designed to function in harsh radiation environments, provide fast response, and give high-fidelity measurements. Development is done in part using modeling and simulation.

1.3.3.1 Neutron detector design for high-dose applications

R&D efforts for nuclear safeguards applications of ^{3}He-free detector technologies have yielded a neutron detection system with performance characteristics similar to ^{3}He tubes. Detector design is done at Los Alamos using MCNP6 simulations to optimize performance. Specifications are then provided to Precision Data Technology, Inc. (PDT) for component and electronics production. This design process has yielded a detector that is comprised of six boron-lined parallel-plate proportional chambers that are interleaved with high density polyethylene (HDPE) for optimum neutron moderation (see Figure 3). The benefit of the technology lies in its inherent capability to sustain high count rates and in design features that allow minimizing its gamma-ray sensitivity and that allow for the capability to extract average neutron energy information from the multi-plate design. Design efforts seek to optimize performance for high count rates and high gamma-ray background applications through maximizing neutron detection efficiency and

development of a fast amplifier with performance capability to match the detector fast rise-time signal characteristics. This system has the potential to outperform ^{3}He tubes in high gamma-ray dose environments that require high count rates capabilities, such as spent fuel and pyro-processing measurements.

To optimize the detector design, an MCNPX model was developed based on the specifications of the original parallel-plate detector design that was benchmarked against experimental measurements (Henzlova, 2016). An optimization study was then performed, where the thickness of internal HDPE layers was varied to find an optimum configuration. The optimization was performed in two stages. The first stage involved variation of the thickness of the front HDPE layer to evaluate interplay between additional neutron thermalization and increasing distance of the first parallel-plate cell from the source. The second stage focused on optimization of the thickness of the HDPE layers between the remaining parallel-plate cells. The results of the MCNPX simulations are summarized in Figure 3 and provided direct input into the optimized detector build. This simulation work expedited design development with commensurate cost reduction.

Future developments related to the boron-lined parallel-plate detector will include the capability to simultaneously measure the neutron and gross gamma counting rates. This dual capability might be useful for both safeguards and PM related to the ratio of actinides and fission products.

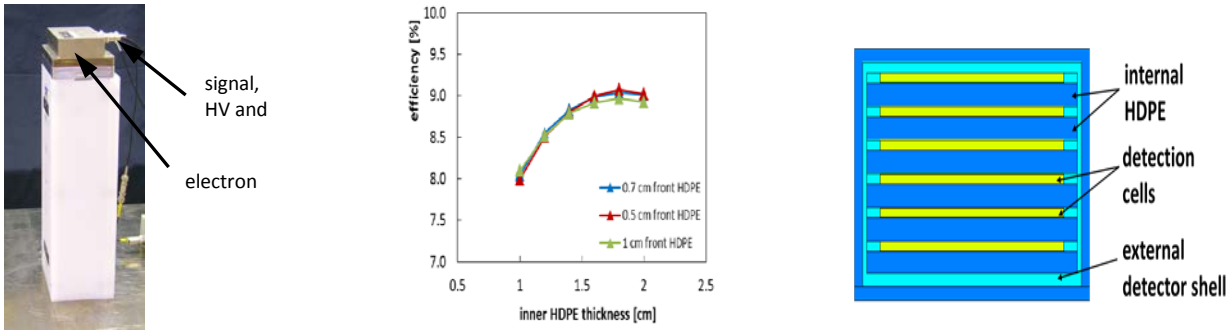


Figure 3. (left) PDT boron-lined parallel-plate neutron detector; center) MCNPX optimization of internal detector layout based on neutron detection efficiency; (right) schematic view of the internal structure

1.3.3.2 ^{4}He detector design for fuel storage neutron fingerprinting

Development of ^{4}He gas scintillator detector technology is being supported with the intent of designing an efficient, gamma-insensitive neutron spectrometer for UNF monitoring in DSCs. This detector, illustrated in Figure 4, uses a single-collision detection mechanism for fast neutrons wherein the neutron transfers its kinetic energy to the ^{4}He nucleus. No moderation is necessary. Tests are demonstrating the ability to clearly differentiate between different energies

of fast neutrons while discriminating from gamma signals at a very high level. By adding a thermal neutron conversion layer to make the "extended range detector," thermal neutrons can simultaneously be detected. This technology enables the measurement of dry storage casks for fingerprinting by providing a unique set of neutron energy markers that correlate to the contents of the cask through spontaneous fission, decay of curium and americium, and multiplication that are all linked back to spent fuel isotopic content. Potential offshoot technologies include enrichment monitoring, isotopic identification, fissile material detection, and reactor physics measurements.

Figure 4. ^{4}He detector for used fuel storage monitoring using neutron fingerprinting.

Detector response is a relationship between the input particle spectra and the registered output spectra. This relationship is characterized using a response matrix. The ^{4}He detector response matrix consists of two components. The neutron kinematic response matrix (NKRM), which relates the incident neutron energy to energy deposited in the detector, is well known. MCNP-PoliMi has been used to assess the NKRM, and the predicted energy-deposition spectrum agrees closely with the analytical predictions, as illustrated in Fig. 5 for a ^{252}Cf source. This is an important step in understanding the response matrix characteristics for this detector. The scintillation light response matrix (SLRM) relates the neutron energy deposition in the detector to the detected energy in terms of scintillation light response. This response is complicated, and is yet to be developed for the ^{4}He detector – inclusive of MCNP-PoliMi. As we have reported (Lewis et al., 2014), the lack of an SLRM has a significant adverse impact on the predicted detector response as gauged by the measured response. Once the tool response matrix is characterized, an unknown incident neutron spectrum can be determined using a detected spectrum.

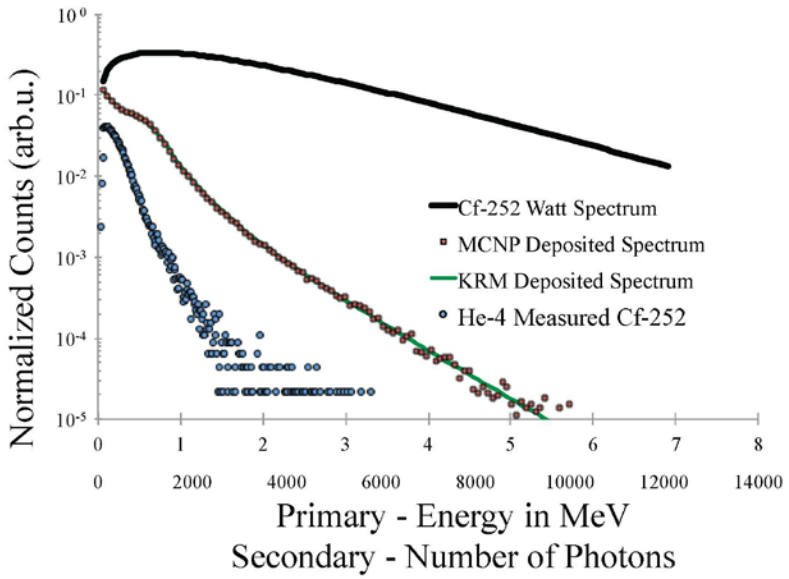


Figure 5. Measured and simulated ^{4}He detector response for a ^{252}Cf source.

1.3.3.3 MIP Monitor

The MIP Monitor is a PM capability that uses multivariate analyses of gamma ray spectroscopy to identify potential process variances upsets in near real time (NLT). This capability was developed at Pacific Northwest National Laboratory (PNNL) and is currently being deployed and tested on a large scale at the H-Canyon separations facility located near Savannah River National Laboratory (Meier et al., 2015).

MCNP6 is being used to model the radiation environment so as to identify detector deployment locations and the effects of shielding and collimation on spectra for the detector rig. MCNP6 can be used with Synth and Super-Synth (gamma spectrum simulators coupled to specific detector materials) to establish a source term of a known geometry and develop gamma ray spectra based upon predetermined burnups, cooldown, reactor types and fuel types.

Processing data is being collected at various sampling locations in the H-Canyon facility. Gamma ray spectra is acquired using NaI and LaBr3 gamma detectors coupled with a Digibase electronics package using Maestro software in list acquisition mode. The data is captured in 5 second time segments and each of these time batches is processed independently. PCA software is used to reduce the variables in the data from 1024 individual channels down to two or three distinct variables that can be plotted onto a Cartesian graph. These plots represent individual data points and make up population clusters. These clusters can be used to understand the relatability of acquired data sets. Figures 6 and 7 represent processed data before and after PCA analysis, respectively. In addition to experimental optimization, modeling and simulation can play and important role in parametric analyses of MIP monitor operational characteristics and sensitivities (Orton et al., 2008).

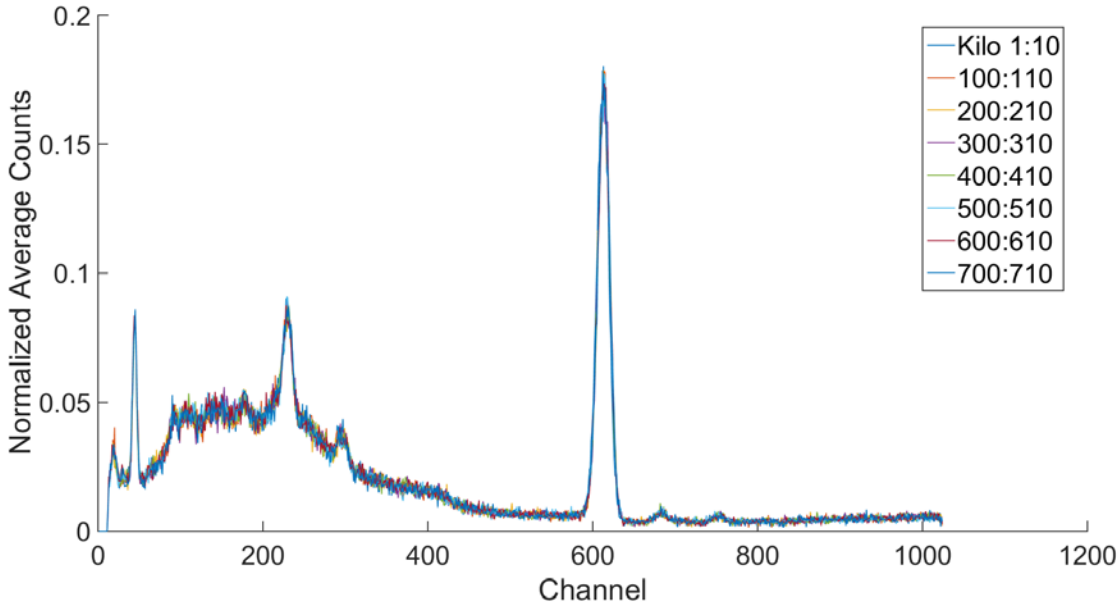


Figure 6. Processed gamma spectra gathered from H-Canyon Separation Facility.

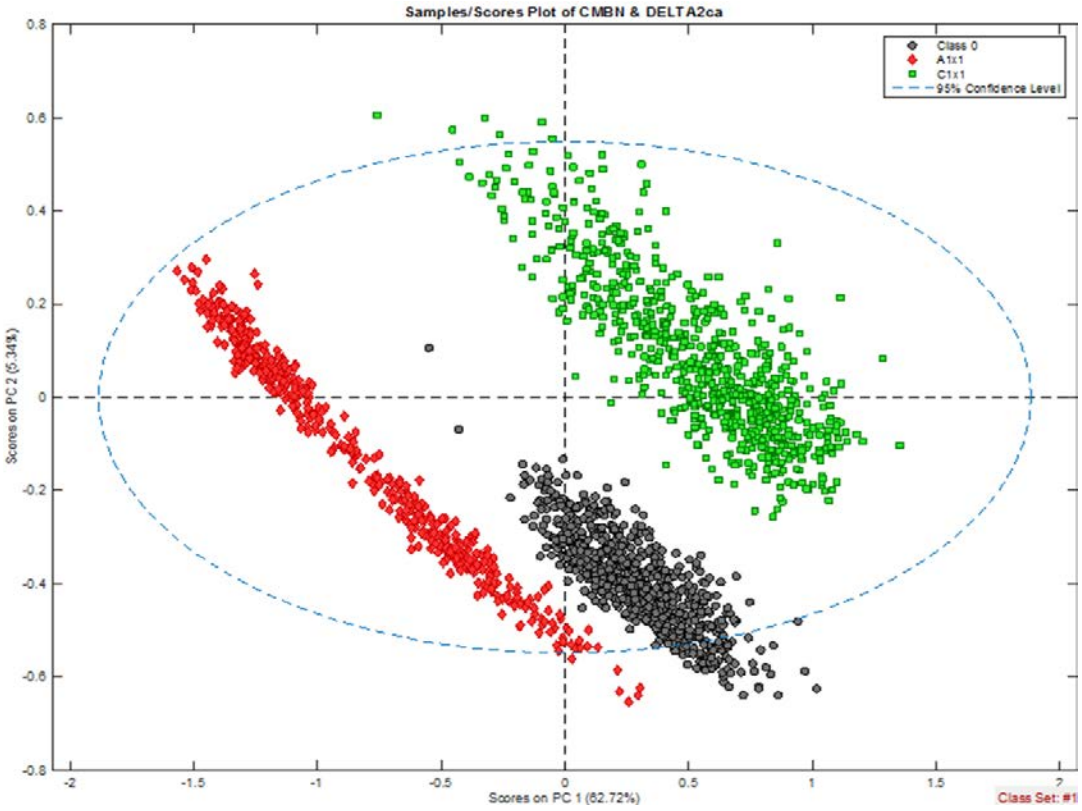


Figure 7. PCA plot of processed data acquired from H-Canyon Separation Facility

1.4 APPLICATIONS TO PROCESS MONITORING

Advances in process monitoring (PM) can be useful for advanced nuclear material accounting and control of advanced nuclear fuel cycles, particularly aqueous and electrochemical processing facilities. PM needs are of particular interest for electrochemical processing because of limited ability to apply nuclear material accountancy (NMA) techniques that are used for aqueous processing. In the following, additional insightful remarks about PM developed in earlier work (Burr et al., 2012) are provided.

PM is not a new technique and is currently used by the IAEA in many types of facilities where it provides added assurance to accountancy verification measure and/or aids in the early detection of misuse of a process or facility. The NRC employs PM trend analysis. A variety of data sources from either independent or shared monitoring systems is used. These data sources include flow rates, temperatures, pressures, volumes, acidity, voltage, electrical current, concentration, mass, reactant volumes and concentration, off-gasses, container item identification, and radiation. Some of the specific uses for PM data include:

- Continuity of knowledge of nuclear material flows and inventories and of design information verification results;
- Portal monitors for storage;
- Thermal power monitors for large research reactors;
- Monitoring of uranium enrichment levels;
- Determination of in-process hold-ups and non-measureable inventories;
- Added assurance to high uncertainty accountancy and timeliness measurements;
- Optimization of inspection and/or measurement/sampling plans;
- Measurement data needed anytime/on demand, such as for electronic mailboxes for short notice random inspections;
- Support to near-real-time-accountancy (NRTA) methods and evaluations;
- Timely detection of process disruptions or equipment mal-functions;
- Assurance that operations are as declared; and
- Reduction of on-site inspector presence (inspection effort).

The following technical issues impact the effective and efficient implementation of PM as a safeguards technique and will need to be addressed with further development work:

- Authentication of monitoring data originating from the operator’s systems;
- Volume of data acquired (probably will perform data processing and reduction on-site);
- Security of data transmission;
- Development costs (e.g., evaluation software, sensors, and data collection and storage);
- Minimization of operating and maintenance costs;
- Protection of confidentiality of proprietary or sensitive data;
- Need for independent conclusion capabilities, particularly when sharing data with the operator;
- Resolution of the question of qualitative assessments vs quantitative results in the facility safeguards effectiveness evaluation;
- Possibility of automated declaration (legal obligations); and

- Validation/benchmarking of simulation models.

Under MPACT, electrochemical processing will be used as an initial example to help define R&D technology requirements to reduce the risk for specific acquisition/diversion paths through the use of nuclear material accountancy (NMA) and process monitoring (PM). NMA and PM have been identified as tools to assess acquisition/diversion path risk consistent with classic domestic material control and accountancy (MC&A) and international [i.e., International Atomic Energy Agency (IAEA)] safeguards. R&D technology requirements will consist of (1) radiation signature maps for electrochemical processing unit operations of interest (e.g., electrorefining, salt distillation, etc.); (2) an NMA standard error in the inventory difference (SEID) model; and (3) a model to combine NMA and PM, all to aid in estimating acquisition/diversion path detection probability (Burr et al., 2015). These R&D requirements can then be used to aid in sensor/instrument development and design which can be deployed to reduce acquisition/diversion path risk.

NMA will be used to calculate the standard error in the inventory difference (SEID) (defined by the NRC)/SIGMA-MUF (defined by the IAEA) for which quantitative requirements have been set by the NRC and IAEA. Process monitoring (PM) is used as an additional NMA measure for which quantitative requirements have not necessarily been set by the NRC and IAEA, with the exception of trend analysis for the NRC. PM is less quantitative than NMA with regards to requirements, which leaves much greater creative space for new approaches and consequent R&D.

1.5 GAPS OR NEEDS AND PATH FORWARD

Deficiency	**Importance**	**Path Forward**
Models of UNF assemblies	Neither enough fidelity in the distribution of nuclides throughout the assembly nor in the structural elements of the assembly to truly say what is happening within an actual assembly	
Source terms for neutron and gamma radiation	Initial review suggests the source terms are provided for the assembly. Also energy spectra are essentially the same for each burnup suggesting simple renormalization has been done.	Pin-by-pin source terms are needed to improve fidelity and detailed spectra are needed for each model.

Burnup data for models	Models of used fuel with burnup from 25 GWd/MTU through 50 GWd/MTU with increments between that at least on the 0.25 GWd/MTU level in the lower part of the range and no more than 1 GWd/MTU at the higher end.	Production of neutron and gamma sources for isotopic inventories.
Interfaces with existing UNF databases	Development and provision of interfaces and database content will enable the creation of a more representative set for use in simulation of new techniques.	
Interface between MCNP6 and an Echem code	An Echem code is needed to provide isotopic and material-density data to MCNP6 for stipulated electrorefining and pyroprocessing conditions.	Discussions with ANL and INL continue. The ERAD code has been acquired from Korea.
Examination of Echem code attributes	Codes need to be assessed to understand capabilities and limitations	At least four new Echem codes are under development, including DyER and AMPERE at ANL, MASTERS at INL, and ERAD in Korea, all of which will need to be assessed.
Measured radiation data (gamma and neutron) for code validation	Code validation using experimental data is critical for benchmarking credibility.	Discussions with program management as well as ANL and INL personnel continue.
Development of detector mockups, especially MCNP6 detector models	The modeling should be as realistic as possible.	Development requires coordination with instrumentation and PM experts
Information exchange pathways between MCNP6 radiation data, instrumentation designers, and process monitoring assessors	All parties involved in design and monitoring activities need to send and receive required information.	Continue the preliminary discussions with ANL, INL, SNL, and LANL personnel.
Additional development of basic radiation-transport tools	Much of the development has been completed, but detector tallies may be simplistic and adjunct codes may be lacking or untested, which is especially true of electrochemical processing codes now under development and testing.	One or more of these codes will be needed to supply data to MCNP6 for electrochemical processing radiation-transport simulations.

Development of a scintillation light response matrix	Once the SLRM is known, the total response matrix (kinematic and scintillation) will be known. It will then be possible to correctly unfold a measured neutron spectrum to infer the incident spectrum. This effort may entail theoretical development, which could entail interfacing with experts in theoretical physics and materials behavior. If a suitable theoretical formulation can be developed, it could be suitable for MCNP-PoliMi implementation and necessitate interactions with MCNP code developers. Experimental validation will be required.	If a suitable theoretical formulation can be developed, it could be suitable for MCNP-PoliMi implementation and necessitate interactions with MCNP code developers.
Development of the new MCNP6 moving-objects capability tailored to Echem applications with moving radiation sources and dynamic radiation signatures.	This is an important effort that will enable the assessment of nominal and abnormal conditions for a variety of applications, and will have uses other than Echem.	Continue MCNP6 code development, and the creation and evaluation of models in consultation with facility experts.
Development of MCNP6 processing unit models within a pyroprocessing facility.	Radiation emission from the electrorefiner and procession units for the uranium cathode, TRUs, hulls, and salt will contribute to the radiation environment throughout a facility.	Initial crude models have been developed. Continue to develop more detailed models of the processing units using specifications from the literature and in consultation with ANL and INL.
Modeling radiation signals for TRUs self-irradiation.	TRUs emit neutrons, which will induce fission and add to the neutron and gamma radiation fields.	Develop models and assess the impact of the self-irradiation effect.
Investigate and discover new delayed-gamma activity ratios (DGARs).	MPACT studies performed during FY14-FY16 suggest that these quantities have potential merit for inferring quantities such as plutonium content using measured radiation.	Develop models inclusive of data mining.
Develop analytic DGAR assessments to augment and	MCNP6 yields DG data which can be used to form DGARs.	Continue development that was started in 2014 when time and

underpin MCNP6 assessments, including extension to nonlinear regimes.	The underlying physics that causes the DGAR structure is masked. This physics needs to be understood so that DGAR information can be used to infer quantities such as Pu content.	funding permit.
Develop multi-DGAR/neutron signal monitoring schemes for inference applications.	The use of multiple radiation signals, as well as other signals, should enhance the ability to infer quantities such as Pu content.	This work will include interfacing with statistics experts.
Study signal dependence on variable irradiation history.	Variations in irradiation history will impact isotopic production and, hence, radiation emission.	MCNP6 can be used to do this analysis. Modeling has yet to be performed.
Upgrade the MCNP6 delayed-gamma cumulative distribution sampling function integration scheme from trapezoidal rule to analytic.	This is an important upgrade that will eliminate issues associated with predicted peak height and enhance the predicted delayed-gamma activity ratio.	The theoretical development for CINDER should be applicable. This effort will require MCNP6 code modifications.
Development the capability to simultaneously measure the neutron and gross gamma counting rates using the boron-lined parallel-plate detector	The dual capability might be useful for both safeguards and PM related to the ratio of actinides and fission products.	Conduct modeling efforts, and use results to do detector development.

2 PROCESS AND CHEMICAL MODELS

2.1 INTRODUCTION

Process and chemical models are at the facility level and are used for the overall design of unit operations, safeguards, and security. Much of the data from instrument and unit operation models can feed into the facility models, but the facility models may also inform the codes/capabilities described in the previous section. The process and chemical models provide key safeguards and security metrics that are used to compare approaches and identify gaps in safeguards and security design. Process and chemistry models can be roughly divided among three major groupings based on the time- and length-scales of the key dimensional parameters, and the complexity or resolution required in the equations that define the system: fundamental models, process models, and facility models. Length and time scales can span nanometers and fractions of seconds for molecular-level interactions to meters and days for facility-level operations. Fundamental models are generally characterized by very fine length scales and high complexity. Among the codes in this group are computational fluid dynamics, nucleation and growth models, and codes that capture nuclear processes (decay, radiation, and material properties). These fundamental models can inform longer length-scale process and facility codes including safeguards modeling and process chemistry, but their complexity results in long calculation times or the use of high-performance computing, limiting their suitability for deployment for distributed systems, as those that characterize nuclear facilities.

Codes that are more suitable for the scale of the unit operations that define the functions within a facility can commonly be described as process models. These are generally comprised of simplified mathematical expressions that describe the physical or chemical conditions or processes, or combination of processes that describe a system. The equations and constraints may capture the chemistry, the temperature distribution, the dimensions or shape of an apparatus, or other factors that define the unit operation. The details and required fidelity ultimately depend on the resolution required in the solution for a given application but are often confined by the quality and comprehensiveness of the available data used to build the model, and the suitability of the set of equations for obtaining a mathematical solution. Process models are essentially zero dimensional since the chemistry and relationships do not depend on the physical size or positioning of the equipment.

Facility models can consist of an integrated set of simplified process models that are linked by chemical streams—that is datasets that describe the chemical and physical state of process - outputs or inputs. These may include models used for overall plant design and process control and models used for safeguards or security analyses. Generally, the chemical models that comprise a facility code are simpler than individual stand-alone process models. This difference in complexity between model scales can arise because stand-alone process models tend to exhibit the significantly higher computational time and mathematical complexity of non-linear systems, but quite often the difference is due to limitations in data that result in a mismatch of model fidelity among operations. Systems models, which are often used for optimization and control, rely on simple mathematical relationships between processes (the processes themselves are defined by simple expressions), and feedback loops are handled readily. Safeguards models fall under this category. Because systems models are intended for defining responses to triggers, the

codes are inherently well-suited to sets of time-varying operations. Facility models can also be applied to broader facility functions, such as security applications, that integrate the movements of personnel into the physical plant. Such codes assign decision logic to dynamic actors (humans) based on a probabilistic assessment of the conditions at the facility.

A key factor includes whether the models are designed for steady-state or dynamic systems. Steady-state process models tend to employ calculated or measured thermodynamic parameters and equilibrium data, and therefore are more amenable to predictive solutions where experimental data may be unavailable for the conditions of interest. However, steady state codes do not capture transitory behavior or highly variable systems that are often the focus of safeguards, process monitoring, and response. Dynamic codes specifically cover transient or time-varying systems which are required for more detailed process, safeguards, and security modeling.

2.2 CODES/TOOLS AND THEIR USAGES

Several applications of modeling and simulation require facility-level models to complete assessments at the systems level. This is needed for overall safeguards and security analyses as well as process control to evaluate performance. In many cases, the modeling capabilities presented in other sections throughout the report can either provide inputs for the facility-level models, or be directly integrated into the facility-level models. The following sections describe the various codes/tools, interfaces, gaps or needs, and path forward.

2.2.1 AMUSE

The Argonne Model for Universal Solvent Extraction (AMUSE) is a computer application that simulates steady-state multi-stage counter-current solvent extraction processes for species of interest to used nuclear fuel reprocessing and radioactive waste treatment (Pereira et al., 2013). The original code (ssAMUSE) was developed to run in Microsoft Excel and is comprised of two major sections. SASSE (Spreadsheet Algorithm for Stagewise Solvent Extraction) is a steady-state mass balance calculator. SASPE (Stagewise Algorithm for Speciation and Partitioning Equilibrium) calculates the equilibrated distribution of species between the organic and aqueous phases (D-values). It contains all of the chemical equations required to perform the calculations. In combination these calculators simulate the steady-state chemical behavior for a user-defined extraction process flowsheet. The library of component data includes over fifty species common to nuclear fuel that are supported with thermodynamic data for several different extraction systems. Figure 8 shows the AMUSE code structure.

The original code has been rewritten in new, more extensible formats to allow relatively easier revision of existing extraction models and inclusion of additional extraction processes. The Fortran version (fssAMUSE) simplifies addition of new species and enables formal standardization of the equations describing the equilibrium chemistry. Required fixed data are fully separated from the underlying program, allowing users to provide new chemistry parameters without changing the internals of the code. The use of data tables and modularized

routines is not possible in Excel. The Fortran version was originally developed to allow better integration with external codes, notably Aspen Technologies' Aspen Custom Modeler® (ACM®) chemical process design software.

The MATLAB® version (dyAMUSE) was developed specifically to simulate process dynamics. Major components of this version include a differential mass transfer term, a description of interstage flowrates, and a rate-based reaction scheme for plutonium reduction. A dynamic representation allows for examination of start-up conditions as well as possible transients due to disturbances. Several non-equilibrium behaviors have been simulated, which should allow for improved process monitoring and prediction of response to disturbances.

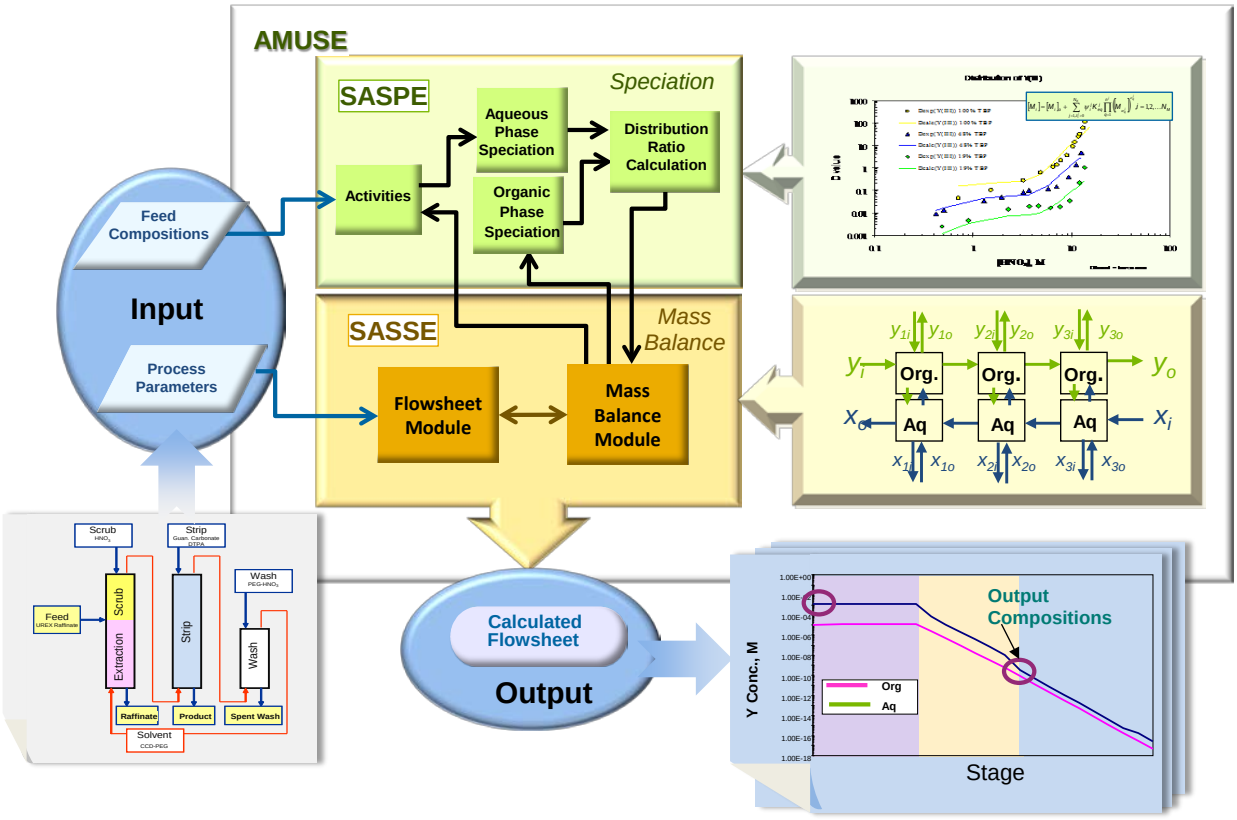


Figure 8. Schematic outlining the AMUSE code structure

2.2.2 AMPYRE

AMPYRE is a flexible mass-balance flowsheet model for metal fuel that dynamically tracks material on a batch-by-batch basis within electrochemical processing facility. Mass balance is achieved by predicting a chemistry-based evolution of the salt, product, and waste compositions in each principle operation of the pyroprocessing flowsheet. The chemical process functions that comprise the flowsheet are configured to capture interdependencies to accurately reflect the

evolution of the state of the physical system. Material is tracked by element as it is converted from one form to another, for instance, from metal to chloride, and as it is physically moved from one operation to the next. Users have the flexibility to specify any ratio of lithium chloride to potassium chloride in the electrolyte, as well as the presence of other soluble species at the start of a simulation. Users also specify the fuel composition, and a set of parameters related to the overall plant operation including: recovery efficiencies, product purities, adhered salt fractions, salt composition targets, and material behavior in transfer operations. After completion of a run, a new scenario with different operational parameters can be initiated with the previous electrorefiner salt composition; the model will adjust and the system will proceed toward a steady state for the new conditions. Figure 9 shows the major unit operations captured with AMPYRE.

All isotopes of an element are assumed to exhibit identical chemical behavior within the system, and changes in material quantities or chemical behavior due to radioactive decay are not currently included. While the model achieves mass balance for each batch processed, the system does not achieve steady state until the amount of material entering the electrorefiner in the fuel and fresh makeup salt is balanced by the material exiting the system as products and waste. The code runs in Microsoft Excel 2010 under the Windows operating system, using Visual Basic for Applications (VBA) to automate the iterative calculations and perform preliminary data processing steps.

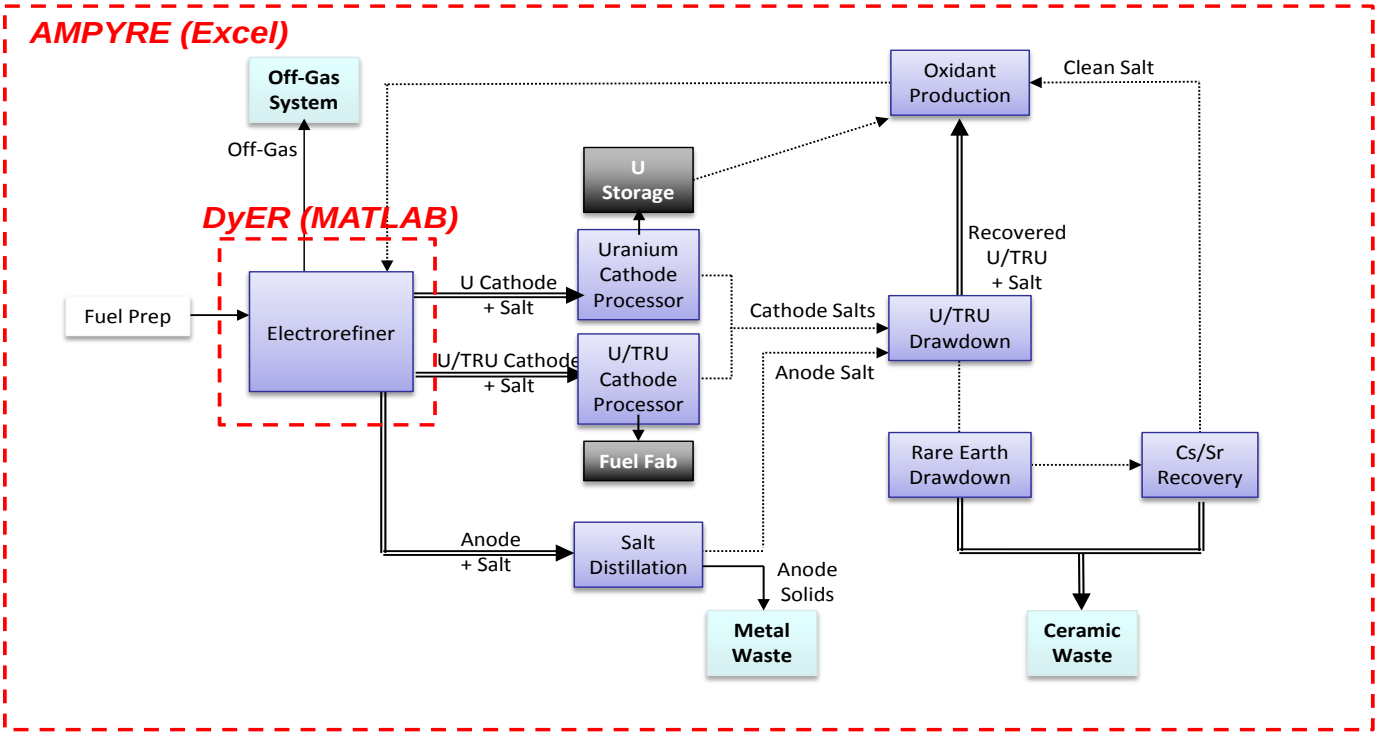


Figure 9. Schematic showing the major unit operations captured in AMPYRE, as well as the interrelation between the AMPYRE and DyER codes

2.2.3 Dynamic Electrorefiner (DyER)

DyEr (Dynamic Electrorefining) simulates the movement of material among the anode, cathode, and salt within an electrorefiner as used fuel is processed into metallic products for recycle or storage. DyER employs chemical expressions derived from fundamental kinetics and thermodynamics for electrochemical processes, and system-specific chemical data developed at Argonne, to produce time-dependent simulations of the electrorefiner operation. Because partial ionic currents (i.e, molar flow rates) are heavily dependent on concentrations, a dynamic model is the most accurate way to calculate real-time compositions and throughputs. The electrorefiner salt can be modeled with either a eutectic mixture of LiCl and KCl at 500°C, or with LiCl at 650°C, with thermodynamic parameters adjusted accordingly. Operationally, used nuclear fuel of a known composition is placed at an anode that is connected with a combination of cathodes at which product is accumulated as fuel is dissolved. At one set of cathodes, a metallic product consisting of essentially pure uranium is collected. At a second set of cathodes, a metallic product consisting of a mixture of transuranic elements and uranium is collected. A potential applied across the system initiates the dissolution of the used fuel and deposition of material onto the cathodes. The electrorefiner simulation is operated in a semi-batch mode with fuel and oxidant added in fixed amounts and cathode products harvested in bulk at single points in time, while the fuel is refined continuously over an extended period. A batch is said to reach "conclusion" when the fuel in the electrorefiner is depleted by a user-defined threshold amount. The model output can be used to predict the changes in transient behavior due to changes in operations or input compositions. The code output can be interfaced directly with AMPYRE to provide a more rigorous simulation of the composition of the products generated in the electrorefiner for a set of user-defined operation conditions, and the overall mass balance in the facility. The code was written in MATLAB, and input parameters can be input directly by the user or imported directly from Excel spreadsheets. The DyER user interface and example results are shown in Figure 10.

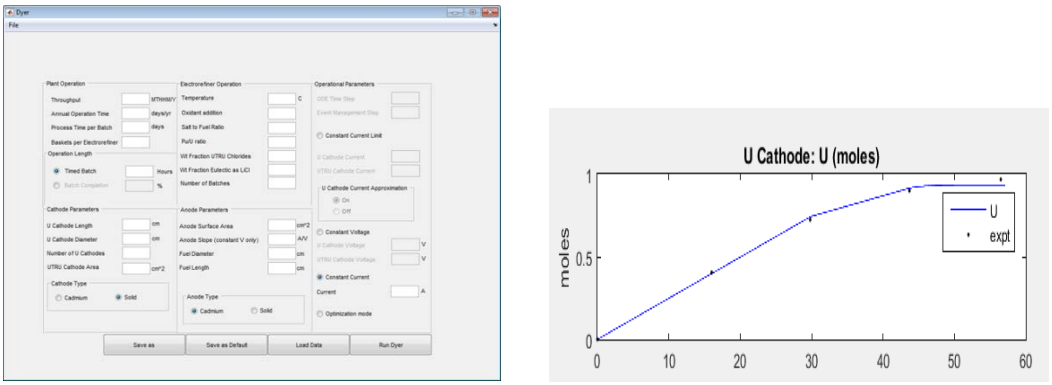


Figure 10. DyER graphical user interface showing some of the user-defined input parameters and example showing deposition of uranium on a cathode over time.

2.2.4 Separation and Safeguards Performance Model (SSPM)

The SSPM is a transient MATLAB Simulink model that tracks elemental and bulk material flow through a reprocessing plant for safeguards design and analysis (Cipiti, 2012). Various versions

of the model exist for aqueous (PUREX and UREX+) and electrochemical reprocessing. The base of the model simulates unit operations including separation of materials and process vessel inventories. Both bulk and materials accountancy measurements are simulated throughout the plant with user-defined measurement uncertainties. These measurements are used to calculate an inventory difference over a specific material balance period as the model runs. Statistical tests are used to set alarm conditions for detecting material loss.

Figure 11 shows an electrochemical version of the SSPM in Simulink. The gray blocks represent the unit operations, and the signals connecting them contain the mass flow information. A great deal of detail is included in each of the unit operation blocks to control vessel filling and emptying, separation fractions, timing sequences, and control switches. Elements 1-99 are tracked along with the bulk materials (salt in the case of pyroprocessing). Chemistry is not modeled unless it has been integrated from another code.

The blue blocks represent accountancy measurements that may be taken throughout the plant. The simulated measurements are fed into a monitoring subsystem that contains all the calculations necessary for the Material Unaccounted For (MUF), cumulative sum (CuSum) MUF, standard error of the MUF (σ_{MUF}), and statistical tests for setting alarms. The model also contains the ability to model diversion scenarios to examine how the safeguards system will respond. Recent work has examined more use of bulk process monitoring data with the overall safeguards balance.

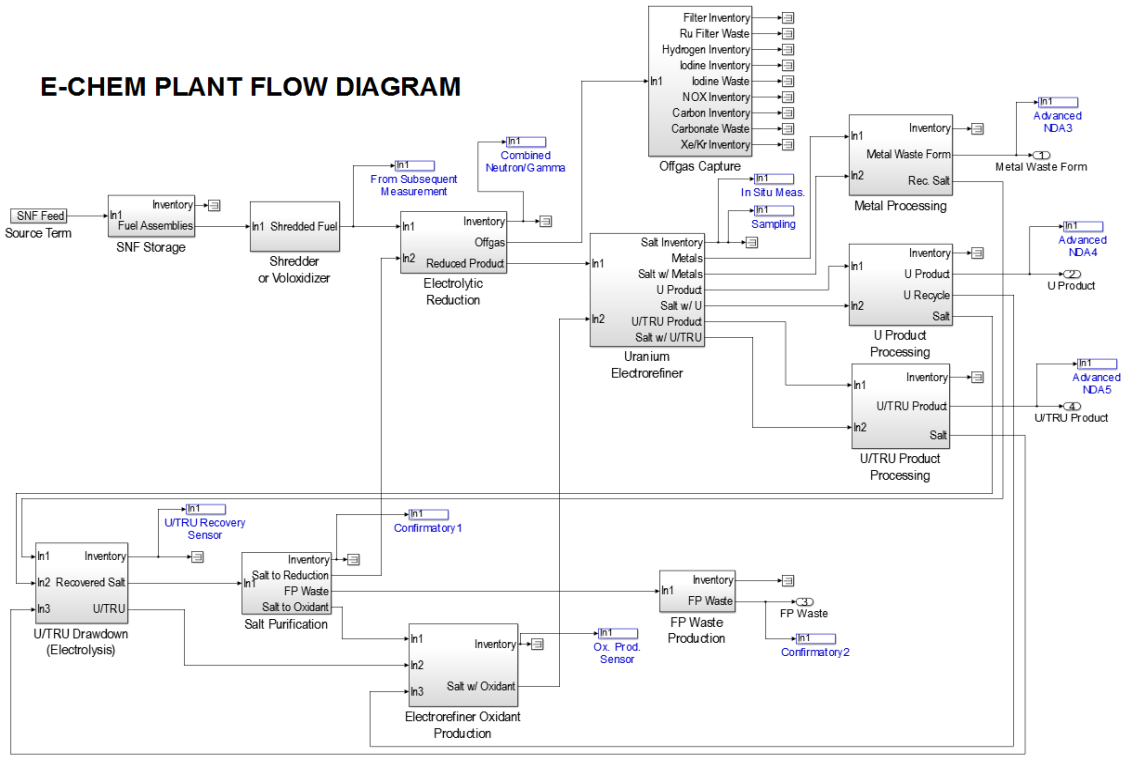
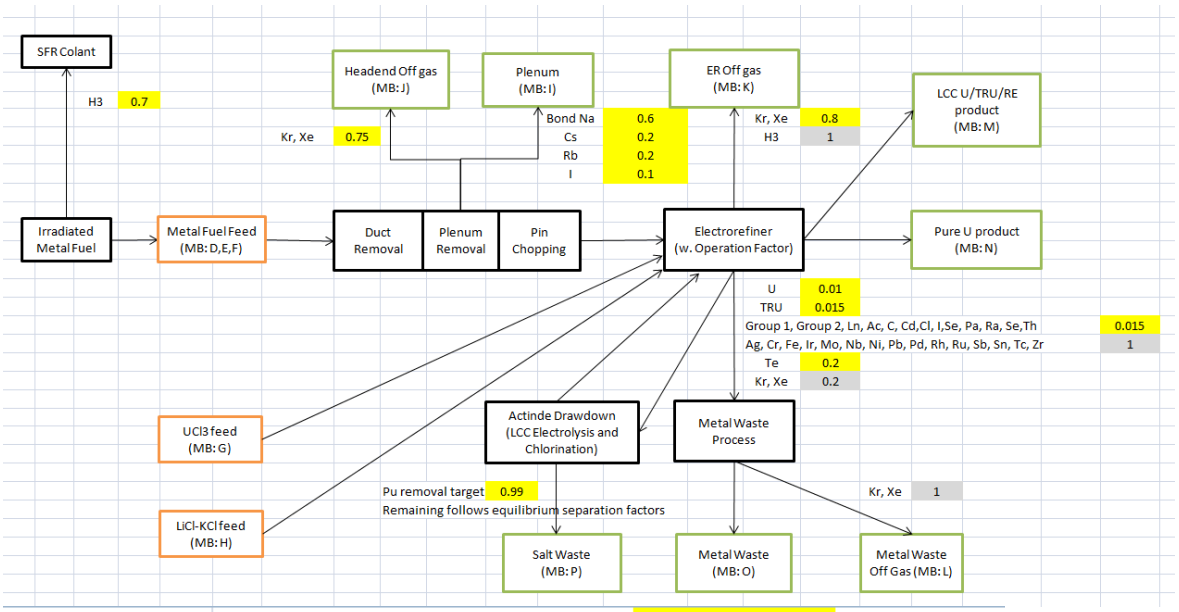


Figure 11. Electrochemical SSPM

2.2.5 MASTERS: Modeling and Simulation Tool for Electrochemical Recycling System

The Idaho National Laboratory (INL) has developed the batch model software based on MATLAB and used extensively for planning purposes for various missions including the EBR-II and the Joint Fuel Cycle Study (JFCS). The developed software aims to simulate various electrochemical recycling system flowsheets. A notable recent addition is a spreadsheet user-interface with Microsoft Office Excel supported by the Fuel Cycle Research and Development (FCR&D) campaign (Yoo, 2015). The addition of the spreadsheet user interface has allowed an easy distribution of the simulation software. This continuing development effort for the simulation tool for electrochemical recycling system is called MASTERS.

The electrorefining process model implemented in MASTERS calculates changes in molten salt electrolyte compositions in the electrorefiner (ER) unit as batches of fuel are treated. MASTERS also relies on domain expertise inputs provided via the user interface. The user also can specify the fraction of undissolved active metals excluding transuranics. The current version of MASTERS assumes all noble metals (Ag, Cr, Fe, etc.) are retained in the anode and report to the metal waste process. Also implemented in MASTERS are selected operational constraints coming from the physical cell size and the criticality related constraints induced by the fissile materials, which are adjustable. This feature allows the user to assess the impact of its physical cell design and criticality consideration to the performance of the flowsheet. Figure 12 gives the snapshot of MASTERS user-input interface. The yellow highlights represent the parameters the user can adjust.



Electrorefiner	Initial salt mass	500	kg
Electrorefiner	Minimum salt mass	350	kg
Electrorefiner	Maximum salt mass	700	kg
Electrorefiner	Initial U3+ concentration (w%)	5	w%
Electrorefiner	Minimum U3+ concentration (w%)	1.5	w%
Electrorefiner	Maximum U3+concentration (w%)	100	w%
Electrorefiner	Maximum fissile material mass	100000	kg
Electrorefiner	Maximum Pu3+ equivalent mass	50	kg
Electrorefiner	Minimal Pu3+/U3+ to initiate TRU recovery	3	
Electrorefiner	Anode Batch Size (HM)	10	kg
Electrorefiner	Minimal LiCl-KCl mass (w%)	70	w%
Electrorefiner	Number of batches	1000	batches
Electrorefiner	Disposed salt (w%)	10	%

Figure 12. Snapshot of the MASTERS user interface

In MASTERS, the key unit process models such as liquid cadmium cathode (LCC) and actinide drawdown processes use the reported thermodynamic separation factor in an effort to eliminate the dependency on the domain expert inputs for tracking the actinides and the lanthanides. For both processes, the product compositions are assumed to follow separation factors of under-saturated cadmium pool equilibrated with the salt. The composition was calculated numerically with a customized search algorithm designed to solve the liquid cadmium/salt equilibrium problem specifically.

MASTERS provides a summary of material partition among various output streams after processing the user-provided number of anode batches. Figure 13 is the snapshot of the material stream information summarized in the format of the flowsheet diagram. The actual isotopic inventories (> 1000 isotopes) tracking results are reported in the separated worksheet as shown in Fig.14.

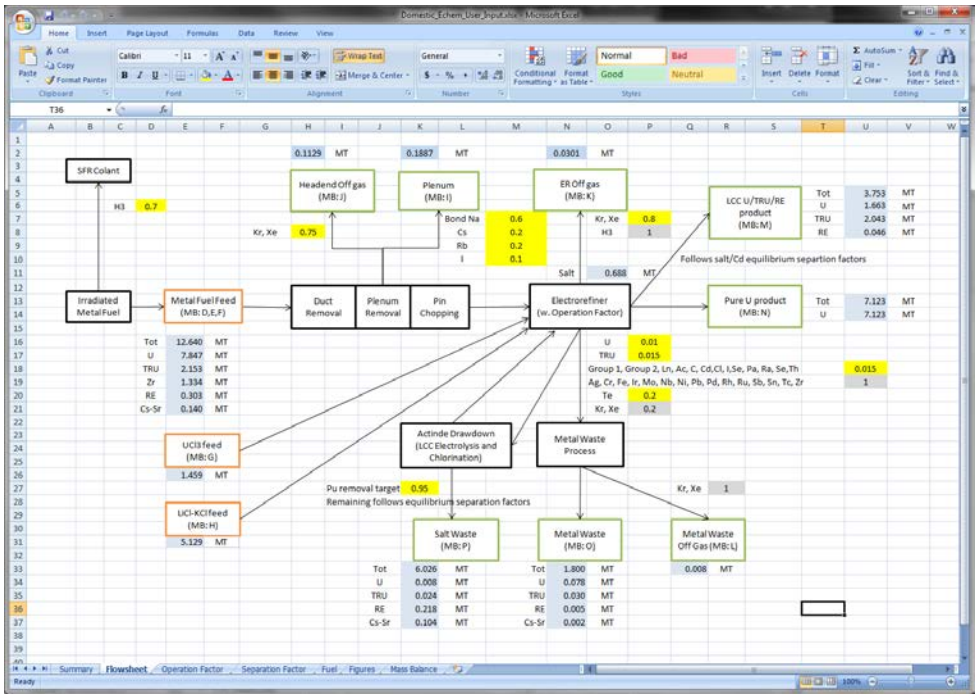


Figure 13: Input and output streams mass flow (Flowsheet Sheet)

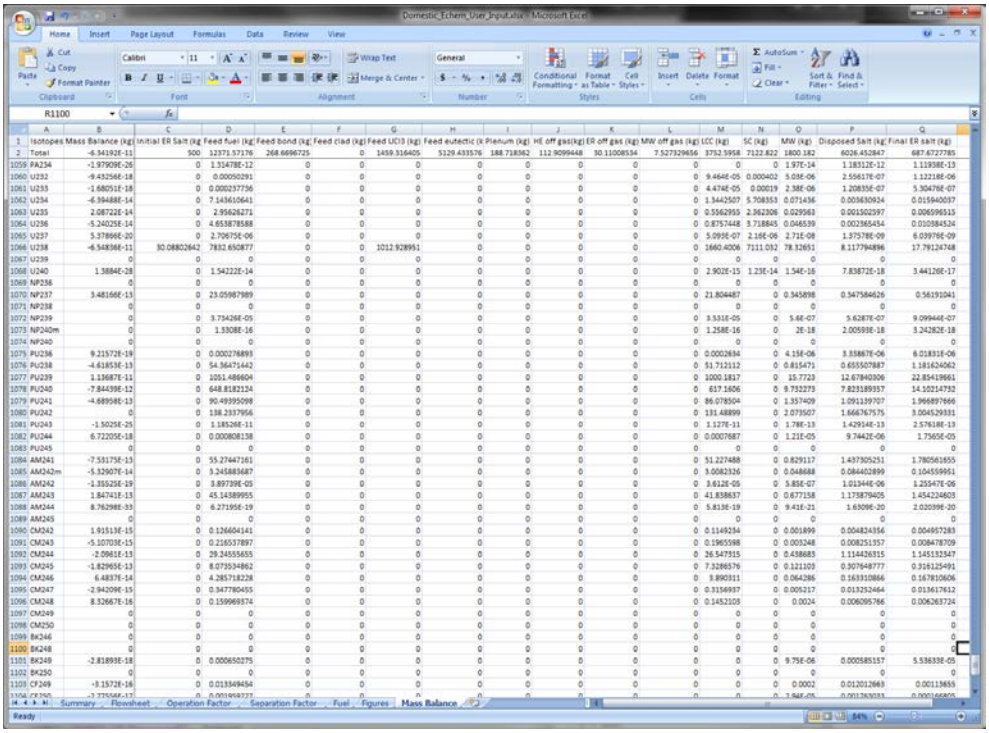


Figure 14: Isotope inventories for salt and input and output streams (Mass Balance Sheet)

2.2.6 PyFOM

The Pyrochemical Facility Operations Model (PyFOM) is an operations model that simulates the physical location and dimensions of unit operations within a pyrochemical reprocessing facility. The code was developed using ExtendSim software (Imagine That, Inc.). Process timing and sequencing of material transfers, as well as the required mechanical movements of cranes, robots, etc., are used to optimize the placement of the equipment and thus to optimize the facility layout, and identify where redesign may be required. Dimensions and time requirements for the various operations within an electrochemical facility are input by the user. The output was used to develop a 3-dimensional layout of a conceptual 100 MT/yr pyroprocessing facility (Figure 15). The code was used to better define the process flowsheet and equipment concepts. It was used to identify process bottlenecks which led to improvements in processing and equipment designs.

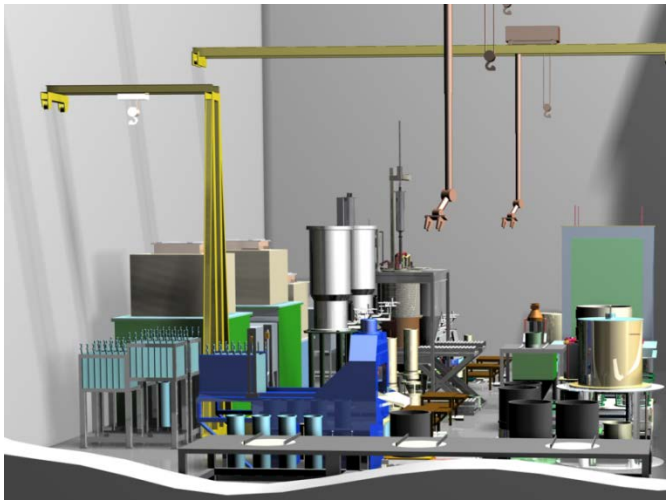


Figure 15. Conceptual 100 MT/yr pyroprocessing facility

2.2.7 Scenario Toolkit and Generation Environment (STAGE)

The STAGE (Scenario Toolkit and Generation Environment) commercial modeling and simulation software has been applied for a variety of security applications, particularly for force-on-force combat engagements for outside adversary attacks (Dominguez et al., 2012). STAGE has also been used to model insider diversion scenarios. One key advantage of STAGE is the ability to fully model a 3D environment, which means that specific safeguards and security scenarios can be modeled. Figure 16 shows both a 3D facility model and a bird's eye view of a facility using STAGE. STAGE contains a library of typical physical security elements (for example sensors, portal monitors, guard forces, etc.) It provides the following capabilities:

- Logic based behavior: Human entities model the ability to "make a decision" based on the current situations and partially controlled by probability analysis.

- Ground navigation: Humans and mobile equipment can dynamically find paths both inside and outside the facility. Sensing abilities possessed by the human entities enable visual detection of other humans and objects.
- Event-based entity missions: Help define the main thread and strategies of the scenarios.
- Scripting support: Provides the ability to integrate data from other codes.
- 2D/3D environment: Provides visual representation of the scenarios.

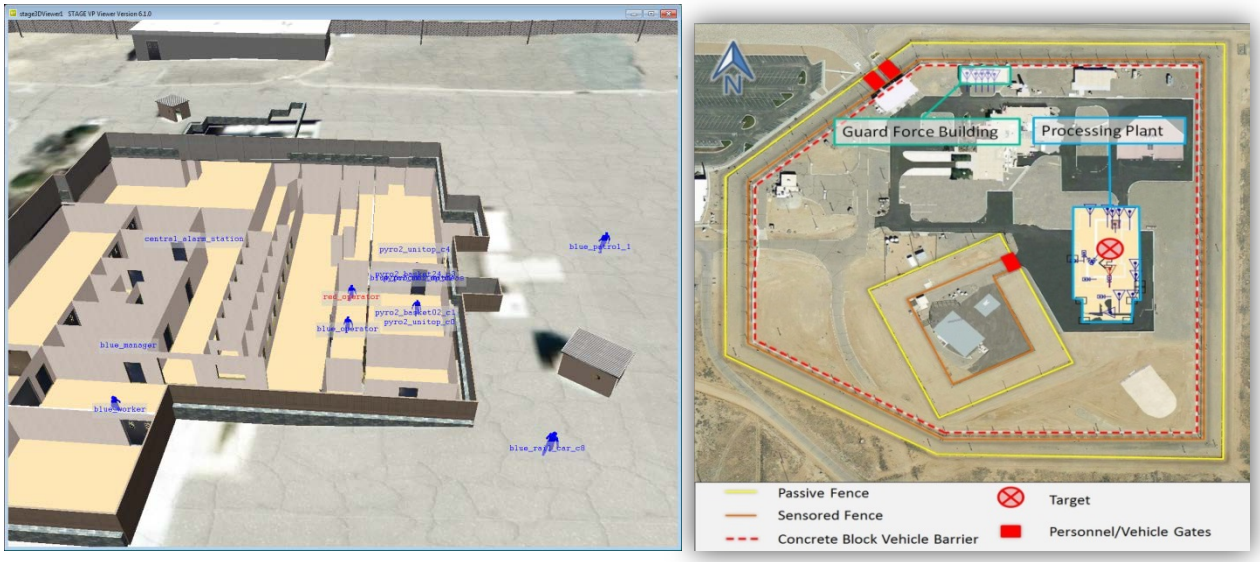


Figure 16. Example STAGE model

2.3 INTERFACES BETWEEN CODES

All of the modeling capabilities described above have individualized strengths and weaknesses for safeguards and security analyses. Together, they can form a robust platform for achieving the Virtual Test Bed. The goal of the Virtual Test Bed milestone is not to unify all codes under one master code. Rather, it seeks to determine how the codes can work together and where those interfaces exist. In some cases, integration of capabilities may be useful, but often just sharing data between codes is a more efficient solution.

The AMUSE and AMPYRE codes are used to develop flowsheets for aqueous and electrochemical processing, and they are based on chemistry modeling and mass balance. They model steady-state behavior. Their strengths are in determining a realistic flowsheet and appropriate process flows and inventories. In addition, they can be useful for examining process monitoring and how process upsets change the material flow. This is useful for distinguishing process upsets from material diversion. Unit operation models, like DyER, and codes like MASTERS can be used to compare for consistency.

The SSPM models the transient nature of the facilities at a higher level, but its main strength is in the design of the safeguards system and generating safeguards metrics (such as overall error and detection probability). It does not include chemistry modeling so is reliant on good assumptions for separation fractions. AMUSE, AMPYRE, and MASTERS can provide data to help improve the fidelity of the SSPM. Past work has already integrated part of the AMUSE code into the SSPM for aqueous plants (Cipiti, 2011). Integration can cause problems such as slowing the models down or requiring multiple licenses. Integration of specific data like an empirical relation would be more efficient. While the SSPM is tailored more for traditional material balances, AMUSE, AMPYRE, DyER, and MASTERS can be used to examine process monitoring and process upsets in more detail.

The STAGE model provides a 3D aspect to the modeling that helps with complete diversion scenario analysis (including the path out of the facility), and security scenario modeling. The PyFOM model can help with the 3D layout of STAGE. Past work has used the SSPM to generate safeguards data that can affect the behavior of the physical protection elements modeled in STAGE. This was a one-way transfer of data that was much more efficient than integrating codes, but it was more than adequate for meeting the modeling need.

In addition to the codes described here, other mod/sim tools can be integrated with these codes as well. Measurement models can be used to provide information about measurement uncertainty that can directly feed into the SSPM. Statistical modeling in the past has already been directly integrated into the SSPM to form the basis for the Page's test for detection material loss. Signatures mapping of the facility could be tied in with the 3D models and also has implications in the design of measurements in a facility.

2.4 GAPS OR NEEDS AND PATH FORWARD

Deficiency	**Importance**	**Path Forward**
Models for fuel fabrication facilities		Branching out to fuel cycle facilities in the back end including fuel fabrication
Limited data for many chemical components that play a key role in the electrorefining process		Validation of models and codes requires significant investment
Conversion of point (zero dimensional) facility models three dimensional representations	Critical to a comprehensive safeguards regime and a direct example of safeguards-by-design approach	
Detailed analysis of the uncertainty and error propagation in processing	There is already some analysis, but the more detailed analysis would allow for better understanding of the natural variability in processing impacts	

	the ability to better maintain a material balance	
Uncertainty quantification and error propagation		the evolution of measurement, material, and processing uncertainties should follow from the evolution of the chemical, and physical, state of the facility and the overall material balance
Optimal safeguards designs for electrochemical facilities	A near term research priority including the use of process monitoring measurements	
Basic accountancy measurements		Much experimental work required
Analysis of process upsets and how process monitoring information can be better utilized		Requires combination of statistical models (updated to take into account process monitoring data), DyER model (to examine process upsets and how measurement parameters can change), and empirical relations (developed to integrate into safeguards analysis from SSPM).
Robust safeguards by design study	Signature mapping can be used to help determine ideal plant layouts for the various NDA measurements required in the process.	Will be made possible by the improved modeling capabilities
		STAGE will continue to be developed to provide a platform for security and complete diversion scenario analyses.
Updated versions of past modeling work on aqueous plants	Much work has already been done on aqueous plants in MPACT program, and revisiting it could cover those capabilities for 2020 milestone	
Modeling of fuel fabrication facilities	Could be used to increase safeguards capabilities and security analyses for back end of the fuel cycle	Modeling capabilities need to stay up to date with experimental work in the Fuel Cycle Program

3 SECURITY ASSESSMENTS

3.1 INTRODUCTION

A range of modeling approaches may be used to evaluate the security, and conversely the vulnerability, of a site or system to a particular threat. First, consequence modeling, seeks to define a source term and the subsequent results of a successful sabotage event. This type of modeling generally uses shock physics and empirical data to estimate the amount and form of radiological material that is released to the environment from the threat scenario. Dispersion codes are then applied to determine the impact of the release at the site and downstream populaces and property. Second, force-on-force modeling allows site planners and operators to assess the effectiveness of various guard force and installation security configurations. These force-on-force simulations are useful in identifying potential security weak points and allow optimization of guard force logistics and tactics. Finally, risk-based scoring permits grading of the difficulty of various attack scenarios against a site. This type of analysis is useful in identifying and justifying potential security improvements.

3.2 SECURITY MODELING – CURRENT APPROACHES

Security modeling is based on evaluating the site response to a defined threat. This includes the response to acts of radiological sabotage and the ability of the security force to effectively react to the threat. The information needed for various modeling of these scenarios is listed below.

Modeling Inputs

1. ***Design basis threat (adversary characteristics)***
    a. Number of adversaries
    b. Allowable weapons
    c. Special tools and equipment
    d. Tactics and level of determination
        - Training and operational effectiveness
        - Skill levels for combat and special tasks
2. ***Site characteristics***
    a. Source quantity of SNF, or material at risk (MAR)
    b. Cask design
    c. Site security configuration
        - Access delay features

- Entry control points
- Vehicle barriers
- Layout of security buildings and systems

d. Definition of guard force
   - Number of guards
   - Weapons and mobility
   - Training and tactics

These inputs inform three different types of security modeling.

1. *Consequence modeling seeks to determine the radiological result of a successful sabotage event.*
2. *Force-on-force modeling examines the effectiveness of various guard force and installation security configurations against various adversary threats.*
3. *Risk-based scoring represents an attempt to assign a difficulty metric to each attack scenario against an assumed physical protection system for a given site.*

Security modeling is often conducted in independent, parallel evaluations. Integration of the different types of modeling serves to provide a more complete security assessment and allow for site optimization as shown Figure 17. The level of integration between current modeling thrusts remains minimal. As modeling progresses in the future, integration is expected to increase, especially as economics are considered more prominently among the figures of merit (FOM's).

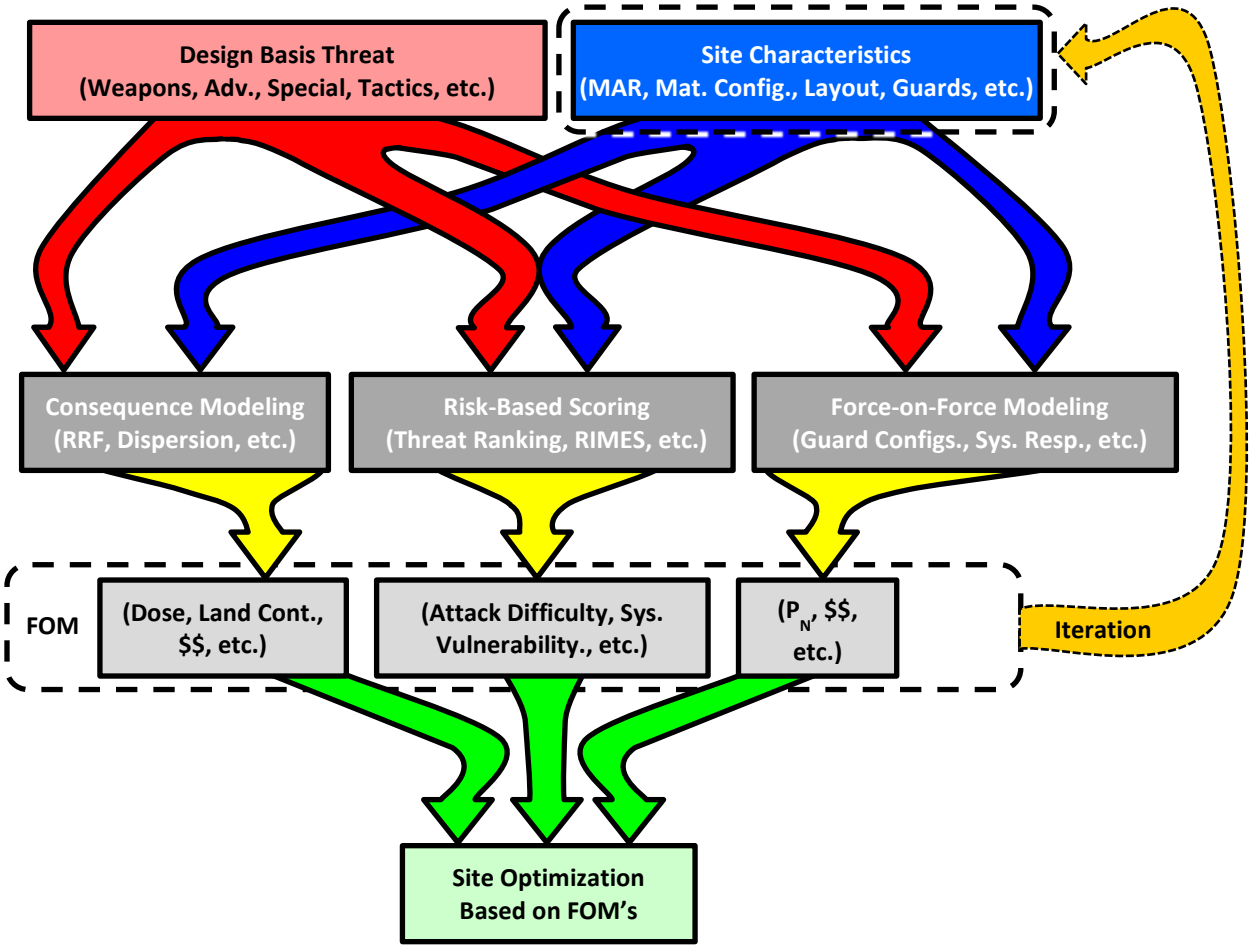


Figure 17. Site security optimization based on multiple modeling figures of merit

3.2.1 Consequence Modeling

Consequence modeling is focused on defining the source term from successful attack scenarios based on information about the cask construction and the adversary toolset and tactics from the design basis threat (DBT). The amount of the source term released, or the release fraction (RF), is determined using information from various integrated, large-scale and separate effects testing, in addition to shock physics modeling. These source terms are then inputted into dispersion codes to calculate different FOM's such as dose, land contamination, or estimated economic impact.

Several of the underlying calculations used to estimate the source term are significantly and inherently conservative. When dealing with spent nuclear fuel (SNF), prime among these calculations are 1) the estimate of the respirable release fraction (RRF) and 2) the spent fuel ratio (SFR). The RRF is estimated from a limited data set of fragmentation analysis of various materials. Previous interpretations of these data appear to have conservative assumptions that deserve reexamination because they likely do not represent the best-estimate RRF and instead portray an upper statistical bound. The SFR is an engineering construct that allows the scaling of results from large-scale sabotage testing with surrogate materials such as depleted uranium oxide

(DUO2) to the response of SNF. A SFR value of 3 is currently accepted for use in source term analyses, but previous data yields values ranging from 0.4 to 12 (Durbin, et al., 2016).

3.2.2 Force-on-Force Modeling

Force-on-force modeling explores the effectiveness of various guard force and installation security configurations against adversary threats using force-on-force simulations. These simulations estimate the probability of neutralization (P_N) of the threat, or conversely the probability of adversary success. Additional security measures such as changes to the guard force or site security layout can also be evaluated using a cost-benefit analysis.

3.2.3 Risk-Based Scoring

A third type of security modeling seeks to grade threats or vulnerabilities by incorporating the degree of difficulty and physical security performance into a risk-based prioritization scheme. The risk-informed management of enterprise security (RIMES) method surveys an expert panel to determine an aggregated metric for an adversary to successfully execute an attack against a site (Wyss, et al. 2013). This metric is assumed to be comparable to the relative difficulty of the attack scenario. By comparing the RIMES score with the consequence, potential deficiencies in the protection performance can be readily identified and corrected.

3.2.4 Site Security Reponses for Underground Storage Systems

From a security response and surveillance standpoint a significant design advantage of a belowground ISF installation is the limited height of the cask lid to provide full cover for adversaries. This design aspect allows the security force to better evaluate an intruder alarm and more accurately determine the scope of the intrusion.

3.3 GAPS OR NEEDS AND PATH FORWARD

Deficiency	Importance	Path Forward
Optimization of physical protection systems for facilities with a broad range of fuel handling capabilities		Requires convergence of several disparate modeling streams and feasibly conflicting optimums. Most obvious means to incorporate and compare information is by assigning economic values to as many variables as possible, allowing for cost-benefit analyses and site optimization as an integrated

		system.
More accurate source term estimate	Would improve the technical basis for licensing and regulation of any facility storing or processing SNF. With the method of calculations, conservativisms for the source term are multiplicative.	
Limited RRF data	Underlying historical data is especially limited for spent fuel samples	
Data using high burnup spent fuel and better aerosol sampling methods	This new data could potentially produce high quality data with reduced scatter. Coupled with shock physics modeling this data could also improve understanding of SFR if DUO_2 samples are also tested	
Error propagation analysis of original experiments that created the data	Would be of additional benefit when used in conjunction with a best-estimate of a source term with statistically defensible uncertainties to portray maximum amount of information	Can be used to evaluate if scatter in data can be attributed to experimental errors, whether some correction in the data is warranted, and what improvements in experimental techniques can be suggested for future testing.
Presentation of a best-estimate RRF with bases	Reduced uncertainty and conservatism in RRF could reduce any associated controlled or exclusion area based on dose-at-distance criteria.	
Evaluation of physical response of an underground storage cask to a DBT-based attack	Analysis needs to be conducted in order to fairly gauge merits of aboveground and belowground storage systems.	If a belowground system offers a more favorable response to DBT, an ISF using belowground storage may enjoy lower life cycle costs.
Evaluation of various non-lethal technologies using force-on-force simulations	May reveal significant benefits as they may extend an adversary's timeline to allow for more effective security response. Some of these technologies may be less useful aboveground than belowground.	

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ACRONYMS

ACM	Aspen Custom Modeler®
AMPYRE	Argonne Model for Pyrochemical Recycling code
AMUSE	Argonne Model for Universal Solvent Extraction
ANL	Argonne National Laboratory
CEA	French Alternative Energies and Atomic Energy Commission
CERN	European Organization for Nuclear Research
CINDER	MCNP6 isotopic transmutation code
CuSum	Cumulative Sum
DBT	Design Basis Threat
DG	Delayed Gamma
DOE	Department of Energy
DOE-NE	Department of Energy Office of Nuclear Energy
DSC	Dry-Storage Cask
dyAMUSE	MATLAB® version of Argonne Model for Universal Solvent Extraction
DyER	Dynamic Electrorefiner code written by ANL
Echem	Electrochemical
ER	Electrorefiner
FCR&D	Fuel Cycle Research & Development
FOM	Figures Of Merit
fssAMUSE	Fortran version of Argonne Model for Universal Solvent Extraction code
FY	Fiscal-Year
IAEA	International Atomic Energy Agency

IFEL	Irradiated Fuels Examination Laboratory
ISFSI	Independent Spent Fuel Storage Installations
INL	Idaho National Laboratory
JFCS	Joint Fuel Cycle Study
LANL	Los Alamos National Laboratory
LCC	Liquid Cadmium Cathode
LIBS	Laser-Induced Breakdown Spectroscopy
LLNL	Lawrence Livermore National Laboratory
M&S	Modeling and Simulation
MAR	Material At Risk
Mark-IV	INL Mark-IV electrorefiner
MASTERS	Modeling and Simulation Tool for Electrochemical Recycling System
MC&A	Material Control and Accountancy
MCNP6	Los Alamos Monte Carlo radiation-transport code
MIP	Multi-Isotope Process
MIT	Massachusetts Institute of Technology
MPACT	Material Protection, Accounting and Control Technologies
MPI	Message Passing Interface
MUF	Material Unaccounted For
NDA	Nondestructive Assay
NGSI	Next Generation Safeguards Initiative
NLT	Near-Real-Time
NMA	Nuclear Material Accountancy

ORNL	Oak Ridge National Laboratory
PCA	Principal Component Analysis
PEER	INL Planar Electrode ElectroRefiner
PM	Process Monitoring
PNNL	Pacific Northwest National Laboratory
pyFOM	Pyrochemical Facility Operations Model
R&D	Research and Development
RIMES	Risk-Informed Management of Enterprise Security
RF	Release Fraction
RRF	Respirable Release Fraction
SASPE	Stagewise Algorithm for Speciation and Partitioning Equilibrium
SASSE	Spreadsheet Algorithm for Stagewise Solvent Extraction
SEID	Standard Error in the Inventory Difference
SFR	Spent Fuel Ratio
SLAC	Stanford Linear Accelerator Center
SNF	Spent Nuclear Fuel
ssAMUSE	Original Argonne Model for Universal Solvent Extraction code
SSPM	Separation and Safeguards Performance
STAGE	Scenario Toolkit and Generation Environment
TCATH	TRUs Cathode
U.S.	United States
UCATH	Uranium Cathode
UK	United Kingdom

UNF	Used Nuclear Fuel
VBA	Windows Visual Basic for Applications
VTT	Technical Research Centre of Finland