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Material Protection, Accounting, and Control Technologies (MPACT)

Advanced Integration 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, simulation and integration.

To aid in framing its long-term goal, during FY16, a roadmap is being developed for advanced integration as applied to next generation nuclear material management. The basic premise is to take full advantage of all information and data streams such that a higher level of facility operational awareness is achieved and ultimately quantified. The ability to extract knowledge, make use of correlations and quantify uncertainty in an integrated manner is expected to perform demonstrably better than current safeguards and security systems that operate largely independent of one another and do not take full advantage of all available information and data.

Traditional safeguards have relied on cost-intensive sampling and inspector presence to determine Inventory Difference (ID) or Material Unaccounted For (MUF) in the various Mass Balance Areas (MBAs) to determine if any nuclear material is missing in each stage of the nuclear fuel cycle. Some of these traditional approaches may not easily transfer over or are cost-prohibitive for advanced fuel cycle and reactor options that are currently being investigated. A goal of the MPACT program is to investigate cost-effective options by which on-line ubiquitous plant monitoring system signatures, advanced radiation, multi-spectral and chemical sensors can be integrated together to supplement, and where appropriate to substitute for, traditional measurements. In addition, the program seeks to integrate security systems and associated information. This approach, generally referred to as the safeguards and security by design, focuses on fully integrating advanced sensor technologies and multi-scale analysis capabilities and incorporating them early in the design of fuel cycle facilities. Achieving full integration, wherein analysts can bring together disparate partially correlated signatures to infer the ability of proposed technologies, together with advanced safeguards and monitoring architectures, should facilitate regulatory acceptance well before the conceptual designs are matured. This objective requires a modular, flexible and integrated forward modeling and analysis capability.

- *Modular* architecture allows an analyst to functionally decompose the process flow sheet into sub-systems (or modules) each of which can be developed, verified, validated and assessed by subject matter experts in that area. It further allows for accurate quantification of underlying uncertainties and their relative contribution to the overall uncertainty at the unit operations level.
- *Flexible* coupling of modules allows the user to rapidly evaluate competing flowsheets and sensor architectures. It also allows for 'on-the-fly' sequencing or timing of various operations.

- *Integration* (or more appropriately Advanced Integration) is vital to physically, chemically and temporally couple otherwise partially correlated set of signatures, measurements and predictions.

We envision this framework to mature with increasing functionality over a period of three phases. During the first phase, we will perform two end-to-end 'use-case' analyses to assess modeling and data gaps and to down-select the integration architecture that best preserves flexibility without loss of accuracy. In this effort we envision virtually tying together multi-scale models, ranging from heuristic models to physics based unit-operations models, which are in different stages of development as part of MPACT or have been developed by other DOE programs. Use-cases act as the forcing function that specifies the 'boundary conditions' for each module and allows for uncertainty quantification at the module level by the Subject Matter Expert (SME). Uncertainty distributions generated at module level will be propagated through the integrated system making use of Bayesian approaches for cross-sensor and cross-modality data fusion. This end-to-end study will provide quantitative insights into the desired level of coupling required to achieve a prescribed level of fidelity. During phase 2 and 3, we will employ increasingly accurate modules and data from sub-scale experimental test beds (e.g., pilot scale facilities) to decrease prediction uncertainty gradually. They will also expand the list of use-cases to cover a range of fuel cycle facilities and/or options. The resulting framework will constitute an enduring tool for the MPACT campaign to utilize in assessing a variety of technologies and options under consideration within the Fuel Cycle Technologies R&D program. A summary of the key findings are listed below.

Gap	Relevance	Path Forward
Uncertainty quantification	System performance assessment	Build on current work and develop new tools/methods
Correlation analysis	Reduces or increases overall uncertainty	Tools and methods for discovery are needed
Process monitoring	Augmentation of NMA	List of PM technologies are needed for specific fuel cycle technologies
Advanced nuclear material accountancy	Push limits within traditional NMA architecture	Emerging technologies being developed (e.g., microcal)
Facility layout	Safeguards and security by design – rapid evaluation	Build on current models, modular capability for specific applications
Advanced information technology/control systems	Automation leads to enhanced access to large data streams such as state-of-health	Identify and demonstrate promising technologies in context of regulatory environment
Diversion analysis	Advanced fuel cycles need assessment	Develop priority facility list and identify areas where new tools are needed
Cost-benefit analysis	Optimization of overall system	Develop priority technology list, overlay regulatory requirements and gaps, identify emerging needs for tools

1. Introduction

The Materials Protection, Accounting, and Control Technologies (MPACT) campaign is working towards the goal of developing and demonstrating the next generation of nuclear materials management for the peaceful use of civilian nuclear energy. A central theme of the campaign is safeguards and security by design, whereby advanced technologies and analysis capabilities are fully integrated and incorporated early in the design of fuel cycle facilities. A major milestone of the campaign is the "Lab-scale demonstration of an advanced safeguards and security system," due in 2020. A key component to achieving this milestone is the development of a virtual facility, distributed test bed that incorporates the instruments, data, analysis tools, and models currently under development and provides a framework to link and normalize the data in a way that simulates a facility, including uncertainty quantification. This virtual distributed test bed will integrate computer simulated facilities that make up a fuel cycle of interest, with distributed test beds located in actual operating facilities and laboratories located throughout the DOE complex. Existing DOE owned facilities poses a variety of lab-scale test bed characteristics that can enable safeguards and MC&A R&D for the nuclear fuel cycle; however, none of these facilities on their own encompass contain fidelity compared to a new, advanced fuel cycle facility. Consequently, a virtual, distributed test bed can integrate these existing facilities to most efficiently represent the facility under study (for example a reprocessing facility) or an entire fuel cycle. Model simulation of prototypic fuel cycle facilities will then enable targeted testing in lab-scale environments with actual or substitute signature sources.

This approach presents both a challenge and opportunity to the research community. The challenge is developing sufficient data from real instrumentation and representative process materials that one can pass results without large areas of extrapolation. Another challenge is the quantification of uncertainty at various levels, as well as aggregating and exploring correlations that may reduce overall uncertainty in the nuclear material control and accounting system.

An example of how a virtual distributed test bed could be implemented is that of an electrochemical processing facility simulation integrated with an actual electrochemical processing test bed, and/or a fuel fabrication facility simulation integrated with an actual fuel fabrication test bed, to enable the estimate of the Standard Error in the Inventory Difference (SEID) and/or Standard Error in the Material Unaccounted For (Sigma-MUF), for the use of advanced instrumentation in full-scale facilities. Another example is the virtual mapping of radiation signatures for the process cell(s) of a full-scale facility, to enable the selection of substitute signature sources for a stand-alone instrument development test bed, thereby facilitating instrument R&D to characterize measurement accuracy and uncertainty in a prototypic environment.

Advanced measurement instrumentation, modeling capabilities, and laboratory test beds all play a role in developing efficient and effective safeguards and security systems for fuel cycle facilities. The purpose of this roadmap is to describe how the individual research results in the campaign (and potentially the larger Fuel Cycle Program) can be integrated, identify gaps, and suggest a path forward.

2. Safeguards and Security Metrics

When designing or analyzing a nuclear facility, a few key metrics are used for safeguards and security. For safeguards, an Inventory Difference (ID) or Material Unaccounted For (MUF) calculation is used in the various Mass Balance Areas (MBAs) to determine if any material is missing. The overall measurement uncertainty is referred to as the Standard Error of the Inventory Different (SEID) or Sigma-MUF for each of those balances. In diversion scenario analysis, the probability of detection is used as a metric, and it can be extended to a probability of detection as a function of time to take into account timeliness.

Security analyses examine the threat of theft or sabotage to a nuclear facility. These threats include both insider and outsider attacks. For security, the metric includes probability of success for either the adversary or response force. However timeliness is also important since it is be desirable to stop a theft before a significant quantity can be removed or stop a sabotage event before it can be successfully completed. Figure 1 shows the relationships and corresponding requirements between safeguards and security as currently implemented under both domestic (NRC) and international (IAEA) regimes.

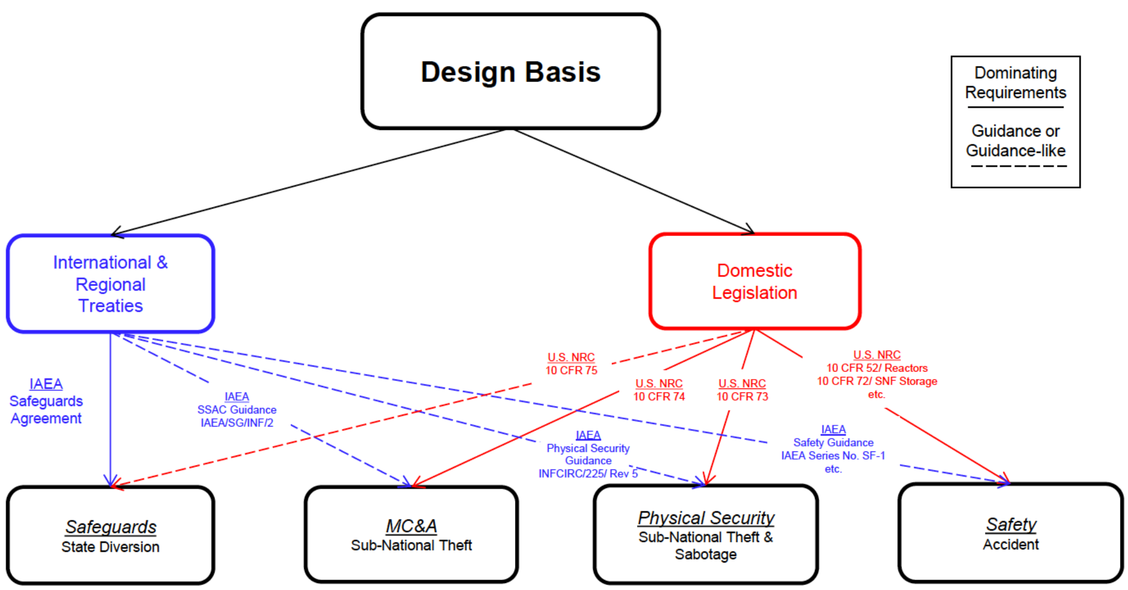

Figure 1. Safety, security, and safeguards requirements for domestic and international nuclear facilities (DeMuth, 2014).

Advanced fuel cycles and associated technologies bring new challenges to existing the safeguards and security framework and as a result research and development continues to be pursued in the MPACT campaign. The campaign has developed roadmaps for safeguards technology development (Smith, 2008), and more recently safeguards and security for used fuel extended storage (Durbin, 2016) and MPACT modeling and simulation (Cipiti, 2016). These roadmaps help to inform program investments and offer a means of communication priorities to external parties (such as NNSA, NRC, IAEA, etc.).

Cost is also a metric for both systems since it is desirable to reduce the burden of safeguards and security on the facility, while maintaining or improving performance. Modern facilities will need efficient and cost-effective solutions that limit the impact on operations. Cost may include equipment capital and operating costs as well as personnel required (see for example Badwan, 2012). In general, cost-benefit analyses for advanced fuel cycle facilities that haven't been built on commercial scale have large uncertainties and new tools are needed for improved fidelity.

3. Data Types

Here we consider data types and their acquisition using nuclear material accounting and process monitoring.

3.1 Nuclear Material Accounting

Nuclear material accounting (NMA) is well-established for existing fuel cycle facilities. NMA includes the key measurements used for input accountancy, inventory measurements, and output accountancy. Facilities such as LEU fuel fabrication, aqueous reprocessing, and thermal reactors, have well-established NMA systems while less mature facility types, such as electrochemical reprocessing, advanced fuel fabrication and fast reactors, need additional work on measurement technologies, approaches, and in some cases regulatory requirements. Overall material balance calculations and analysis tools are well-established for NMA, including facility level performance assessments (Cipiti, 2012).

The primary thrust for R&D in NMA continues to be advancing the state of the art in measurement uncertainty and throughput (see for example Hoover, 2016 and Launiere, 2015), addressing hard to measure samples (such as the direct measurement of Pu in spent fuel or molten salts), and developing concepts and approaches for advanced facilities that have not been deployed at commercial scale (for example fast reactors and pyroprocessing). Advances in this area lessen the advanced integration problem since uncertainty quantification is straight forward and quantitative, direct results obtained. Correlations among a network of sensors exist and are largely unexplored and unexploited. Further work to push the state of the art in instrument accuracy is needed as well as tools for correlation discovery.

3.2 Process Monitoring

Processing monitoring (PM) is used to augment NMA in situations where the combined uncertainty of the inventory difference and facility throughput do not meet goal quantities and timeliness. An example is bulk processing, large throughput plants. PM is often used to help augment the safeguards evaluation by providing trend analyses or additional observational barriers to diversion. These are however, primarily subjective and not subject to strict requirements. PM is also important to achieve timeliness goals by taking advantage of systems that can provide data in a more continuous fashion (as opposed to waiting for a material balance).

PM data generally falls into two categories, and the data can be used in different ways. Quantitative data may be any non-sampling or non-destructive measurement that determines specific quantities of material. These are usually on-line or in-line measurements that produce data frequently or continuously. Examples include bulk level and/or bulk mass measurements (Galbreth, 2016), on-line spectroscopy (Bryan, 2011), and on-line gamma or neutron measurements. Quantitative PM data is much easier in principle to integrate with NMA since it has knowable uncertainties and involves measures of direct interest (for example, Pu) and therefore can be combined with NMA data directly. Analysis and modeling techniques can be improved for integrating quantitative PM data to include discovery and application of correlations.

Qualitative data will not reveal specific quantities of materials, but can indicate off-normal conditions. This can include temperature, pressure, density, current, voltage, and off-gas monitoring. In other cases, the method may involve tradition signature observation (for example gamma-ray spectroscopy as reported by Meier, 2015), but the nature of the data precludes quantification easily. Qualitative data is much more difficult to integrate with NMA data, given the disparate nature of the data sets (including basis value, uncertainty quantification, and correlation). Hybrid approaches have been explored and developed (Burr, 2105) however, additional research is needed. Approaches developed to estimate remaining useful life (Coble, 2011) may find application as well as data driven maintenance.

The MPACT campaign is investigating a number of advanced process monitoring approaches, with particular emphasis on pyroprocessing. These include the development of a potentiometric sensor for molten salt application (Gese, 2012), voltammetry (Tylka, 2015), and *in situ* measurement of metal product (Westphal, 2016). Application of process monitoring has been of interest to the international community for some time (see Burr, 2012). Solving the rigorous integration of PM data with NMA data in of itself would constitute a major step forward in knowledge extraction of facility operations as applied to advanced safeguards and security. We are however, interested in going beyond the integration of instrument related measurements to include disparate data types.

3.3 Containment, Surveillance, Physical Security, and Other Data Types

Where material cannot be measured well, like the front end of reprocessing before the accountability tank, there is more reliance on item accounting of spent fuel assemblies and C/S of the chopped and dissolved fuel as part of traditional safeguards and security. Reprocessing products and wastes, and fabricated fuel contain nuclear material in discrete items, so item accounting and C/S are well suited for use in those locations as well. Generally, existing approaches work for safeguards and security, so these areas tend to have less of a research focus. Additional research is needed for diversion path analysis and integration with the NMA/PM outputs. Reducing costs may be a larger driver for item accounting where automation and remote access of real-time data streams may be taken advantage of perhaps in a manner that is less complicated that bulk processing.

Physical protection elements, such as cameras, guard patrols, access controls, and portal monitors are also well established. However, there is a need to optimize costs since physical security costs can become large with over-conservativism. Analysis tools that can quickly analyze designs and examine ways to reduce costs are useful. In addition, formal integration of data streams from both safeguards and security systems could benefit both areas. Previous research in the program started to address this integration across data types (Izraelevitz, 2009), the key deficiency though was the requirement that correlations were know *a priori*.

One area that has not been explored in detail is ambient intelligence or “smart buildings” that make better use of any data that might be indicative of certain behaviors. For example, access controls that can monitor movement of personnel coupled with sensor data may indicate an off-normal plant condition. Work on ambient intelligence in other fields should be explored for application to nuclear facilities. This is an example where applications with a reduced misuse concern (for example air temperature control for an office building) can provide a forcing function for development but the lens of safeguards and security for nuclear fuel cycle facilities will bring additional requirements and constraints. Investigation into this category, that of future technology in facility operation and maintenance, may provide additional dividends if initiated in the ‘early adopter’ phase where basic modifications can be made more cost effectively.

4. Data Mining

As discussed above, nuclear facilities contain a vast assortment of processes and attendant data. Data mining can be used to develop knowledge from such data. Data mining is the process of discovering patterns and developing knowledge from large amounts of data. The data-mining process can be characterized in several interconnected components (Han, 2012):

- Data cleaning – removal of noise and inconsistent data
- Data integration – combining multiple data sources
- Data selection – retrieval of relevant data from a database
- Data transformation – transformation and consolidation into forms appropriate for mining
- Data mining – use of intelligent methods to extract data patterns
- Pattern evaluation – identification of patterns of interest
- Knowledge presentation – visualization and representation use for user presentation

There are many data mining functionalities, including:

- Characterization and discrimination
- Mining of frequent patterns, associations, and correlations
- Classification and regression
- Clustering analysis
- Outlier analysis

These functionalities are used to specify the kinds of patterns to be found in data mining tasks. Such tasks can be grouped into two categories:

- Descriptive – property characterization of the data
- Predictive – performing induction of the data in order to make predictions

Data mining makes use of techniques from many disciplines, including statistics, machine learning, pattern recognition, database and data warehouse systems, information retrieval, visualization, and high-performance computing. Data mining is an active area of research, including initiatives in multidimensional mining, methods integration, and consideration of semantic ties among data objects (Mena, 2003; Han, 2012).

This overview of data mining serves as an introduction to this important aspect of advanced integration for nuclear facilities. The following sections provide some additional insights into some aspects of data mining for facility applications.

5. Quantifying and Propagating Uncertainties

There are roughly three levels of uncertainty propagation that may be considered for the fuel cycle: the instrument level, facility level, and fuel cycle level. Most of the work here centers on integrating the facility level with the instrument level. This is the logical first step and represents the core of the approach towards achievement of the 2020 milestone. However, the same conceptual framework can be applied at fuel cycle level and investments made in the near term will directly benefit this enduring capability (that could be used for example to compare fuel cycle options).

5.1 Instrument Level

Measurements uncertainties at the instrument level are determined through experimental testing and modeling. Test beds are useful to provide this data. Uncertainty propagation is carried out after accounting for multiple contributions to the random and systematic errors, with the goal of achieving an overall random and systematic error for that particular technology. Correlations that exist between material flows for example are currently largely unexplored and unexploited. A systems level approach is the first step: integration between a network of instruments. The SSPM tool (Cipiti, 2012) provides a platform to study variations of instrument placement and MBA structure where uncertainties (random and systematic) can be varied and SEID or Sigma-MUF calculated. This tool does not account for correlations however or provide a mechanism for discovery.

5.2 Facility Level

At the facility level, uncertainty propagation is well established for NMA and implemented (but not formally adopted by the regulatory or verification systems) in SSPM for including quantitative PM technologies. For example, bulk measurements like mass or tank level are routinely used with sampling measurements in aqueous reprocessing plants as part of the overall balance, but they could also be used for a bulk balance of a vessel or portion of a facility. Online spectroscopic data can measure concentrations of specific elements/species of interest—when combined with the bulk data, can be used to calculate an inventory difference in near real time. As on-line technologies improve, the main difference is that the material balances can be done more frequently (thus potentially benefiting the overall system performance), but the approach and error propagation does not change.

More work is needed on applying uncertainties to qualitative PM data. For example, an electrorefiner may have multiple qualitative measurements associated with it. A combination of input and output measurements as well as a knowledge of real time monitoring operational parameters may be enough to provide assurance that the process is operating as expected or as declared. Multi-variate analysis can be used to take into account multiple disparate data streams to help determine if operation is normal or off-normal. An off-normal operation may lead to a decision to take additional samples or other more detailed measurements to determine the source of variation. Other examples include the use of Bayesian or other statistical approaches to determine what combination of signals would indicate an off-normal event like a material diversion (Burr, 2015; Garcia, 2012).

Qualitative and/or quantitative PM data may also be used with a computer model to predict quantities. Using the same electrorefiner example, various PM data could feed into a model like AMPYRE-DyER to predict actinide inventory as a function of time (Pereira, 2013). This approach needs to take into account both the error propagation from all the measurements as well as the model error. A well-validated model would be needed. It is important to also consider if the use of larger numbers of qualitative data would lead to increased burden for the operator as opposed to relying on traditional sampling approaches. Correlation discovery and application may lead to alternate thinking about optimizing at the facility level.

Facility level modeling also includes physical protection, consequence modeling, and ambient intelligence. All of these areas require further development. Uncertainty propagation for physical protection is based on performance data of specific physical protection elements. Modeling multiple iterations of attack scenarios is used to develop statistics. Consequence modeling may be more or less important depending on the facility type, and there can be very large uncertainties in outputs like release rates or consequence to the public or economy. The concept of ambient intelligence is relatively new and unexplored for this area.

5.3 Fuel Cycle Level

The ultimate level of integration would be at the fuel cycle level, where nuclear material is controlled, tracked, and accounted for from ‘cradle to grave.’ Application at this level would naturally build upon the integration at the instrument and facility level and enable more detailed analysis and potentially optimization for fuel cycle options. This is particularly true when coupled with the technology developers (fuels, material recover, reactors).

Fuel cycle-level analysis and evaluation has been a subject of study from the early 1980’s to the present (Wigeland, 2014). The general result is that nonproliferation considerations tend to reside primarily on the policy side of the house whereas safeguards and security approaches tend to be driven by commercial development of nuclear technology. In the early days of nuclear power and technology development, these two aspects were largely independent. One reason is the lack of rigorous and quantitative analysis at the fuel cycle level that encompasses all domains (technology, safety, economics, safeguards and security, etc.). For the specific case of optimizing and integrating safeguards and security at the fuel cycle level, one can imagine using the same tools as developed for facility level integration with an additional integration level – namely between facilities.

New methods of data analysis and knowledge discovery could be a key enabler at the instrument-facility and fuel cycle levels. Operations research (see for example Ho, 2008), analytics and data mining (see for example Shearer, 2000) are being studied and developed across a wide range of information rich environments (logistics, manufacture, agriculture, etc.) with the goal of optimizing performance based on integration of multiple disparate data streams. Application of such techniques in the safeguards and security realm has been the subject of some investigation (see for example INMM, 2104; Crowley, 2014).

6. Technologies, Models, and Test Beds

A modeling and simulation roadmap (Cipiti, 2016) has been developed in parallel to the advanced integration roadmap. This modeling and simulation roadmap goes into more extensive detail on the codes and analysis tools that are being used in the campaign and the field more generally. There are three major areas of that roadmap including radiation transport and sensors, process and chemical models, and consequence assessments. The table below summarizes the modeling and simulation roadmap. Advanced integration and achievement of the 2020 milestone will rely heavily on the developments and future efforts in modeling and simulation within the MAPCT campaign. Given the strong overlap with the Material Recovery and Waste Form Development campaign, we are planning a joint modeling and simulation workshop in FY 2017. It is anticipated that this roadmap will be updated based on the results of the workshop.

Table 1: MPACT Models, Technologies, and Test Beds

Detector/Instrument Models	**Application/Comments**
Neutron signatures of storage casks	Neutron fingerprinting
Multi-Isotope Process (MIP) monitor	Gamma analysis of reprocessing streams
Delayed gamma	NDA measurements of spent fuel
Neutron detector design	Various uses
Muon imaging of dry casks	Measuring gross defects
Electrochemical radiation signatures	Mapping and design of systems
Process/Facility Level Models	
AMUSE	Aqueous flowsheet development
AMPYRE	Electrochemical flowsheet development
DyER	Dynamic electrorefiner model
PyFOM	3D operations model
SSPM	Safeguards model

STAGE	Physical security model
MASTERS	Electrochemical flowsheet development
Consequence Models	
CTH	Shock physics
MACCS, HotSpot	Dispersion codes
Instrumentation	
Triple Bubbler	Mass, volume, density of molten salts
Voltammetry	Actinide content in molten salts
MIP Monitor	Gamma analysis of various streams
UV-Vis-NIR Spectroscopy	Various species in streams
Microfluidic Sampler	Reducing sample volume
Electrochemical Sensor	In situ measurement of actinides in salt
High Dose Neutron Detector	For measurements in hot cell
Microcalorimeter	Significantly improved gamma spec.
Test Beds	
H-Canyon	Provides aqueous streams for testing
Co-Decontamination Demo	Process monitoring test bed
INL hot cells	Pyroprocessing

7. Virtual Facility, Distributed Test Bed Concept

A major milestone of the MPACT campaign is the 2020 milestone: *lab-scale demonstration of an advanced safeguards and security system*. Since there isn't a single facility available that possesses the attributes needed (advanced fuel cycle, kg throughputs, modern technologies, etc.) for such a demonstration, the MPACT campaign has made the strategic decision to advance the state-of-the-art through a distributed test bed concept, assembling a virtual fuel cycle facility as a result. One or more of these constructs will constitute the 2020 milestone. Advanced integration is a key requirement to accomplish this task and serves the dual purpose of providing an enduring and robust framework to advance the existing safeguard and security paradigm towards the campaign goal of *next generation nuclear materials management.*

Figure 2 shows the concept of the distributed test bed, virtual facility. Individual investigators develop prototype instrumentation, perform bench-scale proof-of-principle testing and then lab-scale demonstration. The testing at this stage uses best-of-class nuclear materials, ideally whose composition and mass are well known, taking advantage of unique assets in the national laboratory system. A series of these individual instruments and results are developed for different key stages in the fuel cycle facility that is being built up. Analysis tools are developed that 1) evaluate the results from instruments, 2) pass key parameters, including uncertainty, between instruments (for example plutonium isotopics that differ from instrument A to instrument B), and 3) integrate the combined data, with correlations and an overall uncertainty.

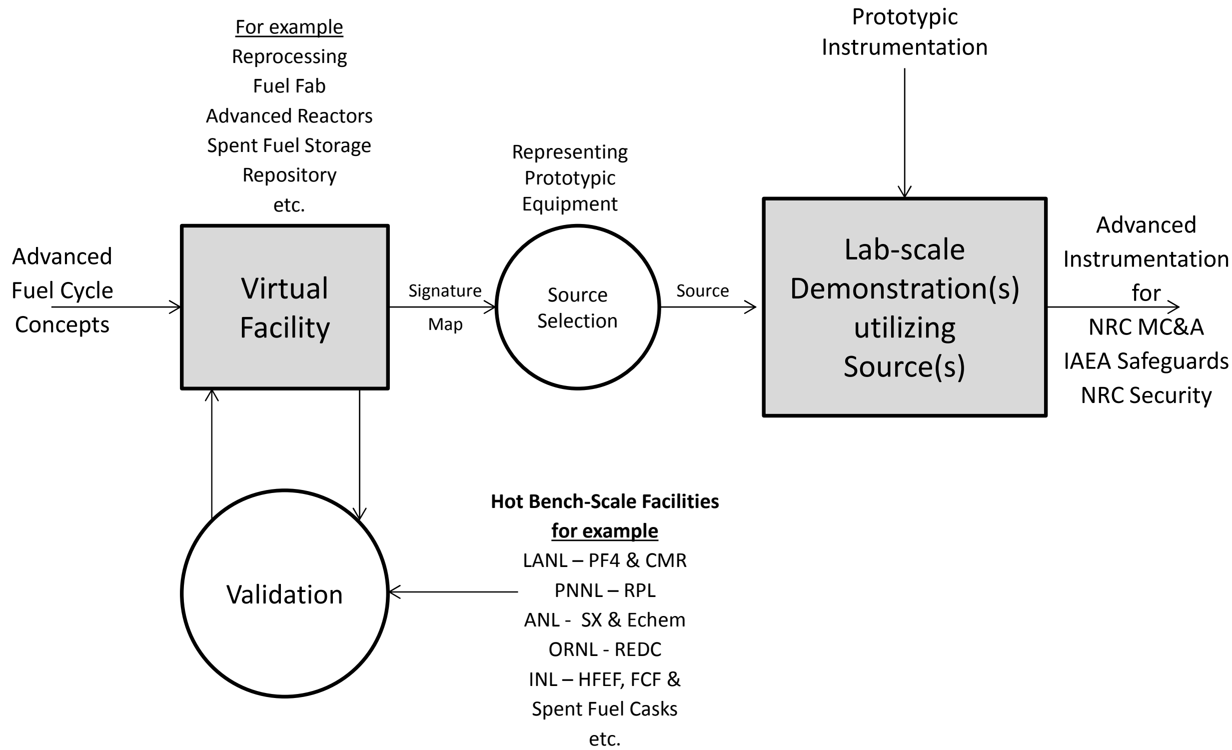

Figure 2. Conceptual design of virtual facility, distributed test bed.

This general concept can be applied a differing levels to achieve a variety of virtual entities. At the sub-facility level, modules could be built up to simulate variations within a common facility (for example different options within a reprocessing flow sheet). At the facility level modules are built up with sufficient fidelity to simulate input-to-output (for example a fuel fabrication facility). Multiple facilities can be built up, with cross correlations built in, to emulate a portion of or entire fuel cycle. The key feature is that all levels are driven by experimental data and supplemented with modeling and simulation where gaps exist. This grounds the virtual facility with real-world constraints and systematics.

8. Advanced Data Integration Path Forward

The next steps in developing MPACT's advanced integration capability and achieving the 2020 milestone are to examine the linkages between various modeling and experimental capabilities. These will vary depending on the type of facility. Figure 3 shows how the various capabilities in the MPACT program can work together for complete safeguards and security modeling of electrochemical reprocessing facilities. The purpose of the figure is to show the linkages between various capabilities. Each capability has a different application or may be focused on a different part of the problem. Together they form a virtual test bed for safeguards and security analyses.

Starting from the bottom, the AMPYRE flowsheet model forms the basis for the facility of interest (in this case, electrochemical reprocessing). Information such as flow rates, unit operation volumes, and separation efficiencies are used to inform the development of safeguards models, a 3D plant layout, and radiation signature mapping. The capabilities are not formally integrated as a single, comprehensive model; rather, information is passed between each component to provide an integrated result. Integration of the various outputs is also needed.

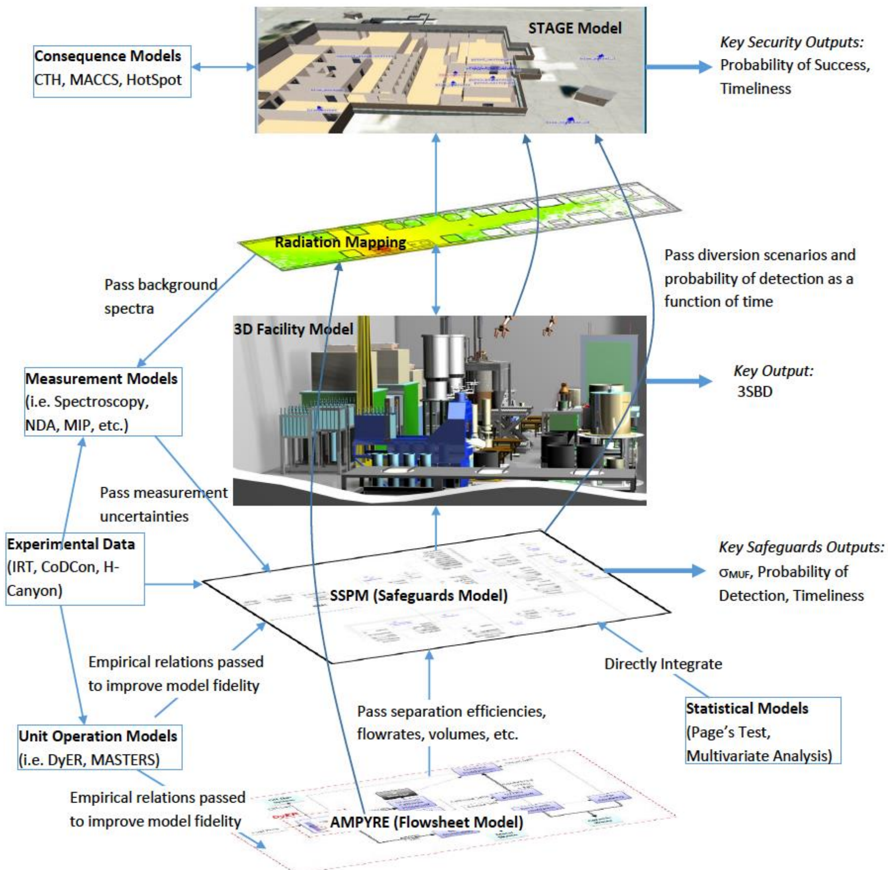

Figure 3. Advanced Integration for Electrochemical Reprocessing.

The SSPM is a safeguards model that is designed for producing the key safeguards metrics for a particular design. There are many data types that feed into it including the flowsheet models, unit operation models, such as the DyER code for modeling the electrorefiner, may be used to increase the fidelity of the flowsheet model and safeguards model. The linkage may be as simple as providing empirical relations or more complex like directly integrating. The MASTERS code at INL could also be useful to fill in gaps in unit operation models that may be needed. Measurement models and test data from experimental facilities can provide the measurement uncertainties that are directly used by the SSPM. Example experimental facilities include the engineering-scale pyroprocessing hot cells at INL, and lab-scale pyroprocessing capabilities at ANL, though there are a number of experimental capabilities at various labs.

The safeguards and flowsheet models can be used to inform a 3D facility model that may be developed as part of the conceptual design. A key output of these models is to develop Safeguards and Security by Design conclusions. Radiation mapping can be informed by the 3D model and flowsheet models, and it serves a role in helping to design measurement models and placement of instrumentation in the hot cell.

The STAGE model is a physical protection model and is informed by the 3D model and the safeguards model. Safeguards data may be passed to STAGE to develop integrated safeguards and security system designs. STAGE produces the key security metrics. Consequence models may also feed into STAGE depending on the type of attacks that are considered.

Together, all of these capabilities serve as the distributed test bed. Other fuel cycle facilities will look similar, but with slightly different codes in some cases. Given the current focus on electrochemical process in the MPACT campaign, we will begin with this facility type to examine linkages between process steps and code/instrument linkages. Additional facility types may be developed to augment electrochemical processing.

8.1 Spiral Approach to Advanced Integration

Whereas Figure 3 presents a final vision for integrated tool set, it is recognized that some or many of the models and test facilities don't exist to the desired degree of fidelity. Therefore a spiral development strategy based on continuous improvement is sought. We commence with adapting and extending the type of analyses described in Burr 2012, Burr 2015, and Miller 2015, each of which examined feasibility and benefits of fusing data from multiple sensors – including traditional NMA measurements and process monitoring (PM) that rely on chemical and radiation signatures. Burr 2015 studied and contrasted various approaches 'fusing' NMA and PM sensor data with model predictions; which was explored in some detail also in Cipiti 2011. Here are some conclusions that can be drawn from these studies.

The Bayesian Approach provides perhaps the best framework for bringing together multiple partially correlated signatures from disparate sensors. Burr 2012 provides a simple data-driven Bayesian approach to fusing the data and for establishing alarming limits at a unit operation level. In general, this study confirmed long held belief that fusing PM data with NMA could result in more timely detection of diversion scenarios at a unit operation level. This aspect was further explored in Cipiti 2011; both of which studied dissolution operations typical of a conventional PUREX operation. Based on further analyses, Burr 2011 concluded that simple data driven fusion may not perform as well when unit operations are combined with transfer operations (that is where inventory is transferred from one tank to another tank for example). One primary reason is that most PM signatures, and some of the NMA samples, are only partially correlated (because they rely on different phenomena: chemical vs multi-spectral vs radiation for example) and are not temporally synchronized. This suggests the need to use a hybrid approach that combines data-driven and period-driven anomalies.

The implicitly hybrid approach of the kind suggested by Burr 2015 requires a functioning systems level model that could be used to tightly couple disparate signatures temporally, physically and chemically. In this hybrid approach, accuracy of modeling each unit operation is not as important as getting the systems dynamics right. In other words, a sub-scale test data can be used to 'tune-in' the model results to generate prototypical synthetic sensor traces that span a spectrum of realities. On the other hand, temporally correlating the traces significantly enhances the ability to detect and examine anomalies. We plan to demonstrate value of this approach for two use cases – that is the value of the proposition that disparate sub-scale experimental PM sensor data can be closely synchronized and coupled, and then scaled up to simulate a real-scale and further that the synthetic data via this process could be used to detect anomalies. Each of the use cases examines an end-to-end process facility, one focused on conventional PUREX/Aqueous Separations process and one focused on PYREX/electro-chemical process. Figure 4 provides types of analyses to be performed and graphically illustrates the anticipated results.

Use Case #1. Aqueous Process. Working with subject matter experts from the Material Recovery and Waste Form Development Campaign, we will develop a flowsheet model for an aqueous separations 'facility' using AMUSE. After calibration, dynamic system parameters from AMUSE will form the basis for a candidate safeguards architecture to be generated and assessed using SSPM. The architecture will explicitly examine various NDA technologies being developed under the MPACT program such that their risk-worth can be quantified as part of the study. Synthetic data that closely approximates what might be observed in a real scale facility will be generated by merging the predictions of a model (for example SEPHIS for counter-flow contactors) with the sub-scale experimental data (for example H-Canyon data). MCNP will be run at the facility scale to output source term environment conditions to which some of the NDA instruments might be subjected to. In the end we would generate a comprehensive set of synchronized time-series (aka synthetic data streams) that could be analyzed to identify and characterize anomalies. Statistical routines available in many scientific packages (e.g., SAS) will be used to perform this last step. Output of the analyses will provide valuable insights of the type shown in the right column of figure 2.

Use Case #2. Electrochemical Process. It will repeat Use Case #1 except for the electro-chemical process. In this case, however, due to the lack of type of information required we would more heavily rely on surrogate materials chemistry (Gd, TC etc.) test facilities and simulations.

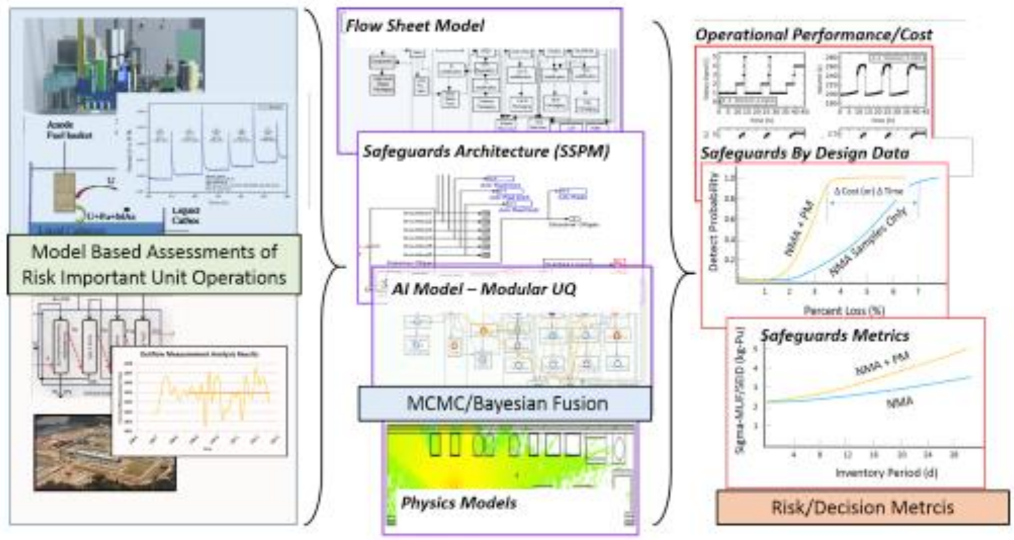

Figure 4: Notional Advanced Integration Spiral Concept

9. Summary

We have outlined the steps needed to develop an advanced integration capability for realization of *next generation nuclear material management*. The approach is data driven, including data generated from prototype instrumentation development and testing within the MPACT campaign. We will also take advantage of analysis tools and associated results that have been developed in the MPACT campaign. The near term goal for this framework is to support the completion of the MPACT 2020 milestone "lab-scale demonstration of an advanced safeguards and security system." In the longer term, an enduring analysis, evaluation, and optimization capability will be realized for safeguards and security by design that can support the safe and secure implementation of advanced civil nuclear energy systems. A summary of the R&D gaps and recommended path forward are listed in Table 2 below.

Table 2: Advanced Integration Gaps and Path Forward

Gap	Relevance	Path Forward
Uncertainty quantification	System performance assessment	Build on current work and develop new tools/methods
Correlation analysis	Reduces or increases overall uncertainty	Tools and methods for discovery are needed
Process monitoring	Augmentation of NMA	List of PM technologies are needed for specific fuel cycle technologies
Advanced nuclear material accountancy	Push limits within traditional NMA architecture	Emerging technologies being developed (e.g., microcal)
Facility layout	Safeguards and security by design – rapid evaluation	Build on current models, modular capability for specific applications
Advanced information technology/control systems	Automation leads to enhanced access to large data streams such as state-of-health	Identify and demonstrate promising technologies in context of regulatory environment
Diversion analysis	Advanced fuel cycles need assessment	Develop priority facility list and identify areas where new tools are needed
Cost-benefit analysis	Optimization of overall system	Develop priority technology list, overlay regulatory requirements and gaps, identify emerging needs for tools

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