MODELLING AND SIMULATION FOR NUCLEAR MATERIAL ACCOUNTING AND PROCESS MONITORING IN NUCLEAR SAFEGUARDS

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ABSTRACT

Nuclear safeguards at inspected facilities aims to deter or detect special nuclear material (SNM) diversion and to do so is increasingly relying on process monitoring (PM) to augment nuclear material accounting (NMA). In NMA, SNM material balances are computed approximately every 30 days, and modeling and simulation are used to predict detector performance, to model SNM flows and inventory, and predict overall NMA performance as measured by the measurement error standard deviation of the material balance, σ_{MB}. In PM, much more frequent and often short-cut measurements (less than full SNM accountability) are used, and modeling and simulation are increasingly used to predict the effects of SNM diversion on normal operating data under various scenarios. This paper reviews traditional modeling and simulation roles in NMA, describes new roles in PM, and illustrates using a case study.

Keywords: *Measurement errors; mixture distribution; nuclear safeguards; process monitoring; process variation.*

1. INTRODUCTION

Nuclear nonproliferation efforts consist of many facets, including nuclear safeguards, which involve monitoring for undeclared nuclear facilities, and monitoring for facility misuse (diversion of special nuclear material, SNM) at inspected facilities. This paper considers inspected facilities where measurements of SNM flows and inventories are periodically used in nuclear material accounting (NMA) to compute material balances (MB). The paper focus is large bulk-handling (primarily aqueous) facilities where MBs are computed approximately every 10 to 30 days.

Modeling and simulation (M/S) have traditionally been used to predict detector performance, to model SNM flows and inventory, and predict overall NMA performance as measured by the measurement error standard deviation of the material balance, σ_{MB}. Nuclear safeguards is increasingly relying on process monitoring (PM) to augment traditional NMA. In PM, much more frequent and often short-cut measurements (less than full SNM accountability measurements, see Section 2.3) are used, and M/S are increasingly used to predict the effects of SNM diversion under various scenarios on normal operating data. This paper reviews traditional M/S roles in NMA, describes new M/S roles in PM, gives four brief examples, then illustrates using a case study.

The following sections include additional background, description of M/S for NMA, M/S for PM, four examples, a case study, and summary.

2. BACKGROUND

This section provides additional background on NMA, containment and surveillance (C/S), and PM.

2.1 NUCLEAR MATERIAL ACCOUNTIG (NMA)

NMA involves measuring facility inputs, outputs, and inventory to compute an MB, defined as $MB = T_{in} + I_{begin} - T_{out} - I_{end}$, where T is a transfer and I is an inventory. The main quantitative assessment of safeguards effectiveness is the measurement error standard deviation of the MB, σ_{MB}.

M/S are used to propagate measurement errors [1] to estimate σ_{MB}. Because many measurements are combined to estimate the terms T_{in}, I_{begin}, T_{out}, and I_{end} in the MB, the central limit theorem and years of experiences implies that MBs will be approximately normally distributed with mean equal to the true SNM loss L and standard deviation σ_{MB}, which is expressed as MB ~ N(L, σ_{MB}) [2]. The magnitude of σ_{MB} determines what SNM loss L could would lead to an alarm with high probability. For example, with a false alarm probability of $\alpha = 0.05$, if MB ~ N(L, σ_{MB}) then the detection probability (DP), $1-\beta$, equals 0.95 for $L = 3.3\,\sigma_{MB}$ (and $1-\beta > 0.95$ if $L > 3.3\,\sigma_{MB}$, where β is the fail-to-detect, or false negative probability) assuming the facility tests for SNM loss only, not for SNM gain.

The factor 3.3 arises from symmetry of the Gaussian, requiring $\alpha = \beta = 0.05$, and the fact that 1.65 is the 0.95 quantile of the standard Gaussian.

For facilities under International Atomic Energy Agency (IAEA) safeguards, one goal is for 1-β to be at least 0.95 if $L \geq 1$ SQ (significant quantity, which is 8 kg for Pu), which is accomplished if and only if $\sigma_{MB\ c}$ SQ/3.3. If σ_{MB} > SQ/3.3, then either measurement errors should be reduced to achieve $\sigma_{MB} \leq$ SQ/3.3 (if feasible), or enhanced material containment and surveillance (C/S) is required; however, the increased C/S effort level is challenging to negotiate and the C/S effectiveness (which can include cameras and remote radiation detection) is difficult to quantify.

Large throughput bulk-handling facilities often try to keep σ_{MB} small as a percent of throughput (perhaps σ_{MB} < 1% of throughput) but cannot achieve $\sigma_{MB} \leq$ SQ/3.3. For example, with a measurement error standard deviation of σ_{MB} = 0.3% of throughput, and the IAEA's DP goals ($\alpha = \beta = 0.05$) for an 8,000 kg annual throughput, the diversion would have to be 3.3 *x* 24 kg = 92 kg or larger [3]. This is much larger than one SQ. One reasonable approach is to evaluate the cost of reducing σ_{MB} and statistical evaluation using M/S is a key tool to estimate σ_{MB} as a function of measurement type(s) and translate the result to a relation between σ_{MB} and cost. One would then choose the cost where the relationship flattens (diminishing returns) and accept the resulting σ_{MB}. It is generally agreed that the resulting σ_{MB} will be too large in large facilities to meet the IAEA goal for slow ("protracted") diversion occurring over one year for example, but there is reasonable hope that the goal can be met over perhaps 10 days or less.

2.2 CONTAINMENT AND SURVEILLANCE (C/S)

Facilities that cannot meet the IAEA DP goal are required to have negotiated levels of additional C/S measures, such as cameras and tamper indicating devices beyond the usual requirements. Smart cameras with context aware image processing can archive scenes involving declared transactions, watch for undeclared transactions, and alert an inspector to sections in the archive that require human review. Image processing for safeguards applications continues to be developed [4].

2.3 PROCESS MONITORING (PM)

The scope of quantitative nuclear safeguards is broadening from NMA to also include PM, which has both C/S and NMA features. PM is a broad term that can include for example monitoring by radiation detectors and monitoring solutions in vessels using pressure-sensing dip tubes, flow meters, or other in-line technologies. Although PM has been used as a component of safeguards, as with C/S, there have been very few attempts to quantify its benefits.

PM goals include support to NMA, but also PM has a "front-line" role to detect changes that could indicate facility misuse and to provide continuity of knowledge to support that the facility is operating as declared. The basic concept is that facility misuse will generate observables that PM can detect. For example, altered material flow rates could imply an attempt to misdirect SNM. Because flow rates are typically monitored for process control, allowing IAEA access to operator flow rate data can provide a quantifiable surveillance benefit. NMA is analogous to a bank periodically confirming that the anticipated cash balance (rounded for example to the nearest dollar so measurement errors are involved) is in the vault. PM can assist NMA in that role, and PM in conjunction with M/S can also provide a surveillance component that is analogous to having cameras in the bank's vault in a way that has a quantifiable benefit.

Radiation detectors fall under C/S and/or under PM, and can monitor either declared SNM transactions (an item was shipped from A to B so the detector should confirm this using detected radiation), can monitor for undeclared transactions (such as portal monitors do), and can in some cases provide rough estimates of holdup (Section 6.4).

Solution monitoring (SM) is a type of PM in which typically masses (M) and volumes (V) are inferred from frequent in-process measurements. Transfers between tanks (which are regarded as sub material balance areas (MBAs)) can be identified in these data, segments of which can then be compared to generate transfer differences. We will refer to these transfer differences as shipper-receiver differences (SRDs) but caution that these are SRDs between tanks, not between full MBAs. A safeguards concern might then be raised if either these SRDs or deviations in M or V data during "wait" modes become significant. Average M and V SRDs should be zero (perhaps following a bias adjustment) to within a historical limit that is a multiple of the standard deviation of the M or V SRD, as should deviations during "wait" modes. Statistical test options can be compared on the basis of their estimated probabilities to detect various material loss scenarios.

In SM, unless there is in-line Pu concentration measurement, then empirical relations linking Pu concentration to in-tank density (D) and temperature (T) for a given nitric acid concentration can be used to indirectly estimate Pu concentration. Together with a volume V estimate using a calibrated relation between measured solution level L and V, an estimate of Pu mass is available. This is an pseudo-measurement because it does not directly measure the Pu. However, it can be adequate for what is known as near-real-time accounting (NRTA). NRTA is almost the same as

NMA but uses much more frequent and often rough estimates of Pu holdup and pseudo-measurements of Pu in inventory. Technically, unless Pu is actually measured directly, one cannot rule out the possibility that some type of operator falsification is being used to mask misdirection of Pu. In current safeguards lingo, NMA refers to less frequent, but full SNM accountability measurements to compute an MB. NRTA refers to very frequent MB closure, usually with short-cut pseudo measurements of some of the SNM in the MB calculation. PM supports both NMA and NRTA, and in some cases could be essentially a form of NRTA with short-cut measurements as just described for Pu [5,6]. A second short-cut pseudo-measurement example involving neutrons produced by Cm is given in Section 6.3.

Generally, some pseudo measurements might be permitted but it becomes obvious that subjective decisions regarding effectiveness arise. For example, in one NMA/NRTA scheme, true balance closures are not done as often as claimed because of the infrequency of actual Pu concentration measurements. True balance closures are less often than weekly, but pseudo-balance closures using empirical relations to estimate Pu concentration are very frequent, approximately daily.

3. QUANTIFYING SAFEGUARDS EFFECTIVENESS

At least two obstacles have historically prevented developing an overall safeguards evaluation methodology. First, there is general agreement that C/S measures add value, but there is no consensus regarding how to take quantitative credit (for example, through improved loss DPs) for C/S in the same manner that improved accountancy measurements are given credit (through reduction in σ_{MB}). Second, there is no consensus regarding the utility of enumerating and characterizing the most likely diversion routes and scenarios. Therefore, some assume that because no system can detect all types of diversion [7], there will be arbitrary decisions made regarding what diversion scenarios the system should detect and therefore what C/S measures will be used. In effect, it is assumed by some that the system design should be decided by arbitrary but reasonable decisions made by the safeguards experts responsible for a given facility.

Alternatively, and in the opinion of the authors, DPs using NMA, PM (and perhaps C/S) in a combined manner, it is possible via M/S to estimate system DPs for a few key specified diversion scenarios. In addition, unspecified scenarios will cause measurable effects on normal plant data, so outlier detection schemes can be devised to detect atypical data associated with unspecified diversion scenarios, without specifying a particular diversion. Current efforts using M/S are therefore underway to quantify the benefits of NMA and PM (but not C/S to our knowledge) in terms of system loss DPs.

Designing an effective safeguards system that is “good enough” without being too costly is a practical goal with significant challenges. A similar goal is to be able to compare and rank candidate safeguards approaches/systems so that the cost/benefit of purported improvements can be evaluated. These two goals are driving safeguards professionals to consider how M/S can be used to quantify the benefit of NMA, C/S, and PM, which are the three key data-driven safeguards systems.

4. MODELING AND SIMULATION (M/S) FEATURES

M/S requirements are strongly problem dependent, so to focus this paper, we consider only NMA and PM.

4.1 PROBLEM DOMAIN

In simulating material flows for NMA or PM, implementations can be batch, continuous, or a hybrid. Real facilities usually are a blend of batch and continuous mode operations.

4.2 APPLICATION

It is often appropriate to ask “why is M/S needed?” Possible reasons that M/S are needed in the context of NMA and PM include:

1) To predict what will actually happen when a plant is built
2) To study misuse scenarios that are not likely to arise in a real plant
3) To compare safeguards options
4) To better understand how plants function (for control systems design and PM)
5) To support NMA by estimating SNM throughput and inventory, including holdup
6) To provide a model-based summary of the real data

4.3 REQUIRED LEVEL OF M/S DETAIL

The required level of M/S detail comes from answering the “why is a simulation needed” question. Performance and/or function prediction ((1) and (4) in Section 4.2) need a model that shows what is actually going to happen. The other applications in Section 4.2 only require levels of detail that are appropriate to the task, but then a very clear idea is needed concerning what the task is. The simulation model must be valid for the task. Mostly validation comes through knowledge of real plant operation, although it can also partly come through comparison with other simulations.

Essentially, the required level of detail will determine the required model fidelity and accuracy. Formal validation and verification (V&V) methods for computer models [8] have rarely been applied to models used in NMA and PM for safeguards. Some V & V methods are considered, however, in codes such as MCNP (MCNP5) [9] which is heavily used for detector design for NMA. MCNP could also be used in PM to predict observables from some misuse scenarios.

A 2007 survey grouped M/S codes into categories including process simulation and modeling, statistical analysis, detector modeling, NMA, physical protection, risk assessment, and training [10]. Although intended uses were briefly mentioned for each code, there was relatively little information provided regarding the actual uses. Therefore, the code use descriptions in [10] will need to be expanded in order to gauge the corresponding required model fidelity. Model fidelity refers to the level of physical detail in the code. Model authenticity refers to a code's ability to mimic reality. Model validity refers to a model's fitness for purpose. Model accuracy then quantifies that fitness. Process design codes are often not that authentic for safeguards purposes; they often falsely assume that installed control systems will compensate for process variations. Similarly, operator training simulators might lack both fidelity and authenticity, if their main purpose is to enable operators to practice procedures.

4.4 EASE OF DEVELOPMENT

Ease of development depends on both the task and the model. For example, is the task intended simply to generate numbers or are graphs needed? If graphs are needed, should they be interactive with the user? Should an equation solver be used that handles batch-wise, continuous-wise, or hybrid unit operations? Are multiple runs needed for example to optimize something? Are the MB equations or other equations amenable to matrix operations?

4.5 EXECUTION TIME

Although NMA simulations for safeguards studies typically cover 10-30 days of activities, they produce output every few seconds, thus generating large data sets. If multiple simulations are needed then this fine-step requirement might need to be carefully considered.

4.6 PORTABILITY AND OPEN SOURCE VERSUS COMMERCIAL TOOLS

Software portability refers to the ease of porting code developed under one operating systems, such as Microsoft Windows to another operating system such as Linux or Mac. Open source code is freely distributed. Commercial tools such as Matlab or Extend require developers and possibly users to purchase a license.

Matlab stands for Matrix Laboratory [11]. It is a primarily a researcher's tool, although real-time applications are possible. It is ideal for manipulating matrices such as occur in mixer-settler/pulsed columns in typical reprocessing facilities. Continuous simulations can be constructed in Matlab directly. It has many toolboxes so for instance the simulation can be linked with an optimizer. One study executed an optimization routine that called a small Matlab continuous simulation about 80 times to locate a diversion [12]. An existing Python hybrid-simulation could also have been used, but that Python simulation was not constructed with optimization in mind. In fact, the "batch-part" of the Matlab simulation is achieved by taking Python outputs as its boundary conditions; that is, the batch operations appear continuous.

Simulink is a block-diagram-based Matlab toolbox intended primarily for relatively small, continuous problems. The block diagramming can get complicated quickly. For example, the top-level of a Simulink simulation of an evaporator tank has several layers of levels beneath it. Simulink ouputs to the Matlab workspace, so that the output can be post-processed easily for example by principal components analysis. Matlab routines can be incorporated into Simulink blocks [1], which has difficulties with batch operations. Matlab/Simulink costs are modest, at approximately $1500 per year per license.

Extend is commercial software for batch processing and is easy to get started but somewhat limited in capability [13]. It is not suited for example to GUAM (glovebox unattended remote monitoring, see Section 6.4) analyses for mixed-oxide power facilities, because GUAM will output continuously. Its cost is similar to the Matlab cost.

Python is a compromise because it is very flexible (incorporates some programming concepts from the LISP language), free, and not as difficult to learn as other object-oriented languages. It has a large number of free libraries including Matlab-style plotting, handlers for large data tables, CSV file handlers, timestamp converters, numerical arrays, etc., and GUI development tools. SimPy [14] is available as an add-on library of simulation tools to link model components according to resource availability. For example, a glovebox that requires input material from an upstream glovebox must enter an idle mode until material is available. Therefore, Python is an excellent choice, particularly if it is important for researchers to all contribute and effectively work together. A current example is the

Glasgow University Reprocessing Plant Simulation Program in Python (GU-RPSP) [12]. GU-RPSP simulates an aqueous reprocessing facility, and includes tank operations plus has a chemical model of the separations area that is based on the SEPHIS model developed at Oak Ridge National Laboratory [15].

Considering simulation in its own right rather than as a tool for a job is quite a major task. Our focus is simulation as a tool for a specific NMA or PM task.

5. M/S FOR NMA/NRTA

M/S are more important to NRTA than to conventional NMA, partly because in the latter, much of the SNM is moved to where it can be measured relatively accurately. This luxury is not available to the more timely NRTA. Here we will not distinguish between NRTA and NMA, but recall that NMA refers to full SNM accounting measurements while NRTA refers to much more frequent but partial SNM measurements.

It is generally agreed that NMA is an essential component of safeguards, but complications include: (1) a lack of transparency regarding where SNM actually is in the plant (holdup material in locations that are inaccessible for measurement such as ducts, pumps, pipes, separations areas such as pulsed columns, etc.; (2) sampling issues such as chemical composition data only being available from samples taken infrequently at a relatively small number of locations; (3) poorly estimated measurement error variances; (4) a limited understanding of systematic measurement errors; for example, results on physical standards is not representative of results on facility material for some flow streams, especially for waste streams, and (5) lack of timely measurement results.

Often, short-cut assay methods such as a weight and assumed SNM purity factor do not directly measure the SNM of interest but are used for some of the measurements. PM overlaps with NMA if PM is used to estimate holdup [16]. Regarding holdup, if there were no measurement error in the transfers and inventory, then the expected value of the MB would equal the change in holdup plus the true loss *L*. The presence of measurement error complicates MB evaluation, and the presence of nonnegligible holdup together with measurement error further complicates MB evaluation. Nevertheless, provided σ_{MB} is well estimated, which is often an engineering challenge constrained by limited time and budget, and which often invokes M/S to estimate holdup and model measurement processes, it is understood as described in Section 2.1 what σ_{MB} implies about loss detection capability.

Simulation for NMA typically involves modeling the flow and inventory of bulk SNM, resulting in a "data generator" that records the transfers and inventory in a manner that mimics real facility data [1, 12,14]. More detail is required if holdup is modeled such as done for powder holdup in gloveboxes [14,16]. One goal for holdup modeling is to anticipate the measurement error associated with holdup measurements. Another goal is to provide a model-based estimate of holdup that could enhance other estimates or measurements of holdup. For example, [17] used FACSIM, which includes a detailed simulation of pulsed columns implemented in C++ to estimate facility holdup in the main holdup locations at a large aqueous reprocessing facility.

Simulation for NMA also models the measurement error process, typically in the same manner that is used in propagation of variance (POV) for estimating σ_{MB}. For example, a common measurement error model is $M = T(1 + S_{item} + S_{inst} + R)$, where *M* is the measured mass, *T* is the true mass, S_{item} is the item-specific systematic error (bias), S_{inst} is the measurement instrument specific systematic error (bias), and *R* is the random error. All errors are random at some stage, which we denote $S_{inst} \sim N(0,\sigma_{Sinst})$, for example, and $N(\mu,\sigma)$ is the normal distribution with mean μ and standard deviation σ [2]. In calculating the variance of a sum of measurements (such as mass(Uranium) = Σ (Volume $\times$ Concentration)), the most common model assumes measurements on two items have nonzero covariance if and only if they are made by the same instrument during the same instrument calibration period, so S_{inst} is the same for the two measurements. The variance of a sum of two measured items with $S_{item} + R$ redefined to be $R_{effective}$ can then be written as $\sigma^2_{M_1+M_2} = \mathrm{var}(T_1(1+S_{\mathrm{inst}1}+R_1)+T_2(1+S_{\mathrm{inst}2}+R_2))$. Because $S_{inst1} = S_{inst2}$ during the same calibration period, it follows that $\sigma^2_{M_1+M_2} = (T_1+T_2)^2\sigma^2_{Sinst} + (T_1^2+T_2^2)\sigma^2_{\mathrm{R\,eff}}$.

M/S are useful for evaluating measurement options and sampling plans. For example, highly accurate destructive chemical assay (DA) is often applied relatively infrequently on a sampling basis [14,16] and mixing rules or less accurate nondestructive assay (NDA) complement DA. M/S can help choose a good allocation of the measurement budget to DA plus sampling and mixing rules and to NDA. Reference [1] illustrates using MatLab how M/S helps allocate measurement budgets to reduce σ_{MB}.

It is then straightforward to derive a useful formula for a given strata with SNM total *T* in *N* items, $\sigma^2_T = T^2(\sigma^2_R/N + \sigma^2_S)$, which is a common approximate result that illustrates the main difference in how random and systematic errors propagate involving division by the number of measurements *N*.

Probably the most commonly used sequential statistical test to monitor for SNM loss in MB sequences is Page's cumulative sum (cusum). For MB sequences, the σ_{MB} concept is slightly generalized to a matrix Σ_{MB} measurement variances and covariances [18,19]. Simulation is typically required to estimate the DP of Page's test.

In summary, M/S for NMA studies require:
- models of material flows and inventories, including material holdup
- models of the measurement error process
- an implementation of the sequential statistical testing procedure

NMA is intended to detect but not necessarily deter diversion because balance closures are relatively infrequent, at least compared to NRTA. In addition, large throughput facilities have large σ_{MB}, so DPs can fail to meet IAEA detection goals. One effective complement to NMA is PM, as discussed next.

6. M/S FOR PM

Simulation for PM is more challenging and less developed than simulation for NMA. The increased challenge arises because PM simulations typically must track more components and be closer to the actual chemistry and physics of the real facility.

We consider four brief examples in Section 6, followed by a more detailed case study in Section 7.

6.1 MULTI-ISOTOPE PROCESS MONITOR (MIPM)

A monitor to detect isotopic composition shifts is being developed (MIPM, multi-isotope process monitor) that could detect certain types of facility misuse [20] on the basis of isotopic shifts.

Three computer codes are currently used in MIP: (1) ORIGEN-ARP to estimate isotopic composition in spent fuel [21]; (2) an interface called AMUSE to a commercial chemical engineering code (ASPEN [22]) to estimate the distribution of elements in organic and aqueous phases after the first separation stage (this estimation requires an estimate from code (1), and (3) Synth [23] or MCNP [10] to model the detected spectra.

MIP is intended to use measured spectra to detect changes, for example, in acid strength that might be associated with facility misuse to misdirect SNM into what should be a low-level waste stream. At least two key M/S concepts emerge in MIPM or MIPM-like studies. First, there is likely to be a systematic mismatch (“model bias”) between the model and the experimental data due to unmodeled effects [8]. For MIPM, unmodeled effects will include aspects of the detector response function, and isotopes that are omitted from the model. Second, the impact of natural process variation is not yet being considered in the MIP context, but should be relatively straightforward to evaluate by varying inputs to the computer codes.

6.2 COLD-STREAM CHEMICAL COMPONENTS CHANGE

The AMUSE code indices that cold-stream chemistry such as acid concentration and flow rate might be important to monitor because operator changes in the cold-stream chemical compositions could misdirect Pu [24]. One monitoring scheme can be thought of as providing a “book value” for SNM in specified streams that is based on the AMUSE model of the unit operation(s). Such a book value could have smaller uncertainty than the uncertainty based on comparing all input and output measurements of SNM. Reference [25] describes the potential impact of AMUSE uncertainty and process variation in corresponding monitoring schemes.

6.3 CURIUM MONITORING

A key safeguards measure in the head end of an aqueous reprocessing facility is based on indirect indication regarding the amount of Pu in the waste generated in the leached hulls following chopping and dissolution of the spent fuel assemblies. The indirect indication is obtained by detecting neutrons emitted primarily by Cm [3]. By assumption and/or continuing design verification, the head end provides no capability to separate the Cm from the Pu. Therefore, if neutron detectors detect no change in the Cm content, it is assumed that there is no change in the Pu content, and therefore, no diversion. This type of PM is semi-quantitative in that it can detect change in the neutron counts but it is difficult to model or estimate what neutron count rate corresponds to various misuse scenarios.

6.4 GLOVEBOX UNATTENDED ASSAY SYSTEM (GUAM)

In mixed-oxide fuel fabrication, the amount of plutonium (Pu) holdup in gloveboxes can be significant and therefore must be monitored. Reference [16] describes the GUAM (glovebox unattended assay system) system for measuring Pu holdup in gloveboxes in real time regardless of the status of the plant operations (static or dynamic). One challenge is that geometric variation in the Pu holdup can impact the measurement error, so M/S efforts using MCNP (MCNP5) are used to minimize measurement errors associated with geometric variations.

NMA that requires GUAM to estimate holdup or holdup change needs to model the random and systematic components of measurement errors (see Section 5). Current estimates of these components are based on MCNP modeling efforts, which will need to be benchmarked using holdup measurement studies. SM can contribute here by providing a "by-difference" estimate of holdup.

7. SOLUTION MONITORING (SM) AND EVALUATION SYTEMS (SMES) CASE STUDY

SMESs are described in [26]. SM can support NMA, for example, by helping to estimate *V* and *M* measurement error models, possibly by enabling *V* measurement bias adjustments, and by estimating SNM holdup. The IAEA's SMES, TaMES [27] (tank monitoring evaluation system) collates sample data with inferred plant status to generate tank inventory estimates. Its extension to process units would require model-based estimation of inventory [12]. Certain SMESs have more of a PM role than a support to NMA role. This is because their main focus is qualitative assurance that tank events such as transfers and sampling are in qualitative agreement with operator declarations. Thus, SMESs provide continuity of knowledge of tank activities.

SMESs currently installed in commercially operated plants were either implemented during commissioning, or after plant commissioning. They were configured, tested, and evolved using real measurement data. Therefore, SMESs are tuned to real operational activities and have had very limited exposure to events such as undeclared removals. There is anecdotal evidence to suggest that they would have benefitted from testing with simulated data prior to software acceptance. There is also anecdotal evidence that inspectors would have benefitted from training on an SMES, driven by simulated data. By using a simple whole plant simulation, [12] demonstrates that current SMESs have limited ability, partly because they lack internal simulation capabilities.

A few SMESs have been described that use model-based reasoning [26], particularly to flag and resolve anomalies. They reason using conservation laws because these laws closely relate to accountancy. A simulation that corresponds to the real SM system is used, which is based on the application of these laws. The simulation can be invoked by a trigger or at regular intervals. Once invoked, simulation boundary conditions (particularly mass transport histories) are estimated from measurement data. The simulation is then executed and its results are compared with measurement data to generate one or more errors vectors that are thought of as "symptoms" to be diagnosed. Reasoning processes then examine these errors to hypothesis, then order, possible causes. A particular hypothesis might be evaluated by re-executing the simulation and using an inverse modelling technique that chooses M/S parameters that best fit the observed data.

There are many types of data potentially available for SM for safeguards applications. Section 2.3 described the commonly-available in-tank (*L*, *D*, *T*, *V*, *M*) measurements. Reference [28] describes a relatively data-rich option that includes measured flows and constituent concentrations in all pipes entering and exiting connected tanks. True material flows and constituent masses for each of three tanks are simulated using first-order approximation to the associated differential equations for mass balances. Associated measured flows are also simulated using basic measurement error modeling. Analysis of the resulting time series of associated vector-valued prediction errors indicates important differences in the measurement error structures compared to those in the more common type of simulated SM data that does not assume flow rate measurements are available to help predict tank contents.

The DP results in [29] are optimistic because they were developed using simulated SM data that is thought to be "too clean" in that real data effects related to process variation and measurement effects are not well modeled. This implies that loss DP results estimated from simulated data are currently too optimistic. Multivariate statistical PM options (e.g., Crosier's multivariate cusum) have more recently been applied to residuals produced from simulated SM data that had no process variation, only random and systematic measurement errors [19].

Figure 1 is a schematic of some of the buffer, feed, and receipt tanks and processing equipment in an aqueous reprocessing facility. Figure 2 illustrates "vanilla" simulated data from the first cycle of some of the tanks and more realistic simulated data in the second cycle of the same selected tanks. The vanilla data was generated using the Glasgow University Reprocessing Plant Simulation Package (GURPSP) [12] in Python.

The estimated start and stop times of the input accountability tank's first receipt and first shipment are marked [ref]. Because the start and stop times are estimated, errors in event marking contribute to the *V* and *M* SRD error.

Figure 3 illustrates V residuals from wait and SRD modes from selected tanks. Such residuals are anticipated to be input to loss detection monitoring schemes. The magnitudes of these residuals will depend strongly on the process variation and measurement error models. Crosier's cusum can still be applied to these more realistic residuals, but the behavior of Crosier's cusum still needs to be evaluated in the no-loss and positive-loss cases. The tank 4 book value is based on a rudimentary model of the first separation cycle, with "tank 4" holding the highly active waste (HAW).

Figure 4 (a) is simulated residuals from 1000 *V* SRD measurements. Figure 4 (b) is a density estimate of the same 1000 *V* SRDs. The shipment measurements were generated using:

$$\text{shipment}_{\text{meas}} = \text{shipment}_{\text{true}}(1 + R + S + PV_1 + PV_2 + e_{\text{marking}}), \qquad (1)$$

where *R* is pure random error, assumed to have a normal distribution with relative standard deviation $\sigma_R = 0.02$, and *S* is systematic error, assumed to have a normal distribution with relative standard deviation $\sigma_S = 0.005$. These relative standard deviations are all relative to the amount shipped, or for receipts, relative to the amount of received material. The SRD is then $SRD = \text{Shipment} - \text{Receipt}$, and simulated receipts were also generated using Eq. (1) with the same values $\sigma_R = 0.02$ and $\sigma_S = 0.005$

There are two process variation terms in Eq. (1). The term PV_1 is also assumed to be normal with relative standard deviation $\sigma_{PV1} = 0.02$. The term PV_2 is a mixture [30,31] with equal (1/3) probability from three random signed values whose magnitudes are normal with relative standard deviation $\sigma_{PV1} = 0.01$. The signed values represent give-and-take quantities due to the solution transfer mechanism. A plus sign indicates a "give" to the pipes/pump and a minus sign indicates a "take" from the pipes/pump. The sign was randomly generated for each event, with a probability 0.5 for plus and 0.5 for minus to model random pattern in the sequence of "giving" and "taking" from the pipes/pump. This PV_2 is therefore a mixture of three mean values, with each value representing an average *M* or *V* amount given to or taken from the pipes/pump during each tank-to-tank transfer. If one averaged over many SRDs then the central limit effect implies that the average SRD should be approximately Gaussian in distribution. However, individual SRDs will exhibit the mixture behavior and because the SM system must also evaluated individual SRDs, the mixture model is needed.

Figure 4 (c) is the same as Figure 4 (a) but is for a second realization of the PV_2 mixture. Figure 4 (d) is the density estimate of the 1000 *V* SRDs in Figure 4 (c). The mixture effect is very clearly visible in (b), and also visible in (d). In Figures 4 (a) and (c), the two horizontal lines are at $\pm 2\hat{\sigma}_{SRD}$ where $\hat{\sigma}_{SRD}$ is the estimated standard deviation of the *V* SRD using the 1000 *V* SRDs from (a) and from (c), respectively. For (a), $\hat{\sigma}_{SRD}$ is approximately 5% relative to the true shipped *V* and for (b), is $\hat{\sigma}_{SRD}$ is approximately 7% relative. Averaged over all realizations of the PV_2 term, $\hat{\sigma}_{SRD}$ is approximately 5% relative to the true shipped *V*. Without using simulation, an incorrect calculation of the relative standard deviation (RSD) of the *V* SRDs assumes the four error terms in Eq. (1) capture all the *V* SRD measurement error. However, imperfect event marking which arises in real data and in our analysis of simulated data also contributes to the *V* SRD measurement error as can be seen by comparing the incorrect calculation $RSD = \sqrt{\sigma_R^2 + \sigma_S^2 + \sigma_{PV1}^2 + \sigma_{PV2}^2} = \sqrt{.02^2 + .005^2 + .02^2 + .01^2} = 0.03$ to the observed 0.05 (averaged over 10,000 realizations of the PV_2 term). This illustrates the that M/S can help assess the impact of marking error [32].

In Figures 4 (a) and (b), assuming a single-component Gaussian leads to overestimation of tail probability. For example, approximately 4% (based on 100,000 rather than 1,000 simulations) of the *V* SRDs exceed $\pm 2\hat{\sigma}_{SRD}$, and the 4% is repeatable across sets of 100,000 simulations to within ± 0.001. In the approximating single-component Gaussian approximately 5% will exceed $\pm 2\hat{\sigma}_{SRD}$. More extreme tail probabilities are also overestimated by a single-component Gaussian, and by a larger relative amount.

In plots 4 (c) and (d), assuming a single-component Gaussian leads to an underestimation of tail probability. For example, approximately 9% of the *V* SRDs exceed $\pm 2\hat{\sigma}_{SRD}$ while in the approximating single-component Gaussian approximately 5% will exceed $\pm 2\hat{\sigma}_{SRD}$. The approximating single-component Gaussian overestimates variance to compensate for ignoring the presence of multiple means. Whether this overestimation of variance leads to over or under estimation of tail area probabilities depends on the realization of the mixture distribution. This implies that *V* SRDs from each facility will have to be evaluated from each tank pair in order to set alarm thresholds. Our M/S software uses Eq. (1) with σ_R , σ_S, σ_{PV1}, and σ_{PV2} chosen so that the $\hat{\sigma}_{SRD}$ from simulated *V* SRDs is in close agreement with $\hat{\sigma}_{SRD}$ from real data.

Figure 5 illustrates that the relation between *V* and *L* impacts the correlation between measured *M* and *V*. Tank *V* is almost never a simple function of solution *L* because these large tanks have atypicial geometry, pipes penetrating the tank at varying levels, and possibly accumulation of organic material that impacts dip tube probe conductivity in different ways as a function of solution *L* [33]. Current M/S implementations do not include detailed tank geometry so the *L*, *V* relation is not modeled from first principles, but instead is chosen on the basis of experience with real facility data. Figure 4 and Equation (1) described process variation and measurement error effects on V. Figure 5 illustrates how our code (in `R`) simulated measured *M* to correspond to measured *V*.

At present, there are no methods to combine NMA and SM data. However, it is anticipated that a safeguards systems that combines NMA and SM will have higher DP for specified diversion scenarios. M/S is being used in the context of combining NMA and SM by: (a) modeling process variation and measurement error effects on *M* and *V* SM data as described an illustrated in Figures 3-5; (b) modeling the effects of facility misuse (misdirection of SNM), and (c) developing simulated training and testing data to evaluate candidate options to combine NMA and SM data. Note that tasks (a-c) have components of all six M/S goals in Section 4.2. For example, Eq. (1) has been developed on the basis of real tank data (refs) and can be regarded as a model-based summary of real data (goal #6 from Section 4.2).

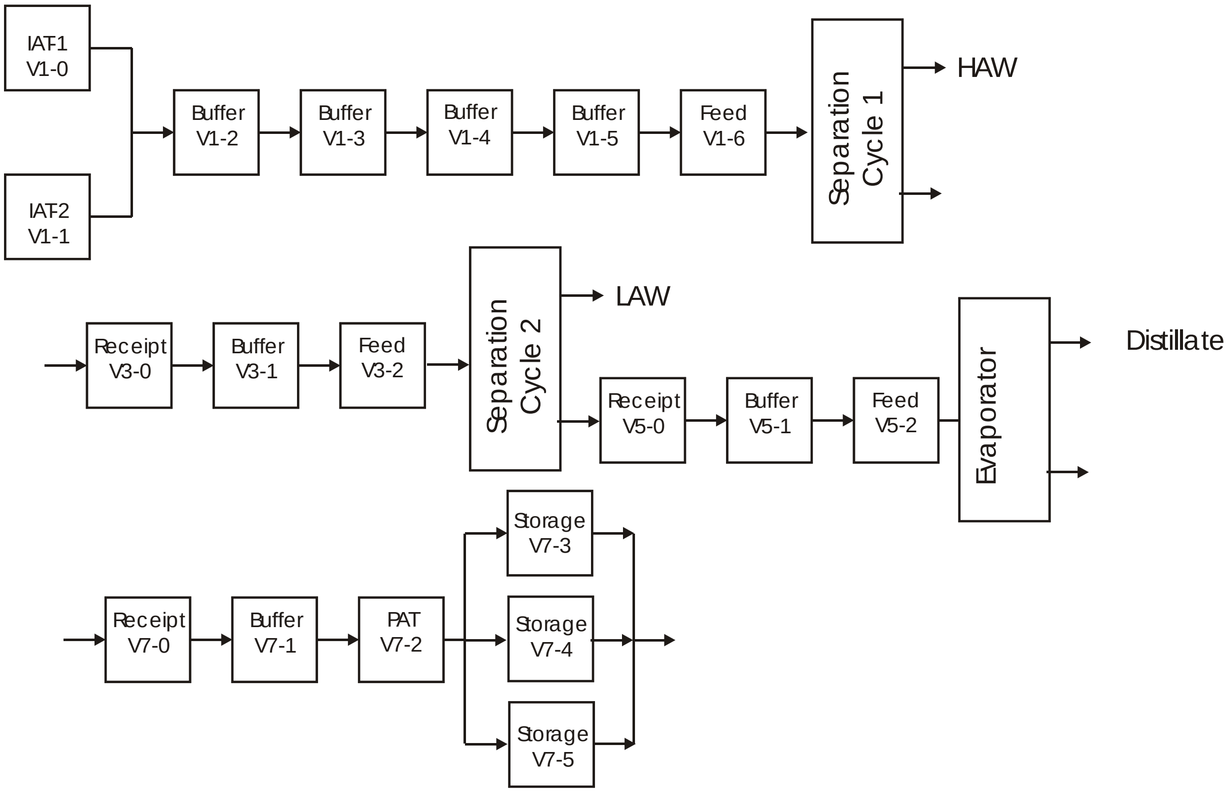

Figure 1. Example aqueous reprocessing facility layout with two input accountability tanks (IAT), one product accountability tank (PAT), several buffer tanks, and feed and receipt tanks surrounding the separations cycles. HAW is highly active waste; LAW is low active waste.

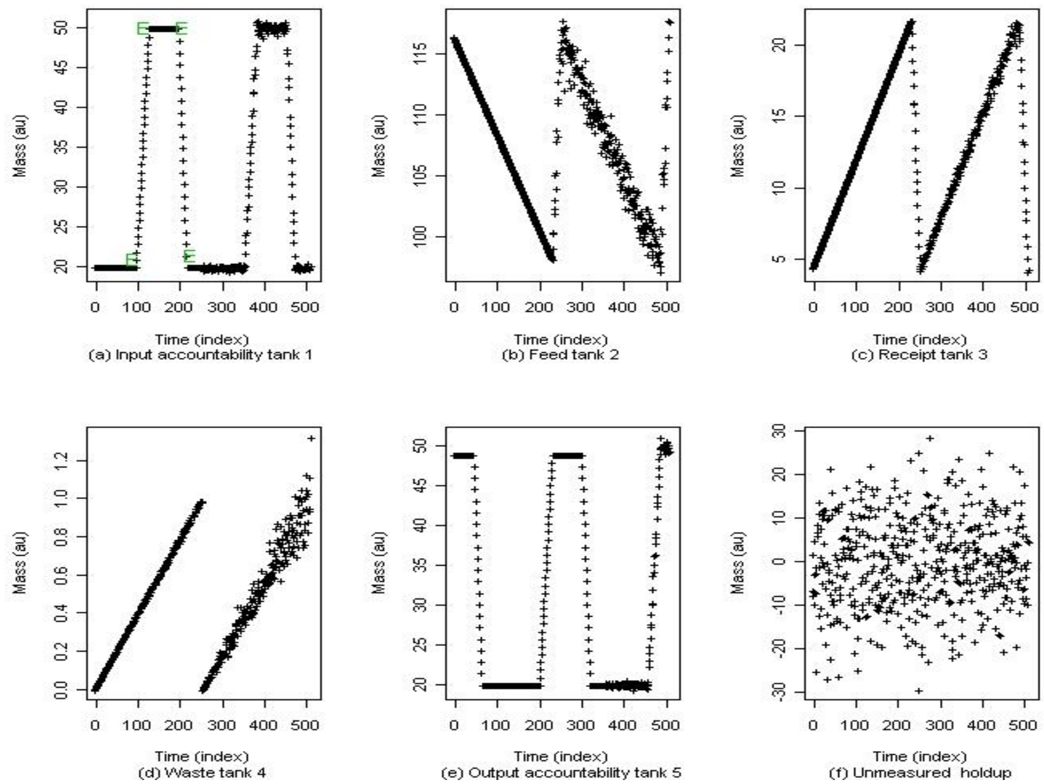

Figure 2. Simulated mass data in arbitrary units every 6 minutes from the indicated tanks. Unmeasured holdup represents the change in unmeasured holdup in the first separations cycle. The first tank cycle has zero process variation and zero measurement error. The second tank cycle includes process variation and measurement error. In (a), the "E" are the estimated start and stop times of the first receipt and first shipment.

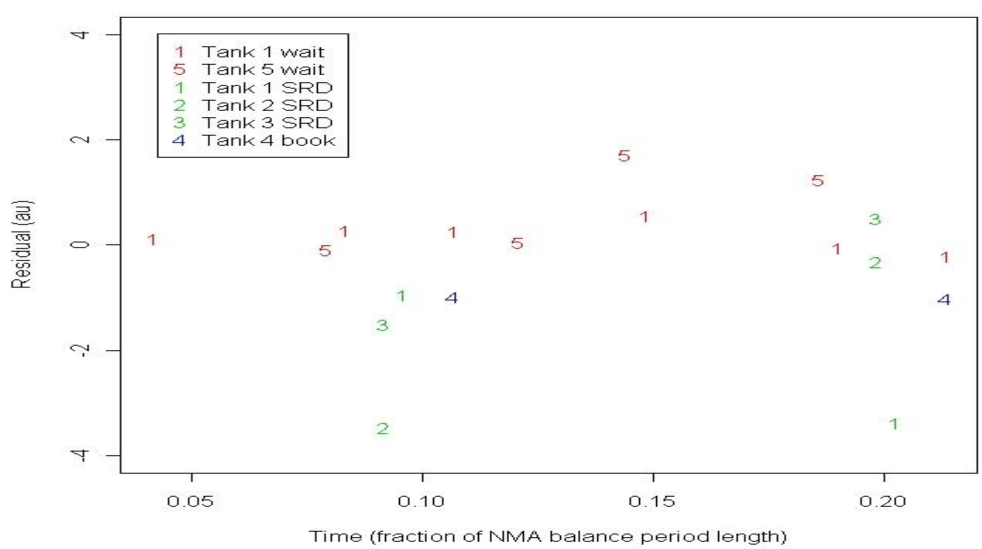

Figure 3. Residuals in wait and SRD modes for the indicated tanks.

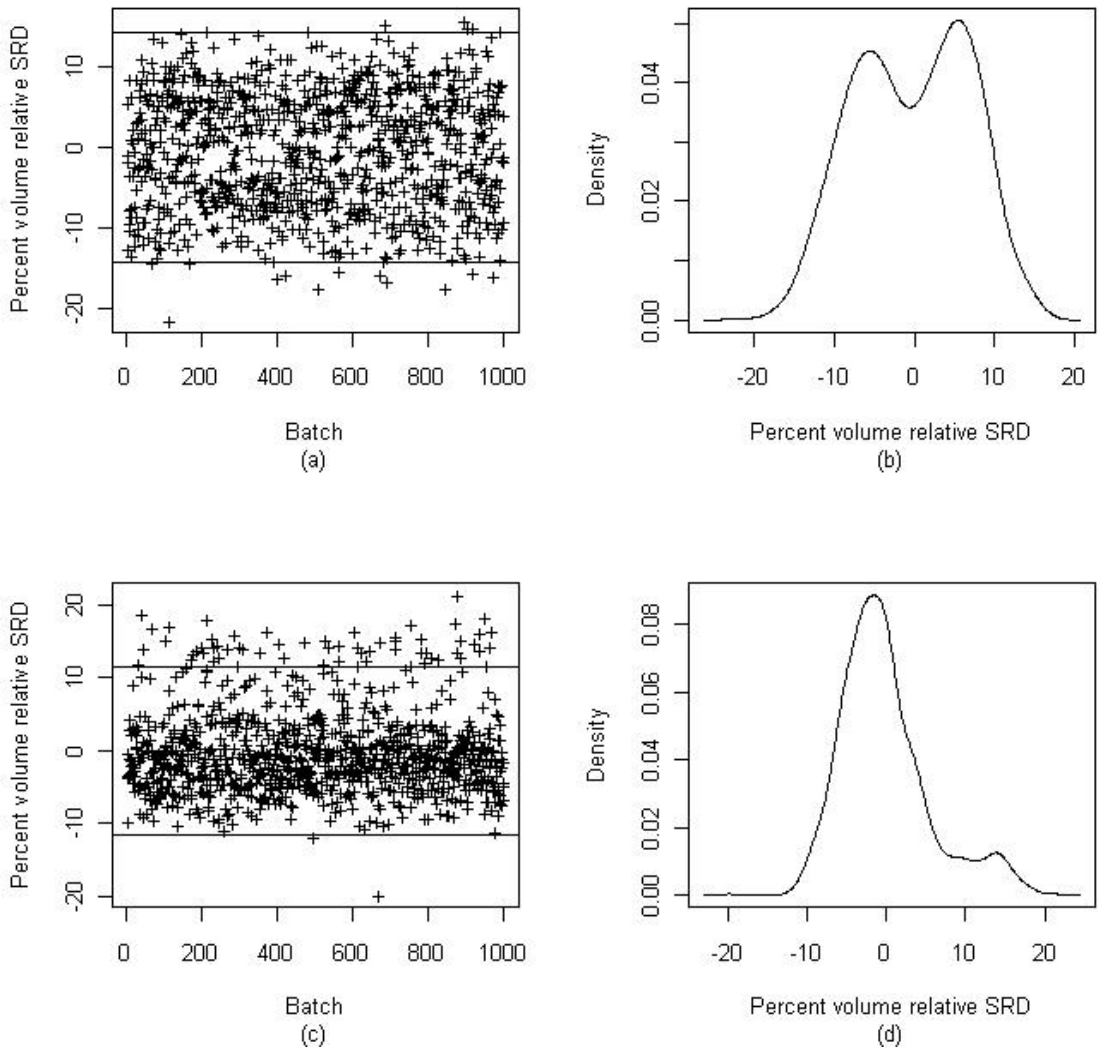

Figure 4. Volume V SRDs from tank1 to tank 2 for two realizations of the process variation 1 (PV1) mixture distribution. Plot (a) is the V SRD for each of 1000 shipments . Plot (b) is a density estimate of the same 1000 SRDs. Plot (c) is the same as plot (a), but for the second realization of the PV1 mixture. Plot (d) is the density estimate for plot (c).

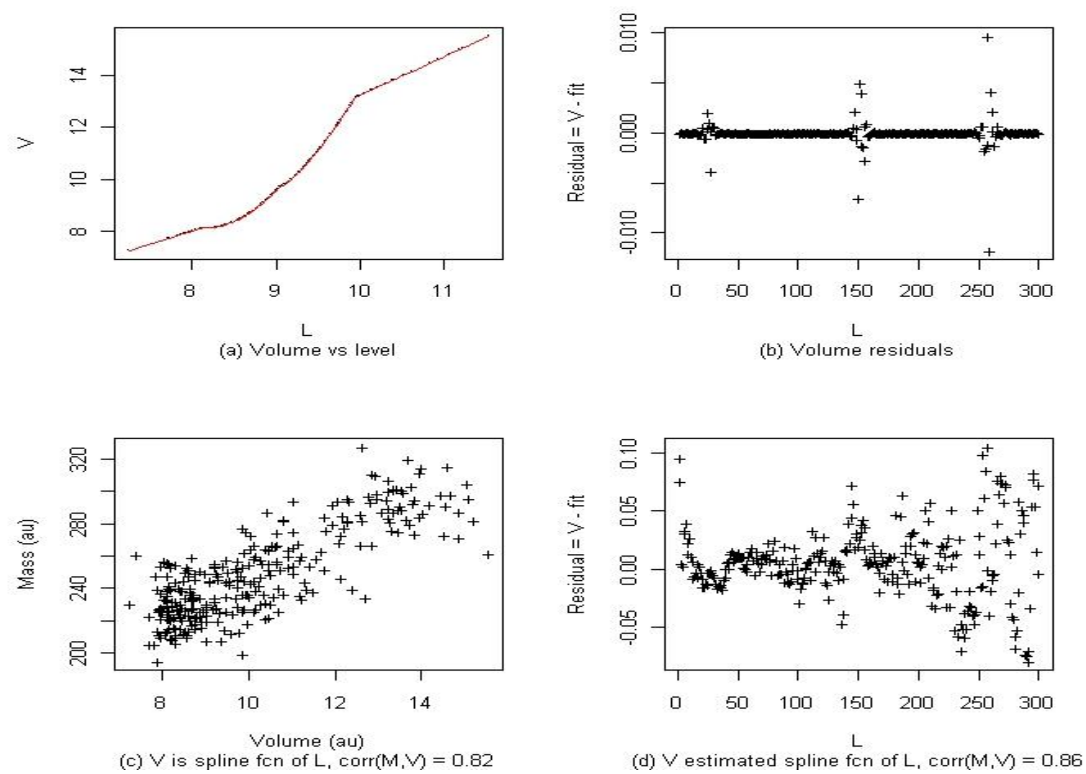

Figure 5. The relationship between *V* and *L* impacts the correlation between M and V, corr(M,V).

8. CONCLUSIONS AND SUMMARY

We have described some of the model and simulation (M/S) goals for nuclear material accounting (NMA) and process monitoring (PM), focusing on the simplest current M/S applications such as those used in solution monitoring that rely mostly on bulk mass and constituent mass balances to simulate real material flows. M/S efforts always require assessment of whether current model fidelity is fit for purpose, and the Section 7 example illustrated statistical modeling (Eq. (1)) of process variation due to details of how material is moved and measurement error effects, neither of which are modeled using first/ physical principles. We do not anticipate requiring a first /physical principles model for how material is moved or measured. However, it is necessary to develop a statistical model analogous to Eq. (1) for different material shipment methods such as pump/pipe, steam jet, or air lift. Analogously, Example 6.1 (MIPM) involving detected gamma spectra relies on first/physical principles to model source and transport terms, but for the modeled detector response relies on empirical assessment of fielded detectors rather than on first/physical principles modeling of the detectors.

The increasing role for PM requires M/S tools to characterize effects of facility misuse so that loss detection probabilities can be estimated for various monitoring options. Others are expanding the M/S goals as the safeguards community further develops M/S tools. For example, M/S is being used to predict SNM amounts in waste streams (Examples 6.2 and 6.3) using models of the dissolution operation in the head end of an aqueous reprocessing facility and using detailed chemical models of the separations process plus on-line monitoring of flow rates and constituent concentrations.

9. ACKNOWLEDGEMENTS

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