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Los Alamos
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OBJECT-ORIENTED PROCESS MODELING FOR MATERIAL-AT-RISK ESTIMATION[a]

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SUMMARY

Nuclear analytical chemistry/materials characterization operations at Los Alamos support many programs related to national security. These operations work with a wide range of material masses (microgram to tens of grams) and several forms (metal, oxide, and liquid). We have used detailed flowsheets for the chemistry and characterization functions to construct a process model of the facility operations. The model, constructed with the commercially available package Extend™, tracks material amounts and forms through the process of sample receiving through data return. The model calculates equipment utilization, throughput, and turnaround-time, as well as the material-at-risk and source term as a function of time for facility safety analyses. We see that the source-term is highly dependent on the material holding time, as expected; thus, proper material management policies are essential to operating a facility within regulatory guidelines regarding material-at-risk. In addition, we see that segregation of operations based on the material used can be beneficial to the overall operations.

I. BACKGROUND

Los Alamos National Laboratory (Los Alamos) currently supports many programs that require processing and analysis of nuclear materials. A key component to supporting the programs is the nuclear analytical chemistry and materials characterization (AC/MC) operations. This function is currently supported in the Chemistry and Metallurgy Research (CMR) Building at Los Alamos. The CMR Building was constructed in the early 1950s and resides on a fault line. Because of the age of the facility, its shortcomings relative to modern standards for nuclear facilities, and its unfortunate placement, Los Alamos and the Department of Energy have concluded that the CMR Building will no longer support nuclear operations in or about 2010. Los Alamos has been planning a replacement of the CMR Building since the mid-1980s. Originally, the Special Nuclear Materials Research and Development Laboratory would replace analytical chemistry operations and provide for aqueous chemistry research. The ending of the Cold War put this project on hold as the Department of Energy decided to reexamine the needs of the entire weapons complex given the potential for changing requirements. In the meantime, the CMR Building has continued to deteriorate and is becoming less useful as various systems degrade.

Nuclear facility construction often contains many more complexities than construction of other industrial facilities. A key component to any new nuclear facility is the calculation of the site-boundary dose in the event of a catastrophic failure of material containment (from fire, seismic, etc.). DOE-STD-3009[1] describes the method by which we can determine the safety-class and safety-significant systems to ensure that no person at the site boundary receives more than 25 rem over two hours. Calculations that address this issue require many assumptions about nuclear material amounts, leak paths, etc. to determine the source term for the accident analysis. In addition, DOE-STD-1027-92[2] describes the means by which a nonreactor nuclear facility is determined to be a Hazard Category 2 or 3 facility according to the material-at-risk (MAR). This paper describes work intended to provide a tool to more rigorously determine the source term for these safety-related calculations, in addition to other operating parameters that are of interest such as equipment utilization and sample turn-around-time.

A. AC/MC Operations

Los Alamos uses several key chemistry functions to determine various qualitative and quantitative

[a] A version of this paper was intended for presentation at the 2001 ANS winter meeting in Reno, NV, but was not presented.

properties of a sample. Most samples at Los Alamos are plutonium. Assay is often performed to determine amounts of plutonium in a sample. Mass spectrometers are used to determine isotopic ratios and abundances of minor constituents in a sample. X-ray fluorescence is used to determine trace impurities and abundances of alloying elements in metal samples. Existence and concentration of several nonmetallic elements, namely carbon, hydrogen, nitrogen, and oxygen is performed with interstitial analysis. Finally, standard radiochemistry operations provide isotopic and concentration information using natural or induced radiation from a sample.

Materials characterization operations are quite varied because they are used to determine many physical properties of a sample, including grain structure, chemistry, thermal/thermodynamic properties, mechanical properties, etc. These capabilities include electron microscopy, auger electron emission spectroscopy, ellipsometry, density measurement, calorimetry, electrochemistry, mechanical properties testing, sample rolling, particle analysis, x-ray diffractometry, and metallography. In general, materials characterization operations require larger samples than analytical chemistry operations.

Several operations must support AC/MC functions. Sample management receives samples into a facility or area, makes sample cuts, and collects data from the individual analysis areas. As with all nuclear facilities, a specialized waste handling area is required. Also, accurate chemistry analyses require a good standards fabrication team.

B. Material-at-Risk and Source Terms

The material at risk is a simple quantity of material in a given facility that is at risk of release in an accident. The source term, ST, uses the MAR quantity plus several other factors to determine the amount of material inhaled by a member of the public at the site boundary. These additional factors in the source term equation account for material that actually reaches the site boundary:

$$ST = MAR \times ARF \times RF \times DR \times LPF \qquad (1)$$

where

MAR = material at risk [g];
ARF = airborne release fraction;
RF = respirable fraction;
DR = damage ratio; and
LPF = leak path factor.

To be conservative, we generally presume that the damage ratio and the leak path factor are both unity. This presumes that the facility itself provides no containment of the material. Given that we track three material forms (metal, oxide, and liquid), the source term equation formally becomes

$$ST(t) = \sum_{i=1,3} MAR_i(t) \times ARF_i \times RF_i \qquad (2)$$

where the summation indices relate to the three material forms. The airborne release fraction and respirable fractions are derived[3] from DOE-HDBK-3010.[4] These quantities are listed in Table 1 for the three material forms of interest.

Table 1. Source Term Data

Quantity	Oxide	Liquid	Metal
ARF	0.045	0.002	0.002
RF	0.88	1.0	0.5

II. PROCESS MODEL

The discrete-event model of analytical chemistry operations, constructed using EXTEND™[5] simulates the functionality of analytical chemistry sample analysis. The model tracks the progress of samples from delivery to the chemistry facility or facilities, through sample management, to various analysis areas that contain sample preparation, measurement, and data reduction operations, and back to sample management for report collecting for delivery of results back to the requester. The sample management operations generally send sample "cuts" of various sizes to the analysis areas. The analysis areas (e.g., radiochemistry, trace elemental analysis, isotopic analysis) process the samples through sample preparation steps, which may involve a change in material form through a dissolution process, then the sample is analyzed, and the results of the analysis are obtained. The sample is then held in the analysis area for a specified time before disposal. We also retain the sample remnant (that which remains after all cuts are sent to the sample analysis areas) in the sample management area for six months. This hold time is intended to model sample retention in the event of a requester asking for more data or reanalysis.

Depending on the assumed suite of available instruments and the demand for their utilization, the time between receipt of samples and delivery of results, or turnaround time, varies between samples. Samples can be randomly returned

within an analysis area for reanalysis, and material holdup in waste containers is modeled as a discrete time delay between sample analysis and disposal. The model can analyze the nature of turnaround time variability as well as the effect of boundary conditions and various aspects of system performance. The residence time of a sample has a direct effect on the time-variable MAR and source term, which is calculated according to Eq. (2). The principal operating parameters required by the model are the process times, sample material form and mass, and information from process flowsheets that indicate where material form changes (e.g., converting a metal to a liquid) occur.

A. Model Assumptions and Parameters

EXTEND™ models use a hierarchical graphical structure to establish the process material and information flow. It allows various components of the model to be governed by parameters that affect operation, such as delays, shutdowns, combinations, and batching. Some of the more important assumptions are discussed in this section, with specific parameters being discussed in the next section.

The model presumes that operations occur for eight hours per day, five days per week. As mentioned previously, the sample remnant is held in sample management for six months, and nuclear material sent to the analysis areas is held there for a prescribed time (0 days, 1 week, 1 month, or 2 months) to model holdback in case of a requested reanalysis. Samples masses vary from 5 to 20 grams, based on the program that sends the sample, and 0.01 g to 15 g are sent as cuts to the analysis areas based on the analysis requirements. The model does not perform isotopic material balances, so all material is presumed to be a 94%/6% mix of Pu-239/Pu-240.

B. Instrument Parameters

The primary model parameters are those that control the amount of time a sample is delayed for processing. These parameters are used in the sample analysis areas. These parameters, along with the flowsheets that define the structure of the model, were obtained from process experts at Los Alamos. Delay times are specified for sample preparation, sample analysis, and data reduction. In addition, the sample preparation delay time is a function of the sample material form. The samples can be prepared or analyzed in batches, so a batch size is also specified. Occasionally a sample is reanalyzed, so a percentage of samples that are rerun is also specified. To model the effects of equipment unavailability due to equipment failure, a general "availability" parameter is defined. This parameter is defined such that it is the percentage of events where a sample is sent to an analysis machine and the instrument is available to process the sample(s). A set of sample model parameters for a few of the instruments is shown in Table 2.

Table 2. Sample Model Parameter

Analysis	Met. Prep. Time (h)	Analysis Time (h)	Batch Size	Avail-ability (%)
ICP-MS	11	11	8	50
Fe Coul.	18	17	6	95
TI-MS	25	13	5	90
Metall.	10	15	1	95

III. RESULTS

As mentioned previously, a variety of model results are of interest to facility planners. The primary results desired are usually equipment utilizations and requirements and sample turnaround times. However, we will focus on the MAR results in this paper.

We run the model over the period of 450 days with 3,765 samples sent for analysis. This sample source is based on informal projections of what programs will reside at Los Alamos in the future and what their sample requirements might be. The number of samples sent to the chemistry operations is uniformly distributed throughout one year, and the remaining time (~85 days) is used to process the samples that arrived late in the year. As mentioned, a primary parameter in the model is the material holdup time in the analysis area after the sample has been analyzed. The model is run for the specified time and the MAR in the task areas is determined as a function of time.

As would be expected in nuclear materials management, the longer residual materials are held in a material area, the larger the MAR will become (without a "sink" term, the material holdings will increase without bound). Figure 1 contains a bar graph of the maximum MAR throughout the year for the individual task areas.

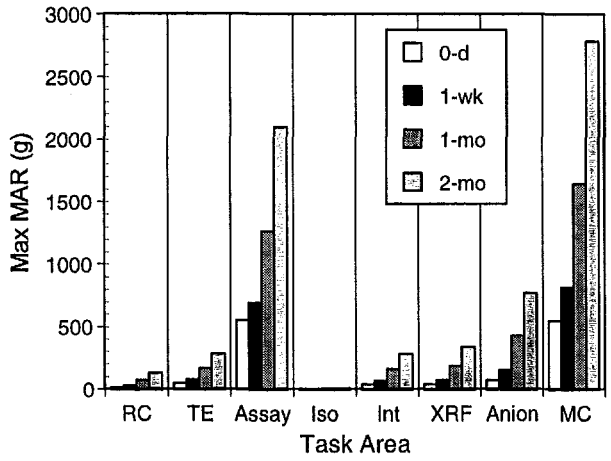

Figure 1. Maximum MAR for task areas.

According to DOE-STD-1027-92, the demarcation between a Hazard Category (HazCat) 2 and 3 facility is 900 g Pu-239; i.e., if a facility typically contains more than 900 g Pu, it should have the safety systems for a HazCat 2 facility. In general, the cost for a HazCat 2 facility is significantly greater than that for a HazCat 3 facility. Based on Figure 1, We see that the assay and materials characterization task areas need to be in a HazCat 2 facility; however, the other task areas could function in a HazCat 3 facility.

Figure 2 contains the total MAR for all the task areas shown in Figure 1 except assay and materials characterization. If we use the 900 g limit, we see that all these functions can be housed in a Hazard Category 3 facility, but that legacy material must be removed from the facility within one month to comply with the DOE standard.

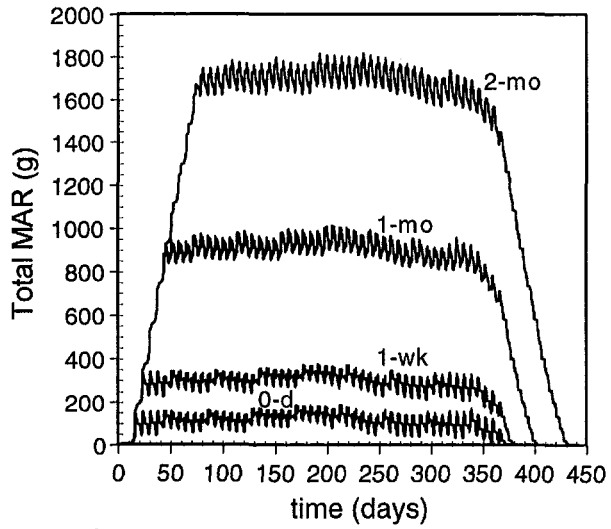

Figure 2. Combined task areas MAR.

The model calculates the maximum MAR (2-mo task area holdup time) in the facility to be 17,000 g Pu, but the vast majority of this mass resides in sample management sample remnant retention (recall we assume these sample remnants remain in sample management for six months). The maximum source term for this case is 340 grams. If we examine the Figure 2 task areas alone, the maximum MAR over the year with a 2-mo holdup time in the task areas is 1,700 grams (maximum source term = 7.9 g).

IV. CONCLUSIONS

Clearly, process modeling can be very useful for nuclear safety analyses. Rather than performing gross estimation, a more rigorous calculation can be performed to estimate material at risk based on actual processing parameters. In addition, the various MAR results can assist facility designers to design multiple facilities for nuclear operations, each of which is suited for the amounts of material housed therein. We anticipate that this tool will be used as conceptual design for a new facility or set of facilities progresses.

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