Simulation of Nuclear Analytical Chemistry Operations

Robert J. Burnside, 505/667-1397
Nelson DeMuth, 505/665-4494
Richard F. Farman, 505/667-3854
Drew E. Kornreich, 505/667-2095
Los Alamos National Laboratory
P.O. Box 1663, Los Alamos, NM 87545 USA

ABSTRACT
This paper describes the object-oriented, discrete-event simulation model of nuclear analytical chemistry operations developed at Los Alamos National Laboratory. Analytical chemistry supports nuclear materials and waste characterization, quality control, and process control. Some major requesting organizations for analytical services are metal preparation, manufacturing, recovery, and waste management. The model tracks the progress of samples from delivery to analytical chemistry through sample management, sample preparation, measurement, data reduction, data management, to delivery of results back to the requester. Analytical chemistry is a key component of material verification and control efforts, and is therefore important to the materials accountability community.

INTRODUCTION
A major mission for Los Alamos National Laboratory (Los Alamos) came in late 1996, when the Department of Energy (DOE) issued a Record of Decision1 to reestablish pit fabrication capability at Los Alamos. In efforts to analyze the requirement for Los Alamos to fulfill the pit-manufacturing mission, focus was placed on analytical chemistry operations and how they support missions related to pit fabrication. Construction of a process model for analytical chemistry operations began in 1997 and resulted in a report describing data collection efforts, including flowsheets, and process model construction.2 The focus of this effort was to determine the equipment needed for various pit-manufacturing missions for Los Alamos. For analytical chemistry and materials characterization work, we used existing and projected data as input to a model of these operations.

Depending on the suite of available instruments and the demand for analytical chemistry results, the time between receipt of samples and delivery of results, or turnaround time, varies between samples. The model can analyze the nature of this variation as well as the effects of multiple shifts, sample batching, overtime, and applications of advanced techniques. The model has been applied to many issues concerning equipment utilization, facility requirements, and conduct-of-operation plans. Since this type of modeling effort directly addresses specific nuclear material items, it can be used to assess the time evolution of nuclear material inventory in an analytical chemistry environment. Application of this model to ascertain the capability of a new nuclear analytical chemistry facility with strict inventory controls will be discussed.
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**Simulation Model**

The discrete-event model of analytical chemistry operations, constructed using EXTEND\textsuperscript{TM}\textsuperscript{3} simulates the functionality of analytical chemistry sample analysis. The model tracks the progress of samples from delivery to the CMR Building 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 top-level representation of the model is displayed in Figure 1.

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. The model can analyze the nature of this variability as well as the effect of boundary conditions and various aspects of system performance. Examples of system performance features that we can study with the model include

1. Instrument performance, availability and reliability (The simulation can use a variety of stochastic models for mean-time-to-failure and time-to-repair.);
2. Inventory of available instrumentation;
3. Methods of sample preparation and batching strategies; and
4. The structure of shift operations.

The structure of an EXTEND\textsuperscript{TM} model is manipulated through a graphical interface that contains symbols representing the functions of the process being modeled. EXTEND\textsuperscript{TM} has the capability of imbedding its components hierarchically, so that complex functions can be displayed as visually simple model components. Figure 1 shows the top-level representation of the analytical chemistry
model.

The principal operating parameters required by the model are the "process times," which are the times required for each unit operation. Values of process time employed in the model were obtained from meetings with the individual analytical chemistry teams responsible for the different processes. Brief descriptions of the major top-level blocks in Figure 1 are provided below.

The Sources block generates the sample input. The model is configured to read two forms of input data. In its original form, the Sources block reads the annual number of samples of each type sent to analytical chemistry and delivers them in periodic batches. Attributes are read from a text file and assigned to each sample. These attributes include flags to identify the sample type, origin, and measurement requirements. This input is configured to send a given number of identical sample types, based on form and measurement requirements, periodically over the year. A new version of the input sends individual samples at given times to the model – each sample is, in principle, unique based on when it enters the system. The block gives each sample a unique identifier and records the time that it entered the system.

The Sample Management block examines the analysis requirements attributes of each sample and routes sample cuts to the appropriate analysis areas. The sample routing to the various analyses is governed by the information attached to the samples coming from the Sources block. A sample attribute list is examined to see if the sample is to be sent to the first analysis. If so, the sample is cloned for further examination to see if it will undergo a different analysis type. If not, the cloning is bypassed and the sample is forwarded down the list to the examination for the next analysis type. This cascades through the checks for all analyses. After checking the attributes, the sample cuts are sent to the task areas for analysis.

The Task Area blocks shown on the right side of Figure 1 represent the various analysis areas (e.g., radiochemistry, trace elements) that perform the analyses on the sample cuts. The model description of the functions of these blocks exists at the next level of detail in the modeling hierarchy, which basically consists of three blocks: sample preparation, analysis, and data reduction. The sample to be analyzed comes in and is sent to the sample preparation area where it is batched. The batching process checks the queue to make sure samples do not wait for a full batch before going to the analysis. These sample batches enter a queue in front of the analysis block, which contains blocks for scheduled and unscheduled downtimes. The unscheduled downtimes are the result of equipment failure and repair. After the analysis, some sample batches are stochastically redirected back for analysis. The data reduction section includes a delay for this operation and then unbatches the samples.

After a sample has been analyzed in a particular task area, it is returned to the LIMS block. In the LIMS block, the samples are collected from the task areas as they are completed. A matching block delays the sample until all analyses are completed. When this criterion is satisfied, the sample is sent to the results block.
The *Results* block receives samples for which all analyses are complete. The block obtains the system time that the sample enters and subtracts from it the time the sample entered the system. This difference is the sample turnaround time, which is recorded in a data block.

**MODEL PARAMETERS**

The sample preparation, analysis, data reduction, and matching blocks contain features that hold a sample for a given time. The delay times are an integral feature of the model because they directly relate to the possible sample turnaround times. In addition to delay times, the model also requires equipment availability, batch size, and rerun frequency information. A value identified as the “process time” represents the nominal rate at which the operation is capable of performing its function. The reason for this condition is that the model needs to capture the average production rate over a repeatable time interval. This interval does not always reflect the actual processing time occupied by the operation. For example, any operation that must be performed in a contiguous time period longer than half of a shift but less than a whole shift can only be performed once per day. Thus, while its actual process time can be less than one day, say six hours out of an 8-hour shift, the effective process time is one complete day. From the viewpoint of the overall production rate of the system, the effective process time of the components governs overall production rate. The specific process times that are in the model for each task area are

1. Sample Preparation Time for Task Area – the time [h] for preparing the sample in the task area based on the sample form (metal, oxide, liquid, or gas);
2. Analysis Time for Task Area – the time [h] for performing the analysis. This is assumed to be the time that the machine is required for the analysis;
3. Data Reduction Time for Task Area – the time [h] for performing data reduction after completion of the analysis;

Occasionally in analytical chemistry operations, a single analysis run can hold several sample cuts. This batching phenomenon is captured in the model where appropriate to accurately reflect the throughput. As expected, the more batching than can be done, the larger the possible throughput is. All processing times apply to the batched quantities, where appropriate.

A sample preparation or an instrument measurement may fail and require repeating. The model simulates this effect with a diverter-block that is triggered by a random number generator. Intentional reruns or multiple analyses for a single sample have not been incorporated into the model.

Availability is the fraction of normal operating time that the instrument or process is operational. It could be inoperative because of a component failure, routine maintenance, facility downtime, and/or personnel unavailability. The model contains logic to randomly impose occasional shutdowns on the processes to simulate this kind of behavior. For example, 90% availability mean that nine times out of ten the machine/equipment is not broken when it is to be used. To show the kind of data that feeds the internal structure of the model, some sample data from the radiochemistry operations are shown in Table 1.
**Table 1. Radiochemistry Model Equipment Parameters.**

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**Some Sample Results**

To estimate the requirements for a replacement analytical chemistry facility, we now examine the performance of the analytical chemistry model given a projected set of samples by program area. The projected sample loading is loosely based on past work, which assumed a pit production level at Los Alamos of approximately 50 pits/yr. Current anticipated projection levels were reduced, so the projected number of samples for the pit-manufacturing program was reduced by a factor of two. Combining the information in these two references along with the analyses performed on samples during 1999 (by program), we estimate the number of samples by analysis type. Other documents may be accessed for information regarding the details of the programmatic activities.

For this analysis, we only run the 100% personnel availability model. This presumes that, for economy, equipment will be utilized as much as possible by hiring enough personnel to operate the equipment. The results of the equipment modeling can then determine personnel requirements based on equipment utilizations.

In all cases, we define the turnaround time as the time within which 95% of the samples will be completed (in terms of a normal distribution, the mean plus two standard deviations). The goal is to add equipment to obtain a 15-day turnaround time. Thus, by providing a desired turnaround time, the equipment requirements can be obtained from the results of the model. Most of the analysis types require only one preparation, analysis, and data reduction station. Figure 2 contains graphical representations of the analysis areas that required additional stations to reduce the turnaround times, where “P” indicates sample preparation, “I” indicates the analysis instrument, and “D” indicates data reduction. For example, if a 15-day turnaround time is required, then nine sample preparation stations are required for TI-MS; however, if 30-day turnaround time is required, then eight will suffice. In both cases, five instruments are required for the projected sample requirements.
MODEL IMPROVEMENTS AND ADDITIONS
The analytical chemistry model is relatively crude compared to other models we have constructed. The random equipment shutdown mechanisms (a simple availability) are very simplistic, and the reduction of all process to three steps is a simplification that disallows certain analyses. We intend to focus on several improvements to the model and the data that support the model in the future.
Quantify Sample Generation and Size
The primary information supplied to an established model usually consists of boundary or initial conditions and operational parameters. We derive operational parameters from the process being modeled, and these parameters are usually independent of the boundary conditions. For analytical chemistry operations models, the key boundary condition is the sample input to the system. This input can be a function of time and function of the analyses required. In general, estimating sample requirements is very difficult and has been performed by using the experience of programmatic personnel. The lack of structure in estimating sample requirements could be addressed by a significant data gathering effort to examine all analytical chemistry sample sources from pit production and elsewhere based on current operations. Subsequent modeling efforts then allow us to quantify the changes in sample generation as programs change over time. Gathering the required data and implementing the facility-wide plutonium-processing model would be a significant effort, but would vastly improve predictive capability of requirements for analytical chemistry operations at Los Alamos.

Improve Model Fidelity
In terms of the analytical chemistry model itself, the current model is relatively crude as compared to other models that we have constructed. Basically, a given analytical chemistry operation is modeled simply as a serial process consisting of sample preparation, analysis, and data reduction. No explicit modeling of personnel availability or equipment failure and repair is modeled. Equipment failure is simply modeled using an equipment availability factor obtained from unit operation details. The fidelity of the analytical chemistry model could be significantly improved by including specific instrument downtime, personnel, and more detailed material flow information. These improvements again will require a concerted data gathering effort and would require significant personnel resources to accomplish. Specifically, we would be interested in how each instrument can fail and how long it takes to repair, how many technicians and staff are required to operate a given instrument, and more detailed flowsheets that show material splits, waste generation sources, etc.

Material Balance Determination
Having material balance information as a model output would allow estimates of equipment, room and building material holdings. This information is vital for facility planning, as the more material is located in the building, the more important safety and security issues are in the facility design and construction. Current plans are to construct a replacement for the facility where nuclear analytical chemistry operations are performed. The current facility was constructed and occupied in the early 1950s and does not conform to current seismic standards; also throughput may be limited by restrictions on the amount of material allowed on the floor at a given time. The amount of material-at-risk in a design-basis accident (earthquake, subsequent fire, and loss of material containment) is limited by the offsite dose limits from the accident; therefore, planning for a replacement facility must include information such as the material-at-risk to ensure the facility will meet programmatic requirements.
REFERENCES

