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# Object-Oriented Process Modeling for Material-at-Risk Estimation

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## I. Background

Nuclear facility construction contains many more complexities than construction of other industrial facilities. Los Alamos National Laboratory has been planning a replacement of its 1950s vintage nuclear analytical chemistry facility, the Chemistry and Metallurgy Research (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.

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 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 a 25 rem over two hours. Calculations that address this issue require many assumptions about nuclear material amounts, leak paths, etc. This paper describes work intended to provide a tool to more rigorously determine the source term for these safety-related calculations.

## II. MAR Calculations

The site-boundary dose calculation relies on a source-term calculation that determines the amount of nuclear material released into the air. The source term is given by the following equation [Ref. 1]:

$$\text{Source Term} = \text{MAR} \times \text{DR} \times \text{ARF} \times \text{RF} \times \text{LPF} , \quad (1)$$

where

MAR = material at risk [g];

DR = damage ratio [conservatively valued at 1];

ARF = airborne release fraction [g];

RF = respirable fraction [g];

LPF = leak path factor [conservatively valued at 1].

The postulated accident can have a significant impact on the values of the ARF and RF, and the variability of the results presented in Ref. 1 can result in engineering judgment being required to estimate the ARF and RF for a given accident. These factors are also a function of material form, such as metal, oxide, or liquid. We use the factors for a fire as given in Ref. 2.

## III. Process Modeling

The discrete-event model of analytical chemistry operations, constructed using EXTEND,<sup>TM</sup> [Ref. 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 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) 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 also 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 source term, which is calculated according to the following formula:

$$ST(t) = \sum_{i=1}^3 ARF_i \times RF_i \times mass_i(t) , \quad (2)$$

where the three components are metals, oxides, and liquids. The principal operating parameters required by the model are the process times, material form and mass, and information from process flowsheets that indicate where material form changes (e.g., converting a metal to a liquid) occur.

#### IV. An Example

We run the model over the period of 450 days with 3,765 samples sent for analysis. The number of samples sent to the chemistry operations is uniformly distributed throughout one year, and the remaining time is used to process the later-time samples. The initial samples vary in size between 5 and 20 grams of nuclear material, and the cuts to the various analysis areas vary from 0.01 to 15 grams. The suite of analyses that is required for a given sample is also defined in the input information. There are 24 analysis types in nine generic task areas.

Figure 1 shows the material in the radiochemistry task area as a function of time. The initial buildup of material is evident, the MAR levels off for all material types, and then the final samples are processed at the end of the year. The difference in MAR between metals and oxides versus liquids indicates that metal and oxide samples are dissolved as soon as they enter the radiochemistry task area. Given the sample generation rate, the MAR in radiochemistry is approximately 20 grams of nuclear material. The maximum MAR in the facility is calculated to be 17,000 grams, but the vast majority of this mass resides in sample management sample remnant retention (recall we assume these remnant remain in sample management for six months). The maximum source term for this case is 340 grams. If we examine the task areas alone, the maximum MAR over the year is 1,700 grams (maximum source term = 5.4 g).

#### V. Summary

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.

## References

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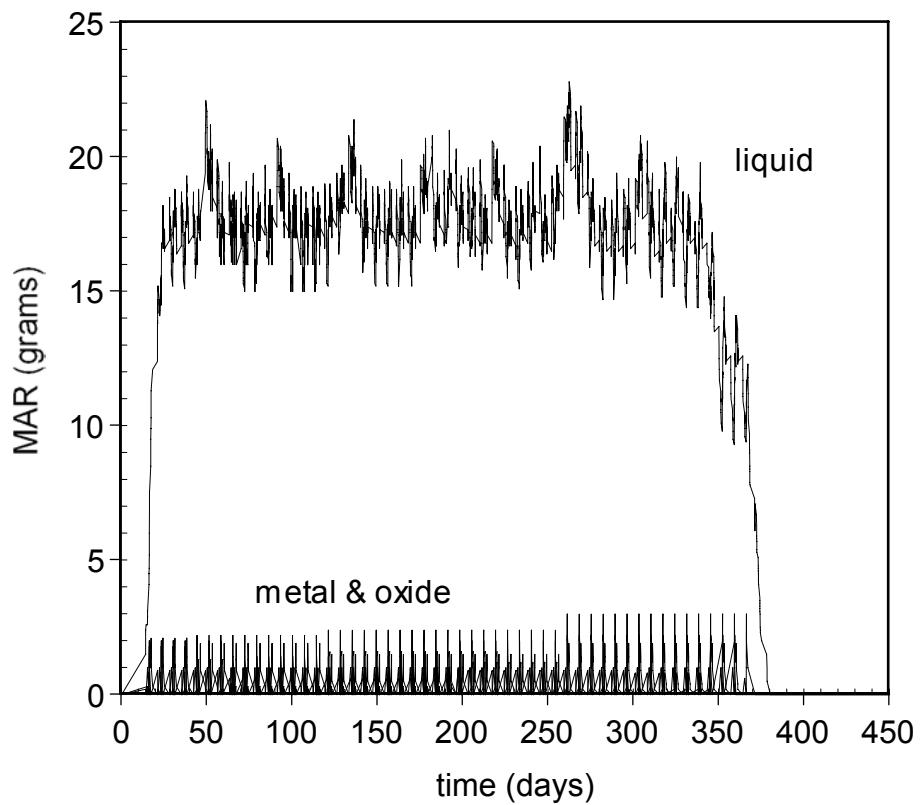


Figure 1. Time variation of material in radiochemistry.