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A VALUE OF INFORMATION APPROACH TO DATA QUALITY OBJECTIVES FOR THE HANFORD HIGH-LEVEL WASTE TANKS

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ABSTRACT

This report summarizes a Pacific Northwest Laboratory[a] review of the organic-nitrate reaction safety issue in the Hanford single-shell tanks. This study employed a decision analytic method known as Value of Information (VOI). VOI analysis is a special form of decision analysis that has an information collection alternative as one of the initial decision choices. This type of decision analysis, therefore results in the ability to specify the preferred information collection alternative, taking into account all information gathering and other relevant alternatives. For example, the risk reduction benefit associated with further sampling to quantify total organic carbon inventory or to improve information on energetics can be compared to the risk reduction benefit of better temperature monitoring, operational restrictions, or mitigation by moisture control. This approach allows freedom from built-in assumptions, e.g., that all tanks *must* be sampled to some degree or that all tanks *must* be deemed intrinsically safe by some means or another. It allows for each tank management decision to be judged in terms of risk reduction from the current state of affairs, and for that state of affairs to be continuously updated to incorporate new information on tank contents, the phenomenology of safety issues, or the effectiveness of mitigation schemes.

ORGANIC-NITRATE SAFETY ISSUE IN HANFORD HIGH-LEVEL WASTE TANKS

This report summarizes a study conducted by the Pacific Northwest Laboratory of the organic-nitrate reaction safety issue in the Hanford single-shell tanks (SSTs). Production of nuclear weapons materials began at the Hanford Site in 1944 and continued until 1990. Radioactive wastes from the reprocessing operations were stored as alkaline liquids and slurries in near-surface underground tanks. One hundred forty-nine SSTs, ranging in capacity from 208 m^3 to 3,800 m^3 (55,000 to 1 million gallons), contain approximately 14,000 m^3 (36 million gallons) of waste damp saltcake (predominately sodium nitrate and sodium nitrite), metallic hydroxides, other insoluble metal salt sludges, plus about 2,300 m^3 (600,000 gallons) of supernatant liquid.

Organic materials were used in several applications in the separations of nuclear materials at the Hanford Site, and many of the waste types generated included organic materials. These included ethylenediaminetetra-acetic acid (EDTA), N-hydroxy-ethylenediaminetetra-acetic acid (HEDTA), sodium citrate, sodium acetate, normal paraffin hydrocarbon (NPH), tri-butyl phosphate (TBP), and hundreds of miscellaneous compounds used in small-scale applications at the Site.[1] An estimated "average chemical composition" of these organic materials approximates sodium acetate.[2] The waste materials have been degraded by radiolytic and chemical attacks in the waste tanks but still retain significant potential fuel value.[3]

The presence of the organic materials in the waste tanks is of concern because of the following: 1) saltcake wastes are rich in $NaNO_3$ and $NaNO_2$, 2) efforts have been expended to remove the bulk of drainable liquids from most tanks, and 3) several tanks contain wastes with significant decay heat. Taken together, these factors could create conditions favorable for an organic-nitrate reaction.

DATA QUALITY OBJECTIVES

Data quality objectives (DQOs) are specifications that describe data that are adequate for a particular purpose. In a typical waste characterization problem, DQOs would specify the analytes to be measured, the sensitivity required (detection limits), the accuracy of individual measurements, the spatial volume of material for which

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measurements are deemed representative, and other such features. In addition to a generic label for this type of data specification, "DQO" has also been used to describe a specific process for deriving these specifications.[4] While some benefit has accrued from applying this method to tank waste problems, the organic-nitrate reaction risk issue was sufficiently complex in terms of phenomenology, number of options, and statistical issues to require structured decision analysis tools.

These decision analysis and risk management tools enhance the standard DQO methodology and allow it to be more responsive to the needs of tank waste characterization. In addition, these methods allowed an integration of the DQO domain (what and how to sample) into a much broader set of risk management decisions: what criteria are appropriate, how conservatively should they be applied, what mitigative actions are "risk-effective," and what incentives exist for developing more effective mitigative measures.

ORGANIC-NITRATE REACTION RISK

The following section describes the organic-nitrate reaction risk. The chemical reaction is introduced with potential initiators and propagation requirements. The reaction risk model is presented with all components. Consequences of the reaction are discussed as well as mitigation measures.

Reaction Initiation and Propagation

The primary hazard of the organic-laden waste is that both fuel and oxidizer are present and intimately mixed. The key mitigative feature is the moisture content of the waste. Waste energetics are characterized by the total organic carbon (TOC) content, expressed as weight percent carbon in the fuel on a dry-waste basis. The reaction of sodium acetate and sodium nitrate is considered a first-order surrogate for the reaction of actual waste (Equation 1) with an ideal heat of reaction of about 7.5 MJ/kg sodium acetate.

$$NaC_2H_3O_2+1.6NaNO_2 \rightarrow 1.3Na_2CO_3+1.5H_2O+0.7CO_2+0.8N_2 \quad (1)$$

Stoichiometry for this reaction corresponds to 11 wt% TOC. The reaction cannot take place unless appropriate energy is supplied as an initiator.

Measurements for dry waste have demonstrated that the reaction does not become exothermic unless the waste is at, or above, the relatively high temperature of about 200°C. The reaction will not propagate through a medium unless the TOC exceeds 6 wt% and the temperature is about 300°C. Moisture in the waste inhibits reactions. Based on the energy release of a stoichiometric mixture, a heat balance indicates that moisture content of 17 wt% would prevent a propagating reaction in mixtures with TOC less than stoichiometry.

The consequences of a hypothetical reaction of organic-nitrate waste involve the heating and pressurization of the tank headspace by hot reaction-product gases and the entrainment of vapors or aerosols from the waste that may be radiologically active. For a TOC value of 6 wt% (the value at which sodium acetate fuel reactions are observed to propagate), a dry reacting volume of 1 m^3 would pressurize the tank headspace to 1.50 atm, or 7 psig overpressure, which is enough to blow out any filter in the system and release gases and aerosols outside the tank through any tank orifice. A 6 wt% TOC dry reacting volume of 2 m^3 would cause a final pressure of about 2.1 atm, or 15 psig overpressure. Structural analysis indicates that a pressure of 14 psi would cause extensive cracking of the concrete dome of a half-million gallon tank, and the failure limit for a million gallon tank is 11.6 psi. This result is important since it indicates that a relatively small reacting volume could be a significant hazard and, thus, that spatial distribution of fuel within a tank is important.

Reaction Risk Model

Although risks of organic-nitrate reaction are thought to be low in most SSTs, the consequences of a major release are high enough to warrant significant investment in ensuring safe storage. In this framework, information on the organic constituents, moisture level, and temperature status of tank becomes a risk management tool. By using a

risk model that embodies uncertainty about the organic constituents, it is possible to show how risk management for a tank benefits from better information on fuel or moisture. Thus, the basic concept of a reaction risk model is to predict the risk of various significant release events as a function of tank fuel, moisture, and temperature (FMT) status, and the uncertainty about them.

The concept was implemented using estimates for probabilities of reaction initiation events and conditional probabilities of reaction propagation (given an initiator was present) expressed as functions of fuel content and moisture level. The basic probability structure of the model is shown in Equation 2.

$$Pr(E_{i_j}|I_k) = Pr[F_l,M_m,T_n]_p \tag{2}$$

where $Pr(E_{ij} \mid I_k)$ = probability that a reaction event will proceed from stage i to stage j given that initiator I_k has occurred in tank p
F_l = fuel state l (one of several discrete states defined by fuel concentration)
M_m = moisture state m (one of several discrete moisture states)
T_n = temperature state n (one of two discrete equilibrium temperature states).

In practice, the probability of an event is a sum of these conditional probabilities weighted by estimated probabilities that a tank is in a given FMT state:

$$Pr(E_{ij}) = \sum^{lmn} [L_p(F_l,M_m,T_n) \times Pr(F_l,M_m,T_n)] \tag{3}$$

where Σ^{lmn} = summation over all FMT states
L_p = estimated probability that tank p is in a given FMT state.

This model was developed using four initiators believed to account for most of the risk of initiation during storage in SSTs. Four event-severity classes were used to define the range of possible consequences of release events. All of the probabilities in this model were estimated by a group of experts familiar with the following: the organic-nitrate reaction, a series of adiabatic calorimetry experiments on waste simulant mixtures, and SST safety issues. Elicitation was conducted by a trained elicitor and confirmed in three separate meetings. Even with experimental basis and consistency checks, the resulting model has substantial judgmental content. The resulting risk model is not intended to accurately represent the absolute risk of uncontrolled releases from the Hanford tanks, but to capture the sensitivity of risk to FMT variables, and uncertainty about these variables.

The overall structure and function of the risk model is schematically shown in Figure 1. This figure illustrates how the probabilities are used in conjunction with statistical estimates of TOC, moisture, and temperature to calculate the risk of a given severity class event. Also shown is the effect of various mitigation measures, which were represented by changing the position of a tank in the FMT space, the initiator probabilities, or both.

Fuel, Moisture and Temperature Definitions

The fuel status for a tank was defined using the following ranges:

$$0 \text{ wt\%} \le TOC \le 2.5 \text{ wt\%}$$
$$2.5 \text{ wt\%} \le TOC \le 5 \text{ wt\%}$$
$$5 \text{ wt\%} \le TOC \le 7.5 \text{ wt\%}$$
$$7.5 \text{ wt\%} \le TOC \le 10 \text{ wt\%}$$
$$10 \text{ wt\%} \le TOC.$$

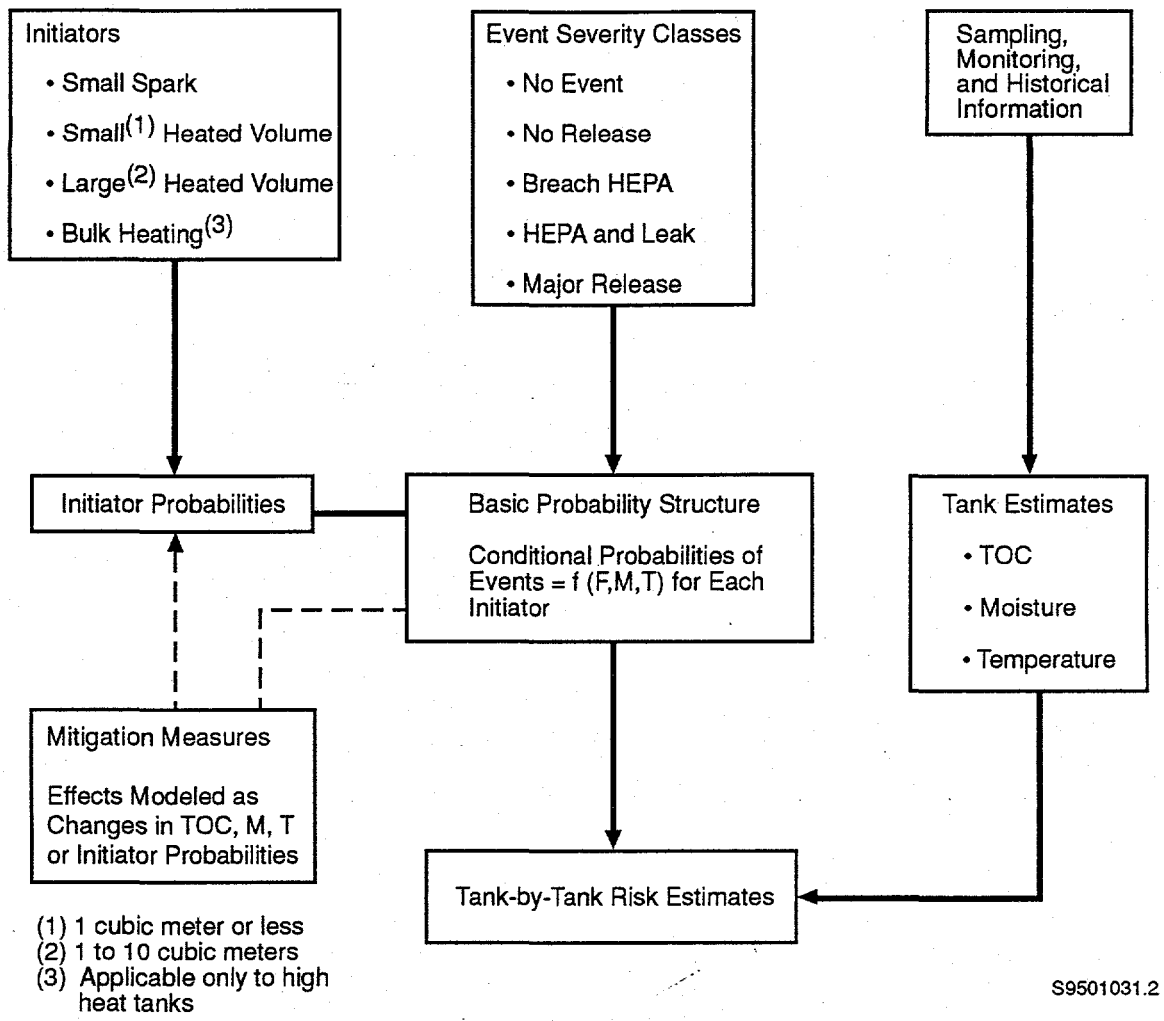

Fig. 1. Overall Structure Organic-Nitrate Risk Model

The model incorporated uncertainty in the spatial variability of TOC within the tank and the uncertainty in specific energy content by using the concept of Maximum Total Fuel Value (MLFV), defined as the product of three independent, lognormally distributed factors (Equation 4):

$$MLFV_p = TOC_p \times EDF \times SCF \tag{4}$$

where TOC_p = mean TOC concentration in wt%, dry basis, tank p
EDF = energy density factor, $[(cal/g)_p/(cal/g)_{NaAc}]$
SCF = spatial concentration factor, $[TOC_{max\ m}{}^3/TOC]$

This model structure accounts for the risk that a small volume of waste, enriched in organic content, can sustain a propagating reaction given a sufficient initiator. It allows for a separate measurement of the VOI on average TOC inventory in a tank, the degree of spatial heterogeneity in the TOC concentration, and the speciation (and energy of reaction) of the TOC.

The moisture status of a tank was represented in the risk model as a set of discrete moisture states analogous to the fuel status. Reaction propagation probabilities were estimated using an assumption that the moisture variable was the moisture of the potentially reacting waste. The number of moisture states were limited to three:

$$M \leq 6 \text{ wt\%}$$
$$6 \text{ wt\%} \leq M \leq 17 \text{ wt\%}$$
$$17 \text{ wt\%} \leq M.$$

The temperature status of a tank was defined with two states:

$$T < 149°C$$
$$T \geq 149°C.$$

Initiator Definitions and Probabilities

In a wet, low temperature condition, organic-nitrate mixtures of even high TOC content are stable to shock and sparks. It is possible, however, for a small spark to initiate a dry mixture. There is also the possibility for a runaway reaction if a source of heat is supplied to some waste volume. These considerations led to the use of four initiators in the risk model. The initiators and the probabilities assigned to them are shown in Table I.

Table I. Summary of Initiator Events

Initiator Event	Life Cycle Probability
Small spark	0.9
Small heated volume (1 m^3)	10^{-2}
Large heated volume (10 m^3)	10^{-5}
Bulk heating	10^{-3} (for high heat tanks only)

A life cycle of 25 years was chosen for analysis as it would represent a reasonable upper limit for tanks that are retrieved late in the retrieval and treatment program and be conservative as an average for all SSTs. These estimates reflected the strong belief of the expert group that a very small spark was essentially unavoidable during routine tank operations (e.g., sampling and waste retrieval operations).

Event Severity Classes

An organic-nitrate propagating reaction in a SST, if initiated, could result in a wide range of event severity cases because of the possible variation in fuel concentrations, the spatial extent of fuel concentration to support propagation, and the moisture concentration in and near the reacting region. Also, the amount of free headspace volume in the tank and the configuration of headspace ventilation would be important in determining the pressures reached and the severity of structural damage and release. Five severity classes were defined in the risk model to represent the potential range of events. The event severity classes are shown in Table II.

Table II. Summary of Event Severity Classes

Release Scenario	Contamination Region	Cleanup Cost
No event	None	$0
No release	None	$0
Breach high efficiency particulate air filter	Filter and local surface contamination x 10	$6 x 10^5
Breach high efficiency particulate air filter and leak	Tank and 75,700 m^3 soil contamination under/around tank	$7 x 10^6
Major release	Widespread surface contamination covering 525 km^2	$5 x 10^{10}

The five severity classes were used as a framework for estimating reaction probabilities and developing estimates of possible consequences.

Mitigation Measures

The final component of the reaction risk model is the development of potential mitigation activities to achieve control of FMT. Fourteen potential corrective actions were studied. The eight shown in Table III were selected as the range of activities that provided the range of information required for this study.

Table III. Summary of Mitigation Measures

Mitigation Measure	Effect on FMT	Total Incremental Life Cycle Cost (operating and construction)
Routine monitor	None	$0
Dry ice addition	Decrease T	$6.74 x 10^6
Bulk water addition	Increase M, decrease T	$2.62 x 10^6
Humidity control	Increase M, decrease T	$4.58 x 10^6
Add water and ventilation	Increase M, decrease T	$4.81 x 10^6
Destroy organics	Decrease FM, increase T	$15 x 10^6
Moist surface spray	Increase M, decrease T	$5.06 x 10^6
Retrieve and transfer contents	Decrease FMT	$6 x 10^7

The total cost includes the number and length of time each intervention would take during the 25-year life cycle.

DECISION ANALYSIS FRAMEWORK

The decisions on how to sample and classify tanks, determine whether any mitigative measures should be applied, and decide which are most effective were represented in a decision tree or decision analytic model. Such a model allows assessment of the best decisions according to some decision rule, based on the probabilities of various outcomes given that certain decisions are made. Data on mitigative measures include effectiveness and cost, where effectiveness is measured by the reduction of either the probability of an initiation event or the probability of a propagating reaction given that an initiator event has occurred; and cost of implementation includes the direct costs of the engineering measures plus, in some cases, indirect or intangible costs. Data required on consequences included at least one measure of value or costs that can be associated with each possible outcome in the decision tree.

The risk model was employed in a decision analysis mode to predict the expected costs of each possible path. Expected costs are calculated using the probabilities of release events given that each of the possible mitigation measures was implemented. All calculations depend on the assessments of fuel and moisture status, i.e., the probabilities that a given tank is in each of the possible fuel and moisture states. The simplest decision rule for such a problem involves minimizing the statistically expected cost (or maximizing the expected value) of the outcomes resulting from a mitigation decision. This risk-neutral decision rule may not be the appropriate one for actually making risky decisions. The appropriate stakeholder (U.S. Department of Energy, State of Washington, the public, etc.) may be willing to pay a premium beyond the statistical expectation of reduced cleanup and social costs saved. However, the focus in this study was on defining the value of different types and qualities of characterization data. For this application, using an expected cost minimization (risk-neutral) decision rule resulted in a lower boundary for VOI estimates, which allows us to determine the minimum that should be spent on efforts to ensure safety through characterization or mitigation.

The value of a given set of information is the decrease in the optimal (minimum expected) cost resulting from making a decision with the information rather than without it (Equation 5).

$$V(I) = \mathrm{Min}[E(C(x_i)|I_0] - \mathrm{Min}[E(C(x_i)|(I_0,I)] \tag{5}$$

where $V(I)$ = value of the information, I
Min = minimum operator (over all possible decisions)
E = expected value operator
C = cost of option x_i
x_i = decision options
I = information to be valued
I_0 = base case or starting information.

In the case of the organic-nitrate reaction problem, the reference information I_0 corresponds to the historical assessments of TOC, moisture, and temperature, and the judgmental evaluations of energy density factor (EDF) and spatial concentration factor (SCF) in this study. The right hand term contains both I and I_0, indicating that the base case is not discarded in making the least cost decision after the prospective information, I, is available. In practice, some synthesis of base case and new information is attempted to take maximum advantage of both. In this VOI application, this was accomplished with a Bayesian updating calculation in which the information set I_0 is the prior distribution and the set (I_0,I) is the posterior distribution.

Figure 2 shows the schematic decision tree structure of the model for evaluating the value of characterization about each tank's organic and moisture contents to support the management of the organic-nitrate safety issue.

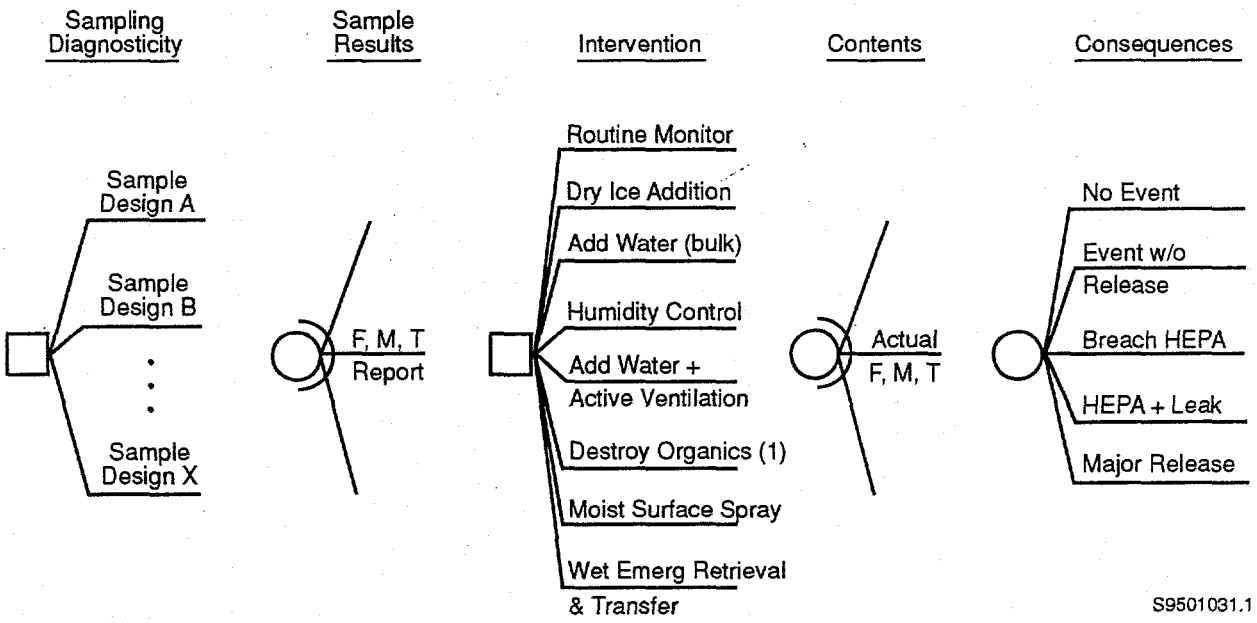

Fig. 2. Overall Structure Organic-Nitrate Value of Information Model

This tree follows all of the same conventions of any decision tree model. Reading left to right, the first decision is whether and what information to gather. This decision is followed, for choices that involve information gathering, with reports on the tank's moisture and fuel (TOC or MLFV) contents. Next comes a decision node that contains the possible mitigative actions, which range from no action to an emergency retrieval and transfer of the tank's

contents. Each mitigative action is followed by an uncertain event node of the tank's actual moisture and fuel contents (before mitigation). The final node is an uncertain event node of outcome severity, which ranges from no event to a major release of the tank's contents.

VALUE OF INFORMATION RESULTS

The model described was used to prepare VOI assessments under several sets of assumptions during the study. The general strategy was to begin with analyses of the value of "perfect" information (e.g., no statistical uncertainty) of various kinds. Following these studies of VOI for perfect information, studies were performed for "realistic diagnosticity" measurements. These studies calculated VOI for MLFV and moisture measurement sets with parametrically defined standard errors (10% to 50%) to assess the sensitivity of VOI to measurement quality.

In general, the results indicate substantial VOI for high TOC, indeterminate moisture tanks, and higher VOI for high-heat tanks than low-heat tanks for a given moisture level. An important observation concerns the degree of discrimination between tanks of significant interest for detailed characterization and those for which tank safety factors and associated risks may not warrant extensive characterization studies. The top 50 or so tanks studied in the case where prior distributions are adjusted for both spatial and energy of reaction factors have a high VOI such that the significant investment in sampling and analysis is a good investment for a risk-neutral stakeholder. The bottom 60 to 70 tanks may not warrant detailed study for this issue. There are 30 tanks in the questionable region. Thus, the study discriminated fairly well among those tanks with high payoff to sampling and those not worth the cost.

Studies separating the VOI for MLFV and moisture showed that perfect information about TOC alone is always worth essentially as much as that about both variables together. However, this should not be taken to mean that priority should go to MLFV determination over moisture measurements. The factors determining MLFV (via its components TOC, SCF, EDF) are much more difficult to measure accurately than the minimum moisture content. Also, from a starting point of considerable uncertainty about both MLFV and moisture, definitive information about either variable will dramatically improve decision-making and is, therefore, of high value.

The VOI statistic for the entire population of 149 SSTs is illustrated in Figure 3 for each of the TOC inventory values and the pertinent adjustments. This figure also shows that the upper limit to the risk-reduction benefit of information is the cost of the least-cost, but substantially effective mitigative action.

Imperfect diagnosticity cases were studied to determine how measurement precision affected the VOI, and, therefore, arrive at acceptable laboratory measurement curves. The standard errors studied are for the tank-scale indicators of MLFV and minimum moisture, and had to be translated to results for individual assays. In general, tanks with high VOI for perfect information retained a high percentage of this VOI as the standard error of MLFV and moisture estimation increased. For standard errors of 20% of the true value for both MLFV and moisture, the VOI was typically at, or near, 90% of the value of perfect information. The results showed that there was not much incentive to estimate MLFV more accurately than about 20% standard error (as a fraction of true mean). Moisture measurements were shown to be tolerated as crudely as 30% to 40% standard error.

CONCLUSIONS

The following bullets summarize the findings of using the VOI approach for applying DQOs to the organic-nitrate safety issue in Hanford high-level waste tanks.

- The decision-making value of tank waste information on moisture and fuel value is substantial.
- Almost all of the information value is concentrated in the top 50 tanks.
- The lowest-cost mitigation option limits the VOI for a tank.
- Extremely accurate predictors of MLFV and minimum moisture (at the tank scale) are not required.
- Fuel information alone is worth almost as much as fuel and moisture information together.

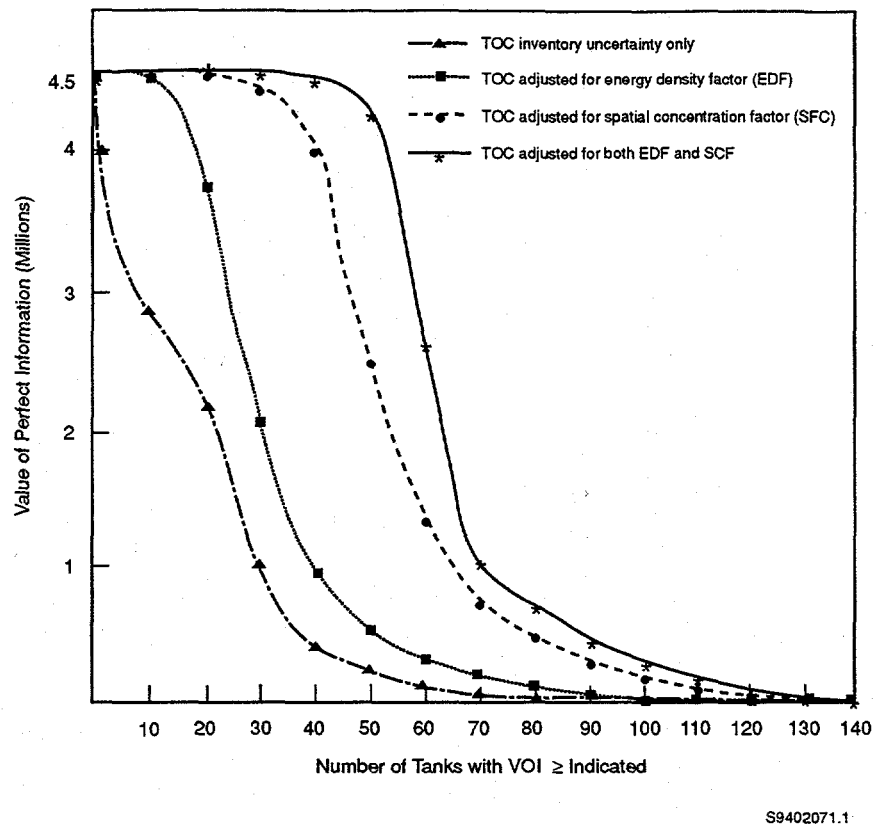

Fig. 3. VOI Statistic for the Population for the Population of 149 Single-Shell Tanks

- Moisture information alone is worth about three quarters of the information on fuel value and moisture together.
- It may not be economical to conduct fuel assessments in wet tanks.
- The uncertainty about spatial distribution of fuel and specific reaction energy warrants investment in tank characterization.

In addition to these specific conclusions, it became clear during and after the study that the VOI model is a general risk management paradigm. With this model, decisions about developing and deploying mitigative measures, restricting operations, and other factors can be integrated and addressed in terms of overall risk reduction and cost minimization.

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