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LA-UR -87-2242

CONF 870713 -56

LA-UR--87-2242

DE87 013134

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SUBMITTED TO 28th Annual Meeting of the Institute of Nuclear Materials Management, Los Angeles, July 12-15, 1987

VARIANCE AND COVARIANCE CALCULATIONS FOR NUCLEAR MATERIALS ACCOUNTING USING 'MAVARIC'*

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ABSTRACT

Determination of the detection sensitivity of a materials accounting system to the loss of special nuclear material (SNM) requires (1) obtaining a relation for the variance of the materials balance by propagation of the instrument errors for the measured quantities that appear in the materials balance equation and (2) substituting measured values and their error standard deviations into this relation and calculating the variance of the materials balance. MAVARIC (Materials Accounting VARIance Calculations) is a custom spreadsheet, designed using the second release of Lotus 1-2-3,† that significantly reduces the effort required to make the necessary variance (and covariance) calculations needed to determine the detection sensitivity of a materials accounting system. Predefined macros within the spreadsheet allow the user to carry out long, tedious procedures with only a few keystrokes. MAVARIC requires that the user enter the following data into one of four data tables, depending on the type of the term in the materials balance equation; the SNM concentration, the bulk mass (or solution volume), the measurement error standard deviations, and the number of measurements made during an accounting period. The user can also specify if there are correlations between transfer terms. Based on these data entries, MAVARIC can calculate the variance of the materials balance and the square root of this variance, from which the detection sensitivity of the accounting system can be determined.

*This work was supported by the U.S. Department of Energy, Office of Safeguards and Security.

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†Trademark of Lotus Development Corporation, 55 Cambridge Parkway, Cambridge, MA 02142.

I. INTRODUCTION

An important element in safeguarding nuclear facilities against the loss of special nuclear material (SNM) is accounting for this material through the periodic measurement of all inventories and input and output transfers. However, due to errors in the measurement instruments, a materials accounting system offers only limited detection sensitivity to the loss of SNM. Determination of the detection sensitivity of a material accounting system requires (1) writing the materials balance (MB) equation for a materials balance area, (2) obtaining a relation for the variance of the MB by propagating the instrument errors for those measured quantities that appear in the MB equation, and (3) substituting measured values and their error standard deviations into this relation and calculating the variance and the standard deviation (sigma) of the materials balance. The application of these steps (with minor differences in each step depending on the facility process description) is necessary for sensitivity studies of all facilities. Implementation of step (3) is particularly tedious for MB equations that contain a large number of transfer and inventory terms. MAVARIC (Materials Accounting VARIance Calculations), a custom spreadsheet designed using the second release of the Lotus 1-2-3, significantly reduces the effort required to make the variance and covariance calculations needed to determine the detection sensitivity of a materials accounting system.

Two recent INMM papers have also reported similar interactive computer programs (EPIC and PROFF) for performing materials balance variance calculations.[1,2] MAVARIC differs from the first program, EPIC, in that MAVARIC is able to perform calculations of the covariance between two transfer terms and in that it can treat more complicated forms of both transfer and inventory terms. Although PROFF, the second such program, is actually the basis for the MAVARIC spreadsheet and is therefore similar to MAVARIC in terms of the complexity of the variance and covariance calculations that can be performed, the basic difference between MAVARIC and PROFF is that MAVARIC uses the very popular and convenient-to-use spreadsheet, Lotus 1-2-3, whereas PROFF is a menu-driven computer program written in TURBO-PASCAL. In addition, MAVARIC does not provide for the calculation of the sigma of the MUF-D statistic contained in the PROFF program (MUF-D is a test statistic used by the International Atomic Energy Agency for verification purposes).

The variance and covariance equations contained in MAVARIC were developed specifically for those nuclear facilities in which the terms in the MB equation can be expressed as a sum over a product of two measured quantities, such as SNM concentration and bulk mass (or solution volume). The stored equations also assume steady-state facility operation. For example, in a series of batch transfers, the SNM concentrations and the batch masses are assumed to have the same nominal measured value, respectively. Although occasions have arisen when the assumption of steady-state facility operation was not valid, these occasions have been rare. Thus, MAVARIC can be widely used for the design of materials accounting systems.

II. TERMS OF THE MATERIALS BALANCE EQUATION

MAVARIC contains variance (and covariance) equations for handling two types of transfer terms and two forms of the inventory difference in the MB equation. One type of transfer term that often occurs in the MB equations of processing or fuel fabrication facilities is of the form

$$T1 = \sum_{i=1}^{N} C_i (BX - LX)_i \quad , \qquad (1)$$

where C is the SNM concentration of a solution (kg Pu/L) or of a bulk powder (in mass percent or fraction, such as kg Pu/kg oxide powder); BX and LX are the gross and tare volumes of the solution (or masses of the bulk powder), respectively; and N is the number of transfers measured during the accounting period (that is, i runs from 1 to N). The form of Eq. (1) assumes that for each C measurement, there are corresponding measurements of BX and LX. In an MB equation, there may be several input or output transfers that have the form of Eq. (1), although the values of the measured quantities (C, BX, and LX) may be different for the different MB terms.

A second type of transfer term that occasionally occurs in MB equations is given by

$$T2 = \sum_{i=1}^{NC} C_i \sum_{j=1}^{NX} (BX - LX)_{ij} \quad . \qquad (2)$$

This form of the MB term shows explicitly that there are NX measurements of BX and LX per C measurement and NC measurements of C during the accounting period. A term like Eq. (2) is necessary for dealing with material from a blender, for instance, where a single concentration measurement is made of a blended sample, but the blended material is subsequently apportioned among several containers, whose individual masses are measured. The form T2 reduces to T1 if NX = 1.

A type of inventory difference term that appears in MB equations is of the form

Beginning inventory - Ending inventory =

$$\left[\sum_{i=1}^{NCi} C_i \sum_{j=1}^{NXi} (BX - LX)_{ij} \right]_B - \left[\sum_{k=1}^{NCf} C_k \sum_{l=1}^{NXf} (BX - LX)_{kl} \right]_E \quad , \qquad (3)$$

where the B and E subscripts refer to beginning and ending measurements of C and X. Although the beginning and ending values are nominally the same for the C, BX, and LX measurements, the two sets of measurements correspond to different material. Such a form of inventory difference might be necessary for boats of material loaded into a calciner, for example, or cans of material in interim storage. A similar form is also used for a number of columns holding SNM solution. Equation (3) allows for different initial and final values for the NC and NX pairs.

The other type of inventory difference that occurs in MB equations is given by

Beginning inventory - Ending inventory =

$$\left[\sum_{i=1}^{Ni} X_i \right]_B - \left[\sum_{j=1}^{Nf} X_j \right]_E \quad . \qquad (4)$$

This form of inventory difference is often used for terms associated with nondestructive assay (NDA) measurements. The values Ni and Nf represent the initial and final number of items in the inventory term, respectively. As with the first type of inventory difference term, the beginning and ending values of the X measurement are nominally the same but correspond to different material.

III. MAVARIC - THE CUSTOM SPREADSHEET

MAVARIC is structured in a spreadsheet format where stored entries are used to perform variance and covariance calculations for the transfer and inventory terms appearing in the MB equation. Within the MAVARIC spreadsheet, the user begins by entering data into one of four data tables depending on the type of transfer or inventory term. The four data tables correspond to input transfers, output transfers, and two types of inventory measurements, NDA and chemical analysis data. At the present time, MAVARIC can accept as many as 20 input transfers, 20 output transfers, and a total of 86 inventory items, 43 for NDA measurements and 43 for measurements made by chemical analysis. MAVARIC is also able to evaluate as many as 40 covariances between the MB transfer terms. For each entry to a data table, MAVARIC requires an identification number and a short description as well as values for the SNM concentration, the bulk mass (or solution volume), the measurement error standard deviations, and the number of measurements during an accounting period.

All variance and covariance calculations are performed by equations stored within the custom spreadsheet. MAVARIC contains four equations for calculating the variance of MB transfer terms, three equations for calculating the covariance between MB transfer terms, and five equations for calculating the variance of inventory difference terms. Variance and covariance equations for the mass (or volume) measurements are included for both the additive and the multiplicative error models. Only the multiplicative error model is used for variance calculations of the concentration measurements.

Once the data have been entered, the user may invoke a designated macro (a predefined sequence of instructions) to perform the necessary calculations. These spreadsheet macros allow the user to carry out long, tedious procedures with only a few keystrokes. To activate a macro, the user must simultaneously press the [Alt] key and the letter key corresponding to the particular macro. In performing a variance (or covariance) calculation, a spreadsheet macro must extract the necessary information from the appropriate data table(s), determine which of the stored equations is to be used (based on the error model and the form of the MB term), and carry out the required calculations to obtain the variance result. Other macros within MAVARIC are "programmed" to perform functions such as reading data from a second spreadsheet, providing hard copies of the data and results tables (with the aid of the program Sideways),* and saving (or deleting) the data and results in the current spreadsheet.

IV. THE MAVARIC DATA TABLES

The first step in using MAVARIC involves making data entries to the four data tables. This may be done by either of two methods. One method begins with the entry of all data to a preliminary "data" spreadsheet, DATA.WK1, before using the actual MAVARIC spreadsheet. By invoking a single macro, the MAVARIC spreadsheet is then prompted to read the data from the DATA.WK1 file and to perform the necessary variance calculations. The second method is data entry directly into the MAVARIC spreadsheet, in which case the variance calculations must be initiated individually for each transfer or inventory term. The general procedure is the same for both methods of data entry with only minor differences in the steps required to perform the variance calculations. We present a set of examples to illustrate the procedure for making entries to the MAVARIC data tables.

*Trademark of Funk Software, Inc., P. O. Box 1290, Cambridge, MA 02238.

Before starting entries to the data tables, the user must complete the START-MENU (Fig. 1), which contains the number of input transfers, output transfers, inventory terms, and the number of days in the accounting period.

START-MENU:

Number of Input Transfers-----------------	1
Number of Output Transfers----------------	2
Number of Inventory Terms-----------------	2
Number of Days in the Accounting Period---	30

Fig. 1.
The number of each type of term in the MB equation and the number of days in the accounting period are specified in the START-MENU.

An entry to the table of input transfers will serve as a generic example of the data entry procedure for a transfer term. Because the four data tables are similar, only the differences in the data entry procedure between each of the other three tables and the table of input transfers will be discussed.

The sample Input Transfer, IT1 (Fig. 2), assumes that mixed-oxide powder (MOX) from a blender is transferred to a single tray, which is to be stored in a materials balance area after the tare and gross masses have been measured. Furthermore, we assume that, to determine the SNM concentration of material in the tray, a single concentration measurement is made of a sample taken from the blender just before the blended material is transferred to the storage tray. Also, the throughput of this facility is such that this procedure is carried out eight times per day. Thus, NC (the number of concentration measurements per day) is 8, and NX (the number of mass measurements per concentration measurement) is 1. The value of the concentration measurement (C) is assumed to be 0.441 kg Pu/kg MOX. The gross mass of each tray (BX) is measured to be 2.75 kg, and the tare mass of each tray (LX) is 0.25 kg. Each of the concentration measurements has an associated multiplicative error model with a random standard deviation, SigEpsC, of 0.36% and a correlated error standard deviation, SigEtaC, of

****
* INPUT TRANSFER TERMS *
****

[Alt]x TO CALCULATE THE C AND X VARIANCES
[Alt]i TO ADD INPUT TRANSFERS
[Alt]o TO ENTER OUTPUT TRANSFERS
[Alt]m TO VIEW THE MAIN MENU

NUMBER	DESCRIPTION	NC	NX	C	BX	LX	SigEpsC (%)	SigEtaC (%)	SigEpsX	Units of SigEpsX	SigEtaX	Variance (C)	Variance (X)
IT1	Input MOX	8	1	0.441	2.75	0.25	0.36	0.21	0.0002	KG	0.0004	3.12518746E-0[illegible]	1.7340[illegible]

Fig. 2.
The table of input transfers containing a sample entry of MOX powder (MOX).

0.21%. The mass measurement scale has associated with it an additive error model with a random standard deviation, SigEpsX, of 0.0002 kg and a correlated error standard deviation, SigEtaX, of 0.0004 kg.

The final two columns in Fig. 2 represent the variance results for the concentration and mass measurements. Clearly, not all eight digits presented in the variance results are considered significant.

The notes in the upper right corner of Fig. 2 are the options available to the user upon completing an entire line of entry. For example, the variance results for the concentration and mass measurements are obtained by invoking the macro corresponding to [Alt]x.

The error model for the mass measurement is specified by the entry to the column titled "Units of SigEpsX." An entry of KG (or L for Liter in the case of a solution) signifies an additive error model, whereas a percent sign (%) specifies a multiplicative error model. The correlated error standard deviation of the X measurements always assumes the same units as the random error standard deviation.

The procedure for making entries to the table of output transfers is exactly the same as that for the input transfer entries outlined in Fig. 2. Hence, there is no sample entry to the table of output transfers.

An inventory term measured by NDA contains FBR fuel pins (Fig. 3) with an initial inventory count, Ni, of 3000 pins and an ending inventory, Nf, of 3000 pins. Unlike the transfers, the inventory items subject to NDA measurement do not undergo specific concentration and mass measurements. Instead, the plutonium content, X, [Eq. (4)] is measured directly. The value of X is given by C(BX - LX), where C, BX, and LX are assigned during calibration of the NDA instrument. In this case the values of C, BX, and LX are 0.176 kg Pu/kg MOX, 0.9 kg, and 0.42 kg, respectively. Random and correlated error standard deviations must be entered for each X measurement. In MAVARIC, these errors are always described by the multiplicative error model and, in this case, are assumed to be 1% for both the random and correlated error standard deviations. The final column in the data table contains the calculated variance of X for the NDA measurement.

A data table corresponding to inventory items that have been analyzed using chemical analysis techniques is shown in Fig. 4. This inventory table contains the number of initial and final measurements for both the concentration and the mass of each item. For the example of liquid waste, the initial and final number of concentration measurements per day, NCi and NCf, are both 1. Similarly, the initial and final number of mass measurements per concentration measurement, NXi and NXf, are both 1. The value of C is measured as 0.0001 kg Pu/liter, with associated error standard deviations of 10% random and 10% correlated. The gross volume measurement, BX, has a value of 20,000 liters, and the tare volume is assigned the value of 0. The volume measurement errors are multiplicative in nature, with random and correlated error standard deviations of 0.05%.

```
*********************************          [Alt]p TO CALCULATE THE X VARIANCE
* X VARIANCES OF INVENTORY ITEMS *          [Alt]v TO ADD NDA DATA
*          (NDA METHODS)          *          [Alt]g TO ENTER CHEMICAL ANALYSIS DATA
*********************************          [Alt]m TO VIEW THE MAIN MENU
```

NUMBER	DESCRIPTION	NI	NF	C	BX	LX	SigEpsX (%)	SigEtaX (%)	Variance (X)
IV1	FBR FUEL PINS	3000	3000	0.176	0.9	0.42	1	1	4.28212224E-03

Fig. 3.
A sample entry of FBR FUEL PINS to the inventory table corresponding to measurements made by NDA instruments.

```
****************************************
* C AND X VARIANCES OF INVENTORY ITEMS *
*    (CHEMICAL ANALYSIS METHODS)       *
****************************************
                                            [Alt]f TO CALCULATE THE C AND X VARIANCE
                                            [Alt]q TO ADD CHEMICAL ANALYSIS DATA
                                            [Alt]m TO VIEW THE MAIN MENU
```

NUMBER	DESCRIPTION	NCi	NXi	NCf	NXf	C	BX	LX	SigEpsC (%)	SigEtaC (%)	SigEpsX	Units of SigEpsX	SigEtaX	Variance (C)	Variance (X)
IV2	LIQUID WASTE	1	1	1	1	0.0001	20000	0	10	10	0.05	%	0.05	8.00000000E-02	2.00000000E-06

Fig. 4.
An inventory table containing terms with concentration measurements made by chemical analysis.

V. CALCULATION OF COVARIANCES AND SIGMA

Covariance calculations are performed when there are correlations between the error standard deviations of two or more of the transfer terms. To obtain the covariance result, the user must complete two covariance menus. The first menu (Fig. 5) requires the identification numbers (e.g., IT1 and IT2) of the two transfer terms. The second menu (Fig. 6) determines the type of correlation (C, X, or both) that exists between the two terms. MAVARIC then presents the covariance result, along with all previous covariance calculations, in a table of covariances (Fig. 7).

```
CALCULATING A COVARIANCE:

Enter the first covariance term:  (e.g., IT1)  IT1

Enter the second covariance term:  (e.g., OT2) IT2

                  ENTER 'QUIT' TO EXIT
```

Fig. 5.
This menu identifies IT1 and IT2 as the two transfer terms involved in the covariance calculation.

```
THE COVARIANCE EXISTS:

     1 --- ONLY FOR C MEASUREMENTS
     2 --- ONLY FOR X MEASUREMENTS
     3 --- FOR BOTH C AND X MEASUREMENTS

            Enter the number of your option:     1
```

Fig. 6.
The concentration measurement is specified as the source of the observed covariance.

```
*************************
* TABLE OF COVARIANCES *
*************************

                     [Alt]m TO VIEW THE MAIN MENU
```

Terms	Covariance (C)	Covariance (X)
IT1 IT2	4. 8245E-02	

Fig. 7.
All covariance results are contained in the table of covariances.

The final results presented by the MAVARIC spreadsheet (Fig. 8) include the total variance, which is the sum of all variance and covariance results contained in the spreadsheet, and sigma, the square root of this variance. MAVARIC also provides the variance contribution from each of the four data tables and the table of covariances. The detection sensitivity of the materials accounting system is determined from the value of sigma calculated by MAVARIC.

```
*****************
* FINAL RESULTS *
*****************
```

VARIANCE CONTRIBUTIONS:	
Transfers:	
Input Terms	3.12542480E-01
Output Terms	3.07689115E-02
Inventories:	
NDA Measurements	4.28212224E-03
Chemical Analysis Measurements	8.00000000E-02
Covariances	1.87872346E-03
TOTAL VARIANCE	4.27595514E-01
SIGMA	6.53907879E-01

Fig. 8.
The final results obtained by the MAVARIC spreadsheet. The value of sigma is used to determine the detection sensitivity of the materials accounting system.

VI. SUMMARY

MAVARIC is a custom spreadsheet, designed using the second release of Lotus 1-2-3, that significantly reduces the effort required to make the necessary variance and covariance calculations needed to determine the detection sensitivity of a materials accounting system. The data tables and spreadsheet macros make MAVARIC convenient to use for the design of such accounting systems.

ACKNOWLEDGMENT

The author wishes to express his most sincere appreciation to Dante Stirpe, Safeguards Systems Group, for hi invaluable guidance throughout the development of MAVARIC.

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