NLO ERROR PROPAGATION EXERCISE: STATISTICAL RESULTS

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ABSTRACT

Error propagation is the extrapolation and cumulation of uncertainty (variance) about total amounts of special nuclear material, for example, uranium or ^{235}U , that are present in a defined location at a given time. The uncertainty results from the inevitable inexactness of individual measurements of weight, uranium concentration, ^{235}U enrichment, etc. The extrapolated and cumulated uncertainty leads directly to quantified limits of error or inventory differences (LEIDs) for such material.

The NLO error propagation exercise was planned as a field demonstration of the utilization of statistical error propagation methodology at the Feed Materials Production Center in Fernald, Ohio (NLO, Inc.) from April 1 to July 1, 1983 in a single material balance area formed specially for the exercise. Major elements of the error propagation methodology were:

- . Variance approximation by Taylor Series expansion.
- . Variance cumulation by uncorrelated primary error sources as suggested by Jaech.
- . Random effects ANOVA model estimation of variance effects (systematic error).
- . Provision for inclusion of process variance in addition to measurement variance.
- . Exclusion of static material.

The methodology was applied to material balance area transactions from the indicated time period through a FORTRAN computer code developed specifically for this purpose on the NLO HF-3000 computer.

This paper contains a complete description of the error propagation methodology and a full summary of the numerical results of applying the methodology in the field demonstration. The error propagation LEIDs did encompass the actual uranium and ^{235}U inventory differences. Further, one can see that error propagation actually provides guidance for reducing inventory differences and LEIDs in future time periods.

I. INTRODUCTION

The DOE Office of Safeguards and Security, through its Material Control and Accountability Branch, sponsored an error propagation exercise at the Feed Materials Production Center in Fernald, Ohio (NLO, Inc.) starting in March, 1982 under the direction of the Technical Support Organization at Brookhaven National Laboratory (BNL) with statistical support provided by the Computer Sciences Division at Oak Ridge National Laboratory (ORNL). The NLO error propagation exercise was planned as a field demonstration of the utilization of statistical error propagation methodology to meet the control limit requirements of DOE Order 5630.2 (1980), which says in part "...each facility shall implement procedures for evaluating special nuclear materials inventory differences. The procedures shall establish control limits....".

The field demonstration was conducted between physical inventories taken April 1 and July 1, 1983 in a material balance area (MBA) formed for the exercise which included the reduction of enriched green salt (UF_4) to uranium metal and casting of the metal into crude ingots. The inventory difference (ID) as typically defined,

$$\begin{array}{rcll} \text{Inventory} & = & \text{Beginning} + \text{Additions} - \text{Removals} - & \text{Ending} \\ \text{Difference} & & \text{Inventory} & \text{Inventory} \end{array}$$

$$ID = BI + A - R - EI$$

was determined separately for uranium (U) and ^{235}U using the computer data base of more than 10,000 transactions (item-by-item BI, A, R, EI) and over 12,000 measurements of weight, U concentration, impurity concentration, and ^{235}U enrichment. The desired control limits, termed the limits of error on the inventory difference (LEID), were determined through error propagation, i.e., the extrapolation and cumulation of uncertainty (variance) about

total amounts of material which results from the inevitable inexactness of individual measurements.

This paper reports on the statistical methodology developed for the NLO error propagation exercise and the results of applying that methodology to the April-June, 1983 field demonstration data. The discussion is divided into the following sections:

Management Summary discusses the nature of and motivation for error propagation, gives numerical exercise results and explains their meaning. It also discusses exercise limitations, and exercise implications for the future.

Methodology provides a detailed description of statistical error propagation methodology, in general concept and as applied at NLO.

Appendices contain detailed statistical and mathematical documentation of various aspects of the statistical work in the exercise.

The intention of the above division is that the paper proceed from a nonstatistical discussion to increasingly statistical discussions.

II. MANAGEMENT SUMMARY

Standard Inventory Difference Control Limits

It is important to understand the standard approach to the determination of inventory difference control limits and the ways in which the control limits it produces may be inappropriate.

The standard approach compares a current inventory difference to the standard deviation of a sequence of historical inventory differences. This is illustrated in Fig. 1 using an uncharacteristically short sequence of five historical IDs given in the second column to develop control limits for a third quarter fiscal year 1983 (FY-83-3) ID of 148 units. The average of the historical IDs is 20 units. The variance around this average, simply the average squared (ID-Average) is 5120, giving a standard deviation of 71.6 units. Statistical observation has shown that many variables like this historical ID that presumably have a long-term average value of zero can take absolute values up to two times their standard deviation without it being particularly unusual, but that larger values would occur only 5% of the time. Thus, control limits, or LEIDs, of $\pm 2(71.6) = \pm 143.2$ would be justified as giving only 5% false alarms. Our FY-83-3 ID of 148 units is not in the interval $(-143.2, 143.2)$, and would thus be considered cause for worry (NLO has used two standard deviation "warning limits" and three standard deviation "alarm limits").

Now suppose that there had been a theft of 50 units in FY-83-2 making its ID 90 units instead of 40 units, as listed in the "Theft IDs" column of Fig. 1. The standard ID control limits would now be $\pm 2(76.9) = \pm 153.8$. The FY-83-3 ID of 148 now falls within the control limits and would be judged insignificant. This illustrates one serious problem with the

standard ID control limits, the fact that they may be inflated by the act of theft or diversion one is trying to prevent, and thus actually mask that act.

Quarter	IDs	(ID-Average)	ID-Average ²	Theft IDs
FY--82-2	120	100	10,000	120
-3	-40	-60	3,600	-40
-4	60	40	1,600	60
FY-83-1	-80	-100	10,000	-80
-2	<u>40</u>	20	<u>400</u>	90
Sum = 100		Sum = 25,600		<div style="border: 1px solid black; padding: 5px; text-align: center;">25,600 5,920 $\sqrt{5,920}$ 76.9</div>
Average = 20		Variance = 5,120		
		Standard Deviation = $\sqrt{5,120}$ = 71.6		
<hr/>				
FY-83-3		ID = 148		<div style="border: 1px solid black; padding: 5px; text-align: center;">148 2(76.9) 153.8 INSIGNIFICANT</div>
		LEID = 2(71.6)		
		= 143.2		
		CONCLUSION = SIGNIFICANT		

Fig. 1. Standard Inventory Difference Control Limits.

Another problem arises in that the variance in the historical IDs may not be representative of the variance in the current ID because changing volumes of material are passing through the facility. In the Fig. 1 example, if the FY-83-3 volume of material is twice that in any of the historical ID periods, there is potential for greater ID variance in the greater number of measurements made on the material. Standard ID control

limits are not directly associated with facility throughput in the current period.

The two problems noted above are in themselves sufficient reason for the action of DOE Order 5630.2 (1980), which specifically prohibits the use of control limits based solely on historical IDs over the long-term (they were permitted as "an interim measure").

What is Error Propagation?

The introduction to this paper stated that error propagation was the extrapolation and cumulation of uncertainty (variance) about amounts of material which results from the inevitable inexactness of individual measurements. The methodology might better be termed "variance propagation", stressing that even the best equipment and analysts produce imperfect measurements, rather than suggesting that we are somehow dealing with large errors made by careless people using poor equipment.

The idea of extrapolation of variance is suggested by the example of Fig. 2. There we suppose we are concerned with an ID for ^{235}U . The weight ^{235}U of a particular item is the product of three measurements, item net weight, U concentration, and ^{235}U enrichment. The variance in these three measurements will extrapolate (or propagate) into a variance in the resulting measured weight ^{235}U . What is the extrapolated variance? This is one example of what the term "error propagation" would mean to most statisticians, determining the variance of a function of variables given the individual variances of the variables in the function.

The error propagation methodology used in the NLO exercise cumulates variance by uncorrelated primary error sources, item by item. These error sources are 1) weight, 2) sampling U , 3) analytical U , 4) sampling ^{235}U , and 5) analytical ^{235}U . The U concentration variance in Fig. 2, for example, will relate both to the fact that only a sample of the item (or lot) is analyzed and to the fact that there is an inherent variability in that analysis, presumed done by the volumetric measurement process. The latter analytical U variance could itself be viewed as a cumulative variance, consisting of random variance, and the variance "effects" of various features of the analysis, such as analytical method, instrument, operator, and time of day.

One issue in error propagation is suggested by Fig. 2. Each of the three previously mentioned measurements at the top of this figure represents a so-called reduced data measurement, that is the particular "final answer" that we sought in using a given measurement process. We have described error propagation in terms of reduced data variance above. However, one can also execute error propagation from the raw data measurement level, recognizing in Fig. 2, for example, that the reduced U concentration is a function of three raw measurements, $(F \cdot V)/W$. Beginning with raw data variances, one would propagate reduced data variances, and then proceed as before. This issue was examined in the NLO exercise.

The extrapolation and cumulation of all measurement variance leads directly to the establishment of the LEID as twice the square root of this

total variance.¹ The two problems noted with the standard ID control limits will clearly not exist for an error propagation LEID. The item-by-item cumulation of measurement variance clearly implies that the LEID will be directly associated with facility throughput in the current period. There is absolutely no path by which the theft or diversion of material can affect an error-propagated LEID.

Fig. 2. Error Propagation Example.

¹ It is our feeling that there is variance to be considered beyond measurement variance. Others in this literature have called it "process variance" or "process error". This is discussed later.

The State of the Art in Error Propagation

There is no broadly utilized general statistical methodology of error propagation in the nuclear materials control area. While the topic of error propagation is frequently discussed in engineering and experimental physics environments, it is rarely emphasized in statistical training environments, and almost all statisticians selected to work in this area would start with a small knowledge base. This was the case in the NLO exercise.

One integrated methodology for error propagation that is available in the nuclear materials control area is called Automated Material Accounting Statistics System (AMASS) and is described in NUSAC, Inc. (1981) (a new version, augmented AMASS, or AAMASS, may now be available). AMASS was developed under contract to the U.S. Nuclear Regulatory Commission (NRC) and has been applied to varying degrees in a number of NRC facilities.

NLO Exercise Error Propagation Methodology

The NLO error propagation exercise methodology was synthesized from Jaech (1973), statistical theory, and AMASS as described in NUSAC, Inc. (1981). There is, however, nothing in the methodology in conflict with AMASS methodology, which we find statistically sound. There were several AMASS concepts that could not be incorporated in the NLO methodology, given constraints of time and an exercise MBA for which there was no historical data.

Steps taken in methodology development were:

- (1) NLO plant familiarization through plant visits and documentation study. We saw the exercise-defined MBA in operation in March, 1982. We watched measurement processes in the NLO analytical laboratory and studied them in Rodden (1972).

- (2) Statistical literature search on error propagation, a rarely mentioned subject in the standard statistical literature. Work studied included Eisenhart (1963), Ku (1966), Youden (1972), Jaech (1973), Lowe and Waterman (1976), NUSAC (1981), Schumacher (1981), and Easterling (1982).
- (3) Formulation of a comprehensive, technically sound error propagation methodology combining our learning from (1) and (2) above with our own perspective as practicing statisticians.
- (4) Estimation of required reduced/raw data measurement variances appropriate to the NLO MBA (as discussed with reference to Fig. 2).
- (5) Application and tuning of the methodology on the April-June, 1983 field demonstration data to produce MEIDs for the exercise MBA's ^{235}U and U IDs for this time period.

The methodology is discussed in depth in Section III. of this report.

Major elements of the methodology are briefly noted here:

- . Propagated variance approximation by the Taylor Series expansion.
- . Inventory difference variance cumulation by uncorrelated primary error sources as suggested by Jaech's (1973) Chapter 6.
- . Provision for random effects model estimation of variance effects due to analytical method, instrument, operator, time of day, if such effects are found to exist, and inclusion of such effects in the error propagation (often termed "systematic error" in the error propagation literature).
- . Provision for inclusion of process error in the error propagation when available data permits. Process error may involve unmeasured inventory, bookkeeping errors, holdup, etc.

- . Exclusion of static material from the error propagation, that is, material that is both added and subtracted in the $ID = BI + A - R - EI$ determination, but is only measured once.

Bias correction was not dealt with in the NLO exercise error propagation methodology.

Results

The focus of error propagation in terms of numerical results sought is clearly the ID and the LEID of selected strategic nuclear materials in a particular facility, enriched uranium and ^{235}U in the case of NLO and this error propagation exercise. However, error propagation requires a great deal of input in terms of reduced/raw data measurement variances and produces substantial useful output beyond the LEID itself, all of which may be termed "results" of the error propagation effort. The full results of the NLO error propagation exercise for the reduced data analysis are reflected in Tables 1 through 16, produced by the error propagation computer code written by the first author of this report specifically for this exercise. The ^{235}U ID of -37,422 grams appears in Table 6, with the associated LEID of $\pm 44,610$ grams in Table 7. The U ID of -1,131,200 grams appears in Table 12, with the associated LEID of $\pm 2,854,200$ grams in Table 13. Thus, both IDs were insignificant when judged against LEID.

The general design behind the results Table 1-16 is as follows (see Appendix A for definitions of terms used in these tables and following descriptions):

Tables 1-3: Input reduced/raw data measurement variances (expressed as relative standard deviations).

Table 4: Input sampling variances for U and ^{235}U (expressed as relative standard deviations). (See Appendix G for material description code (M.D.C.) number list.)

Table 5: Summary of materials represented in the 10,000 transactions in the NLO exercise computer data base, by M.D.C.

Table 6: Summary of ^{235}U material by transaction category and static/active division, with implied inventory difference.

Table 7: Summary of uncertainty (variance) in ^{235}U amounts by variance source, with implied limit of error on inventory difference.

Tables 8-11: Detailed summary of non-zero ^{235}U variance sources in Table 7 (excluding indirect measurement) by scale number, analytical method, or M.D.C., as appropriate.

Table 12, Table 13, Tables 14-16: Repeat the pattern of Table 6, Table 7, Tables 8-10 for U.

For purposes of discussion in the following section, one further results table, Table 17, is provided. It includes, in addition to selected reduced data analysis results extracted from Tables 1-16, the only raw data analysis results presented in this paper.

Discussion of Results

Tables 1-5 establish inputs to the NLO error propagation exercise in terms of measurement variances and material flows. It is the combination of these two forms of input that produces the propagated measurement variance which in turn produces the NLO exercise LEIDs for ^{235}U and U. Selected aspects of the NLO exercise outputs in Tables 6-17 are discussed below, emphasizing the IDs, LEIDs, validity of the LFIDs, and available guidance in the results for reducing future IDs and LEIDs:

Table 1. Relative standard deviations for weighing

Method	Raw Data		Reduced Data	Effects
1-03	.00990	.00170		.00210
4-15	.00280	.00050		.00054
4-20	.00280	.00050		.00054
4-40	.00280	.00050		.00054
5-08	.01160	.00110		.00184
5-11	.00000	.00130		.00130
5-14	.01160	.00110		.00184
5-18	.01160	.00110		.00184
5-22	.00990	.00070		.00123
5-28	.00000	.00100		.00100
6-10	.02540	.00090		.00116
6-24	.00650	.00070		.00105
9-04	.03110	.00290		.00395
9-08	.03110	.00290		.00395
9-18	.03190	.00090		.00153
9-19	.03190	.00090		.00153
9-20	.03190	.00090		.00153
9-26	.00000	.00100		.00100
SP01	.00410	.00120		.00227

Table 2. Relative standard deviations for uranium

Method	Raw Data				Reduced Data	Effects
Gravimetric	.00001	.00001	.00001	.00000	.00025	
	.00000	.00000	.00000	.00000		
	.00000	.00000				
Volumetric- Auto.	.01330	.01070	.00000	.00000	.00410	
	.01640	.00000	.00000	.00000		
	.00000	.00000				
Volumetric- Manu.	.01330	.01070	.00000	.00000	.00410	
	.01640	.00000	.00000	.00000		
	.00000	.00000				
Atomic Absorp.	.14150	.13800	.27520	.23370	.12130	
	.00000	.00000	.00000	.00000		
	.00000	.00000				
Colorimetric	.00860	.01060	.00000	.00000	.00830	
	.00000	.00000	.00000	.00000		
	.00000	.00000				
Emission Spec.	.04440	.03680	.04300	.00000	.03650	
	.00000	.06440	.00000	.06980		
	.00000	.00000				
Leco Carbon	.01350	.00000	.00000	.00000	.01350	
	.00000	.00000	.00000	.00000		
	.00000	.00000				
Micro-Kj Nitrogen	.14150	.00000	.00000	.00000	.14150	
	.00000	.00000	.00000	.00000		
	.00000	.00000				

Table 3. Relative standard deviations for ^{235}U

Method	Raw Data				Reduced Data	Effects
Gas Mass Spec 1	.00827	.00793	.00896	.00894	.00018	
	.00816	.00831	.00000	.00000		
Gas Mass Spec 2	.01090	.01683	.02100	.02051	.00049	
	.01527	.01004	.00000	.00000		
Gas Mass Spec 3	.00040	.00030	.00050	.00050	.00015	
	.00030	.00040	.00000	.00000		
Gas Mass Spec 7	.01492	.01489	.01489	.01483	.00020	
	.01476	.01474	.00000	.00000		
Therm. Mass Spec	.08696	.00094	.07407	.00000	.00074	
	.00000	.00000	.00000	.00000		

Table 4. Relative standard deviations for sampling

Material	Uranium	^{235}U
11	.01009	.00000
17	.01009	.00000
19	.01009	.00000
21	.01009	.00000
28	.01009	.00000
29	.01009	.00000
30	.01009	.00000
34	.12972	.00000
35	.06468	.00000
38	.01009	.00000
46	.01009	.00000
57	.01009	.00000
62	.30759	.00000
65	.01009	.00000
70	.01009	.00000
71	.01009	.00000
77	.01009	.00000
79	.01009	.00000
101	.01009	.00000
104	.01009	.00000
129	.01009	.00000
132	.01009	.00000
135	.01009	.00000
210	.00032	.00000
212	.00238	.00000
218	.00000	.00000
219	.00000	.00000
220	.00000	.00000
224	.00000	.00000
227	.00000	.00000
229	.00000	.00000
230	.00000	.00000
240	.00000	.00000
252	.00000	.00000
300	.00000	.00000
302	.00000	.00000
304	.00000	.00000
307	.00000	.00000
311	.00000	.00000
313	.00000	.00000
314	.00000	.00000
315	.00000	.00000
324	.00000	.00000
327	.00000	.00000
330	.00000	.00000
331	.00000	.00000
333	.00000	.00000
335	.00000	.00000
336	.00000	.00000
337	.00000	.00000
404	.00000	.00000

Table 5. Material summary by material description code

Material Description Code	Number of Lots
11	4
17	10
19	3
21	1
28	2
29	4
30	4
34	11
35	15
38	1
46	2
57	3
62	20
65	2
70	2
71	7
77	6
79	3
101	19
104	6
129	0
132	5
135	2
210	41
212	90
218	13
219	16
220	4
224	9
227	10
229	11
230	0
240	3
252	8
300	5
302	13
304	6
307	16
311	0
313	65
314	16
315	21
324	0
327	0
330	0
331	1
333	43
335	4
336	17
337	1
404	5

Table 6. Static/active material summary grams ^{235}U

		Static	Active	Total
Beginning	To Ending	.29362E+06		
	To Removal	.59168E+05		
	Total	.35278E+06	.27728E+07	.31256E+07
Additions	To Ending	.10694E+07		
	To Removal	.00000E+00		
	Total	.10694E+07	.41201E+07	.51895E+07
Removals		-.59168E+05	-.55298E+07	-.55889E+07
Ending		-.13630E+07	-.14005E+07	-.27636E+07
Inventory Difference		.00000E+00	-.37422E+05	-.37422E+05

Table 7. Variance components summary for ^{235}U propagation
from reduced data

Variance Source	Variance (Grams**2)	% of Total
Weighing		
Random	.93485E+05	.0
Uranium Analysis		
Random	.13917E+08	2.8
Uranium Sampling	.93851E+07	1.9
^{235}U Analysis		
Random	.89118E+04	.0
^{235}U Sampling	.00000E+00	.0
Indirect Measurement		
Uranium Factors	.18269E+09	36.7
^{235}U Class Code	.20335E+08	4.1
^{235}U P.O. Numbers	.40720E+05	.0
^{235}U Shipper's Values	.27105E+09	54.5
Total Measurement Variance	.49752E+09	100.0
[Measurement Variance	-.44610E+05	
[Bounds on ID	+.44610E+05	
Total Process Variance	.00000E+00	
Total of all Variance	.49752E+09	
[Total Variance	-.44610E+05	
[Bounds on ID	+.44610E+05	

Table 8. Variance components summary for ^{235}U , weighing - random

Scale	Variance (Grams**2)	% of Total
1-03	.58864E+01	.0
4-15	.31502E+03	.3
4-20	.00000E+00	.0
4-40	.29680E+02	.0
5-08	.15431E+05	16.5
5-11	.26960E+04	2.9
5-14	.28661E-03	.0
5-18	.51951E+04	5.6
5-22	.27972E+00	.0
5-28	.99498E+04	10.6
6-10	.11670E+04	1.2
6-24	.10372E+05	11.1
9-04	.16742E+04	1.8
9-08	.00000E+00	.0
9-18	.71353E+04	7.6
9-19	.41151E+03	.4
9-20	.25308E+04	2.7
9-26	.36420E+05	39.0
SP01	.15186E+03	.2
Total	.93485E+05	100.0

Table 9. Variance components summary for ^{235}U ,
uranium analysis - random

Method	Variance (Grams**2)	% of Total
Gravimetric	.25733E+04	.0
Volumetric-Auto.	.37810E+05	.3
Volumetric-Manu.	.00000E+00	.0
Atomic Absorp.	.63875E+01	.0
Colorimetric	.59211E+07	42.5
Emission Spec.	.37838E+07	27.2
Leco Carbon	.41717E+07	30.0
Mic-KJ Nitrogen	.00000E+00	.0
Total	.13917E+08	100.0

Table 10. Variance components summary for ^{235}U , uranium sampling

Material	Variance (Grams**2)	% of Total
11	.00000E+00	.0
17	.00000E+00	.0
19	.00000E+00	.0
21	.00000E+00	.0
28	.00000E+00	.0
29	.00000E+00	.0
30	.00000E+00	.0
34	.11728E+05	.1
35	.28438E+06	3.0
38	.00000E+00	.0
46	.00000E+00	.0
57	.00000E+00	.0
62	.86971E+07	92.7
65	.46179E+05	.5
70	.00000E+00	.0
71	.00000E+00	.0
77	.62851E+00	.0
79	.00000E+00	.0
101	.16479E+06	1.8
104	.00000E+00	.0
129	.00000E+00	.0
132	.16775E+04	.0
135	.00000E+00	.0
210	.99314E+03	.0
212	.17824E+06	1.9
218	.00000E+00	.0
219	.00000E+00	.0
220	.00000E+00	.0
224	.00000E+00	.0
227	.00000E+00	.0
229	.00000E+00	.0
230	.00000E+00	.0
240	.00000E+00	.0
252	.00000E+00	.0
300	.00000E+00	.0
302	.00000E+00	.0
304	.00000E+00	.0
307	.00000E+00	.0
311	.00000E+00	.0
313	.00000E+00	.0
314	.00000E+00	.0
315	.00000E+00	.0
324	.00000E+00	.0
327	.00000E+00	.0
330	.00000E+00	.0
331	.00000E+00	.0
333	.00000E+00	.0
335	.00000E+00	.0
336	.00000E+00	.0
337	.00000E+00	.0
404	.00000E+00	.0
Total	.93851E+07	100.0

Table 11. Variance components summary for ^{235}U ,
 ^{235}U analysis - random

Method	Variance (Grams**2)	% of Total
Gas Mass Spec 1	.37319E+04	41.9
Gas Mass Spec 2	.40452E+04	45.4
Gas Mass Spec 3	.20028E+03	2.2
Gas Mass Spec 7	.93426E+03	10.5
Therm. Mass Spec	.22940E+00	.0
Total	.89118E+04	100.0

Table 12. Static/active material summary grams uranium

		Static	Active	Total
Beginning	To Ending	.29307E+08		
	To Removal	.59654E+07		
	Total	.35273E+08	.27511E+09	.31038E+09
Additions	To Ending	.10313E+09		
	To Removal	.00000E+00		
	Total	.10313E+09	.40666E+09	.50979E+09
Removals		-.59654E+07	-.53723E+09	-.54319E+09
Ending		-.13243E+09	-.14568E+09	-.27811E+09
Inventory Difference		.00000E+00	-.11312E+07	-.11312E+07

Table 13. Variance components summary for uranium
propagation from reduced data

Variance Source	Variance (Grams**2)	% of Total
Weighing		
Random	.8600E+09	.0
Uranium Analysis		
Random	.12628E+12	6.2
Uranium Sampling	.10465E+12	5.1
Indirect Measurement		
Uranium Factors	.18048E+13	88.6
Total Measurement Variance	.20366E+13	100.0
[Measurement Variance	-.28542E+07	
[Bounds on ID	+.28542E+07	
Total Process Variance	.00000E+00	
Total of all Variance	.20366E+13	
[Total Variance	-.28542E+07	
[Bounds on ID	+.28542E+07	

Table 14. Variance components summary for uranium,
weighing - random

Scale	Variance (Grams**2)	% of Total
1-03	.60981E+05	.0
4-15	.34412E+07	.4
4-20	.00000E+00	.0
4-40	.33049E+06	.0
5-08	.12768E+09	14.7
5-11	.30106E+08	3.5
5-14	.31959E+01	.0
5-18	.50327E+08	5.8
5-22	.31829E+04	.0
5-28	.75198E+08	8.7
6-10	.11173E+08	1.3
6-24	.97189E+08	11.2
9-04	.16882E+08	1.9
9-08	.00000E+00	.0
9-18	.65403E+08	7.5
9-19	.45129E+07	.5
9-20	.27581E+08	3.2
9-26	.35762E+09	41.2
SP01	.15540E+07	.2
Total	.86906E+09	100.0

Table 15. Variance components summary for uranium,
uranium analysis - random

Method	Variance (Grams**2)	% of Total
Gravimetric	.29708E+08	.0
Volumetric-Auto.	.38027E+09	.3
Volumetric-Manu.	.00000E+00	.0
Atomic Absorp.	.73808E+05	.0
Colorimetric	.52724E+11	41.8
Emission Spec.	.35530E+11	28.1
Leco Carbon	.37617E+11	29.8
Mic-KJ Nitrogen	.00000E+00	.0
Total	.12628E+12	100.0

Table 16. Variance components summary for uranium, uranium sampling

Material	Variance (Grams**2)	% of Total
11	.00000E+00	.0
17	.00000E+00	.0
19	.00000E+00	.0
21	.00000E+00	.0
28	.00000E+00	.0
29	.00000E+00	.0
30	.00000E+00	.0
34	.13459E+09	.1
35	.33173E+10	3.2
38	.00000E+00	.0
46	.00000E+00	.0
57	.00000E+00	.0
62	.96543E+11	92.3
65	.55311E+09	.5
70	.00000E+00	.0
71	.00000E+00	.0
77	.40225E+04	.0
79	.00000E+00	.0
101	.15499E+10	1.5
104	.00000E+00	.0
129	.00000E+00	.0
132	.14602E+08	.0
135	.00000E+00	.0
210	.28437E+07	.0
212	.25347E+10	2.1
218	.00000E+00	.0
219	.00000E+00	.0
220	.00000E+00	.0
224	.00000E+00	.0
227	.00000E+00	.0
229	.00000E+00	.0
230	.00000E+00	.0
240	.00000E+00	.0
252	.00000E+00	.0
300	.00000E+00	.0
302	.00000E+00	.0
304	.00070E+00	.0
307	.00000E+00	.0
311	.00000E+00	.0
313	.00000E+00	.0
314	.00000E+00	.0
315	.00000E+00	.0
324	.00000E+00	.0
327	.00000E+00	.0
330	.00000E+00	.0
331	.00000E+00	.0
333	.00000E+00	.0
335	.00000E+00	.0
336	.00000E+00	.0
337	.00000E+00	.0
404	.00000E+00	.0
Total	.10465E+12	100.0

Table 17. Error Propagation Exercise summary statistics (grams)

	²³⁵ U	U
BI Beginning Inventory	2,772,800	275,110,000
+A Additions	4,120,100	406,660,000
-R Removals	-5,529,800	-537,230,000
-EI Ending Inventory	-1,400,500	-145,680,000
ID Inventory Difference	-37,422	-1,131,200
LEID Raw Data Limit of Error	45,455	2,863,000
LEID Reduced Data Limit of Error	44,610	2,854,200
T (Throughput) = BI + A	6,892,900	681,770,000
Raw LEID/Tx100 (%)	.659	.420
Reduced LEID/Tx100 (%)	.647	.419
Historical Control Limit/Tx100 (%)*	.880	.880

*Calculated FY 1982 to apply to test data period contained in FY 1983.

1. *Inventory Differences (ID's)*. The ^{235}U and U IDs given in Tables 6 and 12, respectively, and repeated in Table 17 as -37,422 grams and -1,131,200 grams both represent gains in material since they are negative (more removals and ending inventory than beginning inventory and additions). About 1% of the exercise U was ^{235}U , as one can see in the Table 17 BI, A, R, and EI transaction amounts. The ^{235}U ID, however, is about 3% of the U ID. This suggests some degree of independence between the ^{235}U and U materials as treated with the exercise computer data base. Previously, NLO would have specified the ^{235}U ID to be .01 times the U ID. There is generally reason to expect ^{235}U IDs to be proportionately larger than U IDs, since one can see from the Fig. 2 example that weight ^{235}U involves all the measurement variance in the weight U and the additional measurement variance in the ^{235}U enrichment determination.

2. *Limit of Error on Inventory Differences (LEID's)*. The ^{235}U and U LEIDs given in Tables 7 and 13, respectively, and repeated in Table 17 as 44,610 grams and 2,854,200 grams based on reduced data measurement variances suggest there is no reason to suspect theft or diversion or any other suspicious occurrence in the exercise MBA during the exercise time period. The absolute ^{235}U ID of 37,422 is relatively close to the LEID of 44,610, but still within the limit. The absolute U ID of 1,131,200 is well within the limit of 2,854,200. It is particularly to be noted that the LEIDs based on raw data measurement variances given in Table 17 are almost exactly the same as those based on reduced data measurement variances discussed above. (These two different sets of measurement variances appear in Tables 1-3.)

3. *Validity of the LEIDs.* No definitive statement of validity can be made about the LEIDs obtained since there are no "true" LEIDs, either known or unknown. We can, however, cite certain evidence of their probable validity. First is the simple fact that the limits obtained were not unrealistically small, as has been the case in some previous error propagation attempts at NLO and elsewhere. Second is the agreement of the raw and reduced data LEIDs noted above, which increases the confidence in the individual LEIDs. Finally, one may compare the exercise LEIDs to NLO's historical control limits using the last four rows of Table 17, where our raw and reduced LEIDs are expressed as a percentage of throughput, and approximate control limits developed via the standard inventory difference procedure for the exercise MBA are similarly expressed as a percentage of throughput. The latter limits are approximate because the exercise MBA was not one of NLO's established historical MBA's, and thus its historical IDs had to be approximated to apply the standard inventory difference procedure. The Table 17 results suggest that the exercise LEIDs are smaller than NLO's historical control limits, .65% to .88% for ^{235}U and .42% to .88% for U (reduced comparison). Specific reasons to expect lower propagation LEIDs in this exercise are the zero process variance estimate in Tables 7 and 13, and the absence of methodology dealing with bias correction. Alternatively, increasing NLO throughput over the past two years should have led to relatively larger propagation LEIDs. In any case, the value of the comparison is greatly limited by the need to approximate historical IDs for a non-historical MBA.

4. *Guidance for Reducing IDs and LEIDs.* A very important benefit of the error propagation approach beyond its provision of statistically

defensible LEIDs is the potential guidance it provides for actually reducing IDs and LEIDs in future time periods. The potential arises in being able to see detailed breakdowns of the measurement variance which led to the LEIDs, as in Table 7 (^{235}U) and Table 13 (U).

Consider Table 7. It shows our ^{235}U LEID of 44,610, which is twice the square root of the total measurement variance of $.49752 \times 10^9$, which is in turn the cumulation of nine different non-zero variances listed above in the same column. One sees that 54.5% of the total variance is associated with using shipper's values in place of actual ^{235}U measurements. One sees that indirect measurement, that is, utilization of uranium factors, standard enrichments, and shipper's values, accounts for 95.3% of all variance. One is directed to study indirect measurement practices for possible reduction of LEIDs and the associated IDs. It should be noted, however, that the validity of this direction is dependent on how typical the material flows in Table 5 are of the "typical" flows in this MBA. The cumulative variances in Table 7 reflect both basic measurement variances and the particular pattern of material flows in the April-June, 1983 period. If the latter were atypical, the percentage distribution in Table 7 variances could change dramatically in future error propagations with no change whatever in basic measurement variances.

The variance picture given by Table 7 is made more specific in Tables 8-11, where direct measurement aggregates in Table 7 are broken down by measurement method, material, etc. In Table 9, for example, one can see the total analytical uranium analysis variance of $.13917\text{E} + 08$ linked to particular analytical methods. The colorimetric, emission spectrometry, and leco carbon methods, all employed to analyze crude ingot impurities, jointly account for 97.7% of the analytical uranium analysis variance.

Thus, if the latter variance were important in the aggregate picture of Table 7, one would be directed to examine these methods for possible reduction of LEIDs and the associated IDs.

The discussion above could readily be repeated in terms of Table 13 and Table 15 and the U LEID of 2,854,200. Tables 7 and 13 might also lead us in other directions. If weighing variance was dominant, we could use Tables 8 and 14 for guidance on possible scale improvement/ replacement. If uranium sampling variance was dominant, we could use Tables 10 and 16 for guidance on possible changes in material sampling procedures. Table 11 breaks down the ^{235}U analytical variance of Table 7 by the five pieces of equipment used to determine ^{235}U enrichment. Overall, we see in these many tables the breakdown of the total measurement variance which led to the LEID, and an ability to see exactly where measurement variance problems should be attacked (assuming typical material flows).

Limitations

The statistical results of the NLO error propagation exercise, like those of any applied data exercise, are limited by the breadth of the statistical methodology employed, and by any inadequacies in the data required to execute that methodology.

The major limitation in the breadth of the statistical methodology employed in the NLO exercise was the absence of any mechanism for the extrapolation and cumulation of bias. The term "bias" is used here in reference to measurement results from a given piece of equipment, operator, or analytical procedure that are on average above or below the true amounts involved over an extended time period (distinguished from the term "systematic error", see below). The extrapolation and cumulation of bias

requires a somewhat different methodological treatment than that used on variances. Constraints of time and a feeling that this would not be a substantial component in determining NLO LEIDs lead us to ignore the bias problem in the NLO exercise.

A known inadequacy in the data required to execute the statistical error propagation methodology designed for NLO was the absence of historical ID data and measurement variance totals for the exercise MBA, which was not one of NLO's standard MBAs. This data would have been used to estimate process variance, or process error, using the approach of NUSAC, Inc. (1981).² Process variance is the variance beyond measurement variance, such as unmeasured inventory, bookkeeping errors, holdup, etc. In certain facilities it may be significant relative to measurement variance, thus expanding LEIDs. Our Tables 7 and 13 reflect zero estimates of process variance in the NLO exercise which were based on very unsophisticated attempts to approximate the missing historical data. We have no faith in these zero estimates. Only the operation of error propagation over a number of inventory periods at NLO will provide all the necessary data, since measurement variance totals are derived from the propagation operation itself.

A probable data inadequacy exists in the area of the reduced/raw measurement variances in Tables 1-3. The reader will note the blank column in these tables labelled "Effects". A cumulative measurement variance can be conceived of as potentially consisting of random variance (unexplained) and the variance "effects" associated with features of the analysis such as

² This approach also requires data on measurement covariance from the historical period.

analytical method, instrument, operator, and time of day. "Effects" is the statistical term for what many in the error propagation literature call "systematic error". Effects can be estimated with appropriate existing data, or data from a designed statistical experiment. Tables 1-3 reflect the absence of any non-zero effects in the NLO exercise (variance associated with these effects would appear in Tables 7 and 13 and additional supporting tables). Some attempts were made to estimate these effects with existing data, but no significant effects were found. Additional designed experiments would have been needed to fully explore the existence of effects (systematic error).

The reduced/raw measurement variance numbers which appear in Tables 1-3 are a possible data inadequacy. There is some support for their overall validity in that the error propagation produced reasonable LEIDs, and about the same LEIDs based on reduced or raw data. However, it should be noted that these variances were estimated largely from existing NLO data, perhaps of some age, in a relatively undocumented manner. This pattern of estimation was not what we would have preferred, a sequence of designed and well documented statistical experiments.

Future Error Propagation at NLO

The enriched materials handled at NLO are accounted for in twelve different MBA's. The single MBA in the NLO exercise focusing on reduction and casting was, however, much more than one-twelfth of the total enriched error propagation problem. NLO personnel estimate that the exercise MBA probably encompassed more than 50% of the total problem. Thus, carrying

error propagation forward from the exercise to all enriched MBA's will not be the enormous task one might suppose it to be as a twelve-to-one extrapolation.

We have made some comments in previous parts of this report that imply certain attitudes about specific paths that should be followed in future NLO error propagation. First, in terms of error propagation methodology, we see that employed in this exercise as adequate to future needs. As previously stated, however, there is nothing in our methodology in conflict with the NUSAC, Inc. (1981) AMASS methodology, other than the terminology of "effects" vs. "systematic error". The now available (or soon to be available) augmented AMASS (AAMASS) will incorporate bias correction procedures and will thus be broader than the exercise methodology. AAMASS would be a worthy alternative methodologically, although there would be practical problems in supplying the historical data needed to estimate process error (as previously discussed).

Second, there is no further general need to propagate error from both reduced and raw data. Error propagation from the simpler reduced data produced results equivalent to those from the detailed raw data in this exercise. We thus feel there is no general need to do raw data error propagation.

Third, in concluding the previous section, the reduced/raw measurement variance numbers in Tables 1-3 were indicated to be less dependable than is desirable. We recommend specific documented experiments at regular intervals, perhaps as part of the on-going NLO recycle-control program, to provide sound input to this fundamental foundation of error propagation. In such experiments, care must be exercised to be sure that measurement

personnel are unaware of previous recycle or true control measurements, for example, by employing double blind checkweights.

Another aspect of future NLO error propagation is the ability to execute error propagation on the NLO HP-3000 computer system. We did experience about two months delay in concluding the exercise after a number of attempts to make error propagation operational on the HP-3000. We were forced to restructure the computer program by a) reducing storage areas, b) segmenting, and c) having it access transactions and measurements data sorted in a special way. The error propagation program does not contain much room for expansion. We feel, however, that since error propagation can be executed sequentially over each of NLO's 12 MBAs, no significant expansion of this program will be required, and the HP-3000 will represent no impediment to whole-plant enriched material error propagation.

Finally, the future importance of subjecting the transactions and measurement data to stringent edit checks is to be stressed. We have seen relatively small errors in the data (for example, a misplaced decimal in one lot's ^{235}U enrichment measurement) produce substantial effects in the ID's and LEID's, particularly when the propagation is done with raw data. The existing error propagation computer program contains numerous edit checks, and these checks were extremely valuable. However, it would be desirable to place as many of these checks as possible closer to the point of entry of the transactions and measurement data.

Summary

Error propagation is the extrapolation and cumulation of uncertainty (variance) about amounts of material which results from measurement error, and possibly from process error. The error propagation methodology suggests a very detailed build-up of variance from the basic level of raw/reduced measurement variances in Tables 1-3 to produce an LEID, twice the square root of total measurement and process error (variance). The error propagation approach avoids two problems of the standard inventory difference control limit approach, a theft or diversion influencing the LEID, and a lack of association of the LEID with facility throughput.

The lessons learned in the applied statistical NLO error propagation exercise were:

- . Apparently valid LEIDs can be determined via statistically based error propagation methodology. The ^{235}U and U ID's were both within the error propagation LEIDs. The LEIDs seemed valid because they were not absurdly small and were essentially the same when produced from raw and reduced data.
- . Tabular variance component summary tables like Tables 8-11 and 14-16 give guidance for actually reducing future IDs and LEIDs, assuming the materials in transactions are typical of a normal material flow. This is an important feature of this approach.
- . Error propagation can be executed on the already reduced final measurement data, disregarding the more voluminous raw measurement data.

- . The raw/reduced measurement variance estimates in Tables 1-3 are the pivotal foundation of the error propagation procedure. Specific documented experiments should be performed at regular intervals to update these variance estimates.
- . There are opportunities for the elaboration of the NLO exercise statistical error propagation methodology to consider bias correction and more fully treat process error as a component of total variance. AAMASS is a statistically sound general methodology that incorporates these two features.
- . It is very important to subject the transactions and measurement data to comprehensive edit checks near the point of data entry.
- . The NLO HP-3000 computer system is capable of handling whole-plant statistical error propagation for enriched material MBAs at NLO.

III. METHODOLOGY

A Note on Terminology

One frequently sees references to the term "systematic error", or the qualified terms "long-term systematic error" and "short-term systematic error" in the error propagation literature. There appears, however, to be little agreement on what systematic error is.

Systematic error was equivalent to "bias" to Eisenhart (1963) and Schumacher (1981), i.e., a non-zero mean error source. To Jaech (1973), in his Chapters 5 and 6, systematic error was the presence of a particular zero-mean error source in multiple observations of an SNM data base, for example, the same operator in a sequence of measurements. In Chapter 5, page 167, Jaech's assumption number eight specifically assumes away bias in the propagation problem and makes it clear that he does not equate systematic error with bias. Unfortunately, in his earlier Chapter 3, Jaech very confusingly mixed the Chapter 5 and 6 concept with the concept of bias. Generally speaking, the error propagation literature has left many people working in nuclear material control understandably confused by the term "systematic error".

It is very easy to drop the term "systematic error". If we want to talk about zero-mean error (or variance) sources that impact more than single observations, we can say "effects", using the conventional statistical terminology of analysis of variance (ANOVA), as discussed by Easterling (1982). The effects which can be considered in the context of the NLO data base are analytical method effects, instrument (e.g., scale) effects, operator effects, and time of day effects. We have, then, dealt with systematic errors as zero-mean error sources that impact more than single observations, and chosen to call them "effects". This follows conventional statistical terminology.

Conceptual Methodology

The conceptual error propagation methodology developed in the process of the NLO exercise combines elements of Jaech (1973), the statistical theory of random effects ANOVA models, and concepts we first experienced through our study of the AMASS methodology in NUSAC (1961). Here, we briefly summarize the major components of what we feel would represent a comprehensive, technologically sound error propagation methodology:

1. *Variance Approximation by Taylor Series Expansion.* Statistical error propagation focuses on determining the variance of a quantity of interest, say Q , which is a function of a number of variables $X_1, X_2, \dots, X_m$, say $f(X_1, X_2, \dots, X_m)$. Assuming no covariance between the X 's, the variance of Q may be approximated through a Taylor series expansion around the means of $X_1, X_2, \dots, X_m$ by

$$\sigma_Q^2 \doteq \sum_{j=1}^m \left[\left. \frac{\partial f}{\partial X_j} \right|_{\underline{\mu}} \right]^2 \sigma_{X_j}^2, \quad (1)$$

where $|\underline{\mu}$ specifies evaluation of the partial derivative at the mean level vector $\underline{\mu} = (\mu_1, \dots, \mu_m)$ with $\mu_j = E(X_j)$, and X_j has variance $\sigma_{X_j}^2$ (see Appendix B).

In the nuclear material control measurement context, the following represents a fundamental example of the propagation process:

Q = weight uranium

X_1 = net weight

X_2 = uranium concentration

$Q = f(X_1, X_2) = X_1 X_2$

Equation (1) then suggests that

$$\sigma_Q^2 \doteq \mu_2^2 \sigma_{X_1}^2 + \mu_1^2 \sigma_{X_2}^2 . \quad (2)$$

The theoretical exact variance for Q, as seen for example in Lowe and Waterman (1976), is

$$\sigma_Q^2 = \mu_2^2 \sigma_{X_1}^2 + \mu_1^2 \sigma_{X_2}^2 + \sigma_{X_1}^2 \sigma_{X_2}^2 . \quad (3)$$

By comparison of (3) and (2), one sees the approximation will be adequate when σ_{X_j} is small relative to μ_j , that is, when the third term in (3) is small relative to each of the two other terms.

For purely additive functional forms of covariance-free X's, the σ_Q^2 from (1) will be exact irrespective of any other considerations. Quotient functional forms, such as $Q = X_1/X_2$, produce results similar to that in the multiplicative functional form example above, adequate approximations when σ_{X_j} is small relative to μ_j . A point of primary importance in the nuclear material control context is that σ_{X_j} represents the standard deviation of a measurement around the true value, not the standard deviation of X_j unconditionally across a general population. Thus, σ_{X_j} should indeed be small relative to μ_j in this context, and (1) will produce a good approximation to σ_Q^2 for multiplicative and quotient forms of Q.

For simplicity of computation, it is also notable that a function $Q = f(X_1, X_2, \dots, X_m)$ of a perhaps large number m of variables can be propagated sequentially in many instances, that is, considering operations on just two variables in sequence. For example, $Q = f(X_1, X_2, X_3) = X_1 X_2 X_3$ is also

$$\begin{aligned}
 Q &= f(X_1, X_2, X_3) = g(X_1, X_2)h(X_3) \\
 Q &= X_1 X_2 X_3 = (X_1 X_2)(X_3)
 \end{aligned}
 \tag{4}$$

The application of (1) to the function g , sequentially followed by another application to gX_3 , gives the same result as one application of (1) to the function f (see Appendix B). The sequential process does not work on a function like $f(X_1, X_2, X_3) = (X_3 - X_2)/(X_1 - X_2)$.

2. *Variance Aggregation by Uncorrelated Primary Error Sources.* An inventory difference is formed through the addition and subtraction of many quantities of interest, Q , whose individual variance propagation was just discussed. The variance associated with the inventory difference cannot, however, be determined by simple addition of individual variances because there are covariances between the individual Q 's that must be considered.

The existence of covariance has been the primary problem preventing the determination of ID variance through the classical representation in terms of beginning and ending inventory, additions, and removals as $ID = BI + A - R - EI$. Covariances between the four components BI, A, R, EI must be considered. There is, however, no reasonable way to derive these covariances.

Jaech's (1973) Chapter 6 discussion of variance aggregation by uncorrelated primary error sources provides the blueprint for a process which circumvents this covariance problem. His Table 6.2 and 6.3 rules detail the aggregation of variance by the uncorrelated primary error sources of weighing, analysis and sampling for element, and analysis and sampling for isotope. It is intuitively clear that errors in any of these five sources should be uncorrelated with errors in any of the others.

Within each primary error source, there may be error covariance that needs to be accounted for, for example, because multiple measurements are done by the same method, instrument, person, or at the same time of day. This is what Jaech terms "long-term systematic error" and "short-term systematic error" in his Table 6.2 and 6.3 rules. As was discussed at the beginning of Section III, we prefer to call this covariance "effects", using the statistical language of analysis of variance. In principle, one can associate an effect with any number of specific aspects of measurement processes that may be repeated in different measurements. Jaech essentially limits himself to two such effects with the generic names "long-term systematic error" and "short-term systematic error". Whatever the terminology, the Table 6.2 - 6.3 rules reflect an appropriate way to aggregate variance that does consider the covariance within primary error source. Appendix C contains the equivalent rules for the simplified measurement environment of the NLO exercise, a one-sample, one-analysis environment.

3. *Random Effects ANOVA Models.* There must be a mechanism for estimating the basic measurement variances of (1), the $\sigma_{x_j}^2$, so-called reduced data measurement variances, or the more micro-level raw data measurement variances which would propagate through (1) to approximate the reduced data measurement variances. As discussed above, we are also concerned with the possible association of parts of the variance with so-called effects, which might imply covariance across measurements done by the same method, instrument, person, etc. We can estimate these variances and any association with effects using random effects ANOVA models, as discussed by Searle (1971).

For purposes of illustration, suppose that canisters of some material are weighed on one of two scales by one of three operators. A model that can be used to describe the weight measurement W_{ijk} corresponding to the i th scale, j th operator, and k th canister is given by:

$$W_{ijk} = \mu + \alpha_i + \beta_j + \epsilon_{ijk} \quad (5)$$

$$\begin{aligned} i &= 1, 2 \\ j &= 1, 2, 3 \\ k &= 1, 2, \dots, n \end{aligned}$$

where

μ = overall mean value.

α_i = effect of the i th scale.

β_j = effect of the j th operator.

and ϵ_{ijk} = random error.

We assume that the scale, operator, and random error terms in (5) are random variables which are mutually independent. In particular, the α_i represent a random sample from a population with mean zero and variance σ_α^2 , denoted by $(0, \sigma_\alpha^2)$. Similarly, the β_j are a random sample from a population distributed as $(0, \sigma_\beta^2)$ and the ϵ_{ijk} a random sample from a population distributed as $(0, \sigma_\epsilon^2)$. It then follows that the variance of a particular weight measurement is given by

$$\sigma_W^2 = \text{Var}(W_{ijk}) = \sigma_\alpha^2 + \sigma_\beta^2 + \sigma_\epsilon^2 \quad (6)$$

Since each of the variances σ_α^2 , σ_β^2 , σ_ϵ^2 is a component of σ_W^2 , these individual variances are termed "variance components". These variance components can be estimated using data from a properly designed experiment.

σ_{ϵ}^2 is associated with random error. σ_{α}^2 and σ_{β}^2 are associated with scale and operator effects, respectively (systematic error). It is, of course, possible that $\sigma_{\alpha}^2 = \sigma_{\beta}^2 = 0$ and σ_W^2 is entirely random error variance, $\sigma_W^2 = \sigma_{\epsilon}^2$.

The presence of non-zero effects such as represented by σ_{α}^2 and σ_{β}^2 does imply a covariance between measurements within primary error source. Suppose in the above example that two single canisters are weighed by two different operators on the same scale. Denoting the two weight measurements symbolically as W_{ijk} and $W_{ij'k'}$, the covariance between them is given by

$$\begin{aligned} & E [(\alpha_i + \beta_j + \epsilon_{ijk})(\alpha_i + \beta_{j'} + \epsilon_{ij'k'})] \\ &= E [\alpha_i^2 + \beta_j \beta_{j'} + \epsilon_{ijk} \epsilon_{ij'k'} + \text{crossprod.}] \\ &= \sigma_{\alpha}^2, \end{aligned} \tag{7}$$

the variance component associated with scale effect. If the same operator weighed the two canisters on the same scale, the covariance would be $\sigma_{\alpha}^2 + \sigma_{\beta}^2$. To properly accumulate these covariances, one must accumulate over measurements where the characteristic associated with an effect is the same. Part of the function of Jaech's (1973) Chapter 6 rules (related to what he calls long-term or short-term systematic error) is the proper accumulation of covariance terms which arise in the manner demonstrated above.

The random effects ANOVA model can be applied separately to each relevant measurement process. For example, in determining the amount of ^{235}U in an item we need to obtain the net weight of the item, the U concentration, and the ^{235}U enrichment. Each of the three individual

measurements can be modeled and the variance components estimated. These estimates can then be used in determining the variances to be propagated through equation (1) in the pattern of Jaech's Table 6.2 - 6.3 rules.

The remaining elements of our conceptual error propagation methodology were concepts we first experienced through our study of the NUSAC (1981) Automated Material Accounting Statistics System (AMASS) error propagation methodology developed for the United States Nuclear Regulatory Commission. This methodology is being extended in current work under the designation AAMASS, augmented AMASS. AMASS begins with Jaech's error propagation approach, maintaining the terminology of "systematic error" which we replace with "effect". However, AMASS goes well beyond Jaech, placing the concepts of bias correction, process error, static inventory, and strata within the context of a conceptually complete error propagation methodology:

4. *Bias Correction.* Whatever the confusion created by his earlier Chapter 3, Jaech (1973) is not propagating bias in his Chapter 5 - 6 methodology. He states the following assumption on page 167 of Chapter 5: "All error-component random variables are unbiased; i.e., they are distributed with zero-means. This means that, if any known measurement biases exist, the data are appropriately corrected." Jaech assumes bias correction. AMASS as summarized in NUSAC (1981) does not include bias correction methodology, but such methodology will be included in the extended AAMASS.

Bias correction is intuitively a simpler process than any attempt to propagate bias in measurements through functions of these measurements, akin to the variance propagation in Equation (1). Bias propagation would ultimately lead to the uncomfortable question of how to combine the previously discussed variance propagation with the bias propagation to form LEIDs. Bias correction allows application of the usual error propagation to the corrected data, recognizing, as Jaech (1973) did in his Chapter 3, that the act of correction is itself an effect whose variance should be propagated.

5. *Process Error.* Error propagation in nuclear material control has often focused entirely on measurement error. AMASS emphasizes the potential role of other sources of error that can impact inventory differences, for example, unmeasured inventory and bookkeeping errors. These other sources are lumped under the label "process error". LEIDs based on measurement error to the exclusion of process error may be understated.

NUSAC (1981) provides methodology for estimating the process variance associated with process error, assuming it to be constant over time (see Appendix D). The estimation requires as data a sequence of historical inventory differences, propagated measurement variance totals in each inventory difference period, and propagated measurement covariance totals between inventory difference periods. The statistical theory behind AMASS's simultaneous consideration of measurement and process error is sound in our opinion. Some question did arise about the acceptability of the methodology under the guidelines of DOE Order 5630.2, which does not permit long-term use of LEIDs based solely on historical inventory

differences. However, the AMASS process error methodology combines information from historical inventory differences and measurement error propagation to formulate LEIDs.

6. *Static Inventory.* Static inventory is material in beginning inventory (BI) or added (A) that is carried to ending inventory (EI) or removed (R) during a period without remeasurement. Thus, there are four paths involved (BI → EI, BI → R, A → EI, A → R), one of which does not even involve material that was in an "inventory" category. Such material cannot contribute to inventory differences since the error present in its measurement cancels out in the $ID = BI + A - R - EI$ determination. Thus, one should exclude static inventory from the error propagation process. It is readily seen in Jaech's (1973) Chapter 6 rules that failure to exclude static inventory would upward bias random error propagation. Jaech, however, does not mention this important concept in any direct way.

7. *Strata.* AMASS seeks to divide material into strata containing like materials, following common error paths in terms of weighing, sampling, and analysis, with like sign in the inventory difference aggregation, and roughly equal amounts of nuclear material. Data processing involves only strata totals. Jaech (1973) also mentions this concept in Section 9.3.

Applied Methodology

The error propagation methodology applied in the actual conduct of the NLO exercise naturally consisted of the elements of the conceptual methodology that could profitably be employed within the realistic limitations imposed by the exercise environment. These limitations were 1) no history of error propagation at NLO, 2) the use of an MBA that was not a historical NLO MBA, 3) time duration of the exercise, and 4) the data collected on individual transactions and measurements. The data collected is summarized in Table 18. Below, the treatment of each element of the conceptual methodology in the final applied methodology is summarized:

Table 18. Transaction and measurement data

Transaction	Measurement
Lot Identification ³	Lot Identification ³
Item No.	Item No.
Sublot No.	Sublot No.
Plant No.	Laboratory No.
MBA No.	Measurement Method
Transaction Date	Instrument No.
Transaction Time	Measurement Date
Transaction Operator No.	Measurement Time
Transaction Type ⁴	Measurement Operator No.
Total Uranium Grams	Measurement Type ⁵
Total ²³⁵ U Grams	Item Type ⁶
	Raw Measurements (up to 10)
	Reduced Measurement

³ Components are purchase order (P.O.) number, source, class code, material type, and lot sequence number.

⁴ Addition, inventory, removal.

⁵ Control, replicate, routine.

⁶ Item, sample (lot measurement).

1. *Variance Approximation by Taylor Series Expansion.* Equation (1) was used either directly or sequentially in all NLO exercise variance approximations.

There are three distinct areas in which propagation of variance by (1) was used. First, the fundamental propagation of variance into weight ^{235}U or weight U from reduced data measurements of net weight, $\bar{X}\text{U}$, and ^{235}U enrichment was executed by Appendix C equations similar to Jaech's. Second, when the propagation was started from the raw data level, (1) was used to propagate reduced data variances, directly in some cases, and sequentially in others, as summarized in Appendix E. Third, approximate variance propagation was needed in some special operations, such as the subtraction of impurities in determining final U concentration, and considering uncropped ingots which were analyzed only after cropping as the MBM output (see 10 below).

It should be noted that, following the pattern of Jaech (1973) and his Chapter 6 equations, all propagation was executed in terms of relative standard deviations rather than variances, that is, the square root of the variance divided by the value of the variable being considered.

2. *Variance Aggregation by Uncorrelated Primary Error Sources.* Table 7 reflects Jaech's five uncorrelated primary error sources - weighing, uranium analysis, uranium sampling, ^{235}U analysis, ^{235}U sampling - and the aggregation of variance in the NLO exercise by these sources. The individual scales, analytical methods, and materials sampled that are aggregated over to produce variance in these five uncorrelated categories can be seen in Tables 1-4. Appendix C contains the detailed formulation of this variance aggregation.

3. *Random Effects ANOVA Models.* The computer code developed for the NLO exercise error propagation provides for the potential of effects (systematic error) associated with the four measurement characteristics

analytical method, instrument, operator, time of day. The limitation to these four characteristics was imposed by the measurement data collected, as summarized by Table 18. One or two effects can be associated with each individual scale in Table 1, the first three analytical methods in Table 2, and each analytical method in Table 3 (program variables WE, UE, U2E in BLOCK DATA and MNE, NWE, NUB, NU2E in SUBROUTINE INIT), by supplying relative standard deviations associated with the effects (which will then be printed in Tables 1-3). The effects propagation was tested during code development and judged to work satisfactorily.

Random effects ANOVA model estimation of variance effects on available data was performed at Oak Ridge National Laboratory using the Statistical Analysis System (SAS) software package. (See Appendix F for further discussion and results.) The analysis indicated no significant effects that should be included in the NLO exercise error propagation. Thus, the exercise results in Tables 1-3, Table 7, and Table 13, make no reference to effects (except in column headings over empty columns). If significant effects had been uncovered, there would in fact have been additional results tables breaking down effects variance by individual scale and/or analytical method. Thus, the NLO exercise computer code includes the "effects" element, but the NLO exercise results do not.

It should be noted that much of the available data was of limited value for estimating effects. The absence of significant effects reflects data inadequacies moreso than the real existence or absence of the effects. Designed experiments need to be performed to obtain accurate estimates. The data used in the NLO exercise was taken from undesigned experiments. Such data is susceptible to several other effects that are not accounted

for, but can confound and confuse the effects being analyzed. In many cases, the data was only useful in estimating the reduced/raw data random measurement variance, while effects such as instrument, operator, etc, could not be evaluated.

4. *Bias Correction.* There was no attempt to implement bias correction in the NLO exercise. Given the limited time duration of the exercise, our small initial knowledge base, and the absence of any generally utilized statistical methodology of error propagation, it was unreasonable for us to establish a goal of producing a totally comprehensive error propagation methodology for the NLO exercise. It was felt that bias would be a relatively smaller component of the uncertainty that would ultimately be reflected in LEIDs. In addition, the work required to handle bias estimation in terms of methodology development, conduct of experiments, etc., would have been extensive and costly compared to that needed to develop other elements of a reasonably comprehensive methodology. Thus, all factors suggested that bias correction receive a low priority.

5. *Process Error.* There was an attempt made in the NLO exercise to estimate process error (variance) and add it to measurement variance to determine LEIDs based on the combined variance. This can be seen at the bottom of Tables 7 and 13. Note, however, that the process variance estimate in each case is listed as zero, essentially saying we were not able to estimate process error with the available information.

All of the historical information needed in the Appendix D procedure for estimating a constant process error - a sequence of historical IDs, propagated measurement variance totals in each ID period, and propagated

measurement covariance totals between ID periods - was unavailable for the NLO exercise MBA. There was no history of propagation at NLO for any MBA, and in addition, the NLO exercise MBA was not one of NLO's historical MBAs. Thus, all of the required historical information had to be approximated, or removed from the process error estimation.

In our attempt to at least roughly approximate process error for the NLO exercise, we took the following steps:

- . Used a sequence of nine historical quarterly IDs (1981, 1982, first quarter 1983) from the historical NLO MBA which most closely approximated the exercise MBA (MBA 82). (One apparent outlier in the second quarter of 1982 was replaced by the average of the other eight IDs.)
- . Approximated historical propagated measurement error in the ID periods as proportional to that in the exercise period (second quarter 1983) using the relative throughput (BI+R) as the factor of proportionality.
- . Ignored propagated measurement covariance in the Appendix D formulas.

The zero estimates in Tables 7 and 13 in fact indicate that the approximated process error was negative. It is not particularly suprising that the result was less than satisfactory, given the crudeness of the attempt in the absence of all of the required historical information. By making the attempt, however, we emphasize our feeling that LEIDs based on measurement error to the exclusion of process error may be seriously understated. Indeed, we have seen in Table 17 that the NLO exercise LEIDs are not as large as NLO's approximate historical control limits.

6. *Static Inventory.* The NLO exercise error propagation excluded all static inventory. Tables 6 and 12 give an accounting of the amounts of such material found in the transactions data base in each of the four possible paths ("To "). It should be noted that the exclusion of static inventory was a major task in the error propagation computer code. This task must receive considerable thought at the point of designing and ordering a transactions data base.

7. *Strata.* Table 5 indicates that there were about 50 basic materials involved in the NLO exercise. Appendix G gives a more complete picture of the range of materials in terms of presumed uranium and ^{235}U content. The number of distinct materials in the NLO exercise MBA was not large by most standards in the nuclear material control area. Thus, we felt no need to use material strata in the NLO exercise. Nevertheless, the stratification concept is a useful one in general, particularly given intentions to estimate random effects ANOVA models.

There are aspects of the NLO exercise error propagation application beyond the treatment of the elements of our conceptual methodology that need to be documented here. They are as follows:

8. *Reduced/Raw Data Measurement Variance (Relative Standard Deviation) Estimation.* The numerous relative standard deviations of Tables 1-4 had to be predetermined as input to the execution of the error propagation computer code. These numerical expressions of measurement uncertainty, combined with other uncertainties documented in 9. below, are the foundation of the error propagation.

The mechanism for estimating the Table 1-3 relative standard deviations is the random effects ANOVA model, previously discussed in 3. above with respect to the estimation of effects. The random effects ANOVA model estimation estimates variance components. Among these components are effects, and the reduced/raw data random measurement variance leading to a relative standard deviation in Tables 1-3. See Appendix F for a more detailed explanation and the supporting data.

The Table 4 relative standard deviations relate to the act of sampling material to measure uranium or ^{235}U content, and reflect uncertainty due to that sampling resulting from material heterogeneity and the sampling procedure employed. These relative standard deviations are based on NLO sampling experiments performed over a span of time before the error propagation exercise.

9. *Unique NLO Propagation Features.* Any error propagation will inevitably have features which are unique to the facility (or even the MBA) for which the propagation is being executed. Here we document those unique features for the NLO exercise.

Primary among these unique features is the intentional choice of a facility not to measure the ^{235}U or U in a particular material, but rather to use some average historical value, or assumed "true" value, in place of actual measurements on the current material. This is referred to as "indirect measurement" in the results Tables 7 and 13. These indirect measurements may also be used in cases where analytical measurements are being done, but have not been completed as of the time of execution of the error propagation. Whenever indirect measurements are used in place of direct measurements, some uncertainty (variance, relative standard

deviation) must be associated with them and fed into the error propagation process, resulting in the Table 7 and 13 cumulated indirect measurement variance.

In the absence of direct ^{235}U enrichment measurements at NLO, there are three paths that one might follow to get an indirect measurement. Those paths and the associated uncertainties assumed in the exercise error propagation are:

- . Indirect measurement is the enrichment corresponding to the one-character class code in the material's lot identification number. Uncertainty is represented by a relative standard deviation of $(.003/\text{enrichment})$. NLO must supply receivers material which is within $\pm .006$ of specified enrichment. It was assumed that $.006$ represented two standard deviations.
- . In cases where the one-character class code is 0 or 2, the class code is not tied to a specific enrichment. The indirect measurement is the enrichment corresponding to the combination of the class code and the purchase order (P.O.) number which begins the material's lot identification number. Uncertainty is represented by a relative standard deviation of $(.003/\text{enrichment})$, justified as above.
- . When the purchase order (P.O.) number which begins the material's lot identification number begins with "S", the material was received from an external shipper. The indirect measurement is the enrichment appearing in the 2nd through 4th characters of the P.O. number.

Uncertainty is represented by a relative standard deviation of (.00075/enrichment). NLO requires external shippers to supply material which is within .15% of specified enrichment. It was assumed that .0015 represented two standard deviations.

In the absence of direct U concentration measurements at NLO, the indirect U measurement is obtained from a standard list of "Factor Assays for EDP Application". These U factors represent average historical values obtained in planned direct measurement experiments at various times over approximately the past 15 years. A standard deviation is associated with each factor based on the variability in the original experimental results. These factors and associated uncertainties are listed in Appendix G. Note that factors may vary with any of the material characteristics of material type, source, or class code, all of which are components of the lot identification number. The factors and associated uncertainties were accessed by the error propagation computer code from data set "FACTOR-MASTER" in the absence of direct U concentration measurements for a transaction.

Other possibly unique features of the NLO exercise propagation were as follows:

- . All NLO analytical work relevant to the exercise MBA was done on a one sample - one analysis basis. This simplifies the propagation equations in Appendix C.
- . The uranium concentration in measured green salt material results from the difference of a gravimetric uranium measurement and an atomic absorption impurities measurement. Variance must be allocated between these measurements in some way.

- . The uranium concentration in measured ingot material results from the subtraction of three impurities measurements (colorimetric, emission spec, leco carbon) from 1.0. Variance must be allocated between these measurements in some way.
- . The end-point of the exercise MBA was defined as an uncropped ingot product (M.D.C. 240 and 404). Analytical uranium measurements however, were for the ingot after top cropping. To adjust to the uncropped ingot basis for M.D.C. 240, a proportion .857 of total ingot weight was assigned to the cropped ingot with standard deviation .024, and the top crop was assumed to be a proportion .993 uranium with a standard deviation .002. Similar numbers for M.D.C. 404 were .928, .0098, .995, and .002. The uncertainties involved in this top crop correction were propagated into analytical uranium variance.
- . Some of the NLO exercise materials analyzed for uranium by the volumetric measurement process were in fact analyzed in two separate portions, one finely ground, the other coarse. An entry on the measurement record allowed the error propagation computer code to utilize the one portion with relatively substantial uranium content. The other portion corresponding to a second volumetric measurement record was ignored.

10. *Computer Code.* An error propagation computer code was written specifically for the NLO exercise to implement the applied methodology discussed above. Written by the first author of this report, the FORTRAN code includes about 1700 lines, inclusive of comment lines, and is listed in its entirety in Appendix H. It was originally our intention to document

the computer code in a separate report. However, when it became clear that this code would not be used in subsequent NLO error propagation efforts, there was no longer any reason to fully document it from our perspective.

The computer code was written to operate directly on NLO HP-3000 system, accessing data from the HP Image Database Management System (data sets named LOT-MASTER, TRANSACTIONS, MEASUREMENTS, FACTOR-MASTER are accessed). It was necessary to segment the code before it would execute on the HP-3000, as summarized in Figure 3. The relative standard deviations printed in Tables 1-4 are specified in the BLOCK DATA program unit. Other set-up parameters are specified in the INIT program unit. There is no external input to the program during execution other than from the four data sets named above.

Figure 4 briefly summarizes the sequence of operations performed by the MAIN program unit, making reference to the sequence numbers in the Appendix H listing (which contains much more detailed comments on program operations). Two particular features of the MAIN program unit are particularly noted:

Segment	Program Units
SEG (Main)	MAIN, BLOCK DATA, FINDL, VPROP
ONE	INIT
TWO	VCCUM
THR	PROCESS
FOU	INP
FIV	MATSUM
SIX	VCSUM

Fig. 3. Error propagation computer code segments.

- . Extensive edit checks were made on the data coming into the program to catch errors in data entry, etc. Errors caused a message to be written out to unit 8. This is an extremely important feature of the program since one wrong record can substantially impact error propagation results.
- . The program code is very dependent on an assumed order of the records in the TRANSACTIONS and MEASUREMENTS data sets. These data sets were sorted by Item No. (Table 18) within chains of records having the same Lot Identification. This sorting greatly reduced program execution time by minimizing the need to repeatedly read the same records.

Sequence Number Range	Operation
71 - 76	Initialize variables.
78 - 86	Data base opened and locked.
87 - 113	Calculate number of lots of each material for Table 5.
118 - 244	Access transactions, add to material summaries, identify static inventory, proceed with transaction that is active.
257 - 323	Begin measurements access for active transaction.
324 - 369	Weight measurements propagation.
370 - 623	Uranium measurements propagation, separate sections for volumetric, gravimetric - atomic absorption, colorimetric - emission spec-leco carbon.
624 - 759	^{235}U measurements propagation, separate sections for gas mass spec, thermal mass spec.
760 - 852	Indirect measurements propagation, entered when no more direct measurements for transaction.
853 - 870	Finish cumulation of propagated measurement variance, calculate process error, output results.
876 - 880	Data base unlocked and closed.

Fig. 4. Error propagation computer code sequence of operations.

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APPENDIX A

Definition of Terminology Associated with Results Tables

Definition of Terminology Associated with Results Tables

Active material. Material that appears in the material balance area in a single transaction type (beginning inventory, addition, removal, ending inventory). This material can contribute to a ^{235}U or U ID, and measurements made on it can contribute to variance that should be reflected in the LEID.

Addition (A). A transaction where material comes into a material balance area sometime between the beginning and ending inventories. (Also receipt.)

Beginning inventory (BI). A transaction indicating that the material was on hand in a material balance area at the beginning of a defined material accounting time period.

Effect. A specific characteristic of a measurement with which some of the measurement variance may be shown to be associated, such as analytical method, instrument, operator, time of day, etc. (Also systematic error). (None present in NLO exercise result tables.)

Ending inventory (EI). A transaction indicating that the material was on hand in a material balance area at the end of a defined material accounting time period.

Indirect measurement. The substitution of a "standard" value for U concentration or ^{235}U enrichment when no analytically measured value is available, whether by design or because of natural time lags in completing the laboratory analysis. Thus, indirect measurement is actually no measurement, for example, using U concentration factors from a standard

factor list, or assuming a ^{235}U enrichment is the exact value associated with an NLO class code or purchase order (P.O.) number, or specified by a shipper.

Inventory difference (ID). The accounting quantity defined in terms of the various transaction types as the sum of beginning inventory and additions minus removals minus ending inventory, or $ID = BI + A - R - EI$. ID would be identically zero in the presence of perfect measurement capability and the absence of material theft, diversion, or misplacement.

Limit of error on inventory difference (LEID). A number indicating the acceptable deviation of an inventory difference from the desired zero level. LEID should reflect imperfect measurement capabilities (measurement variance), and the potential for equipment holdup, bookkeeping errors, etc. (process variance).

Measurement variance. Variance inherent in stated amounts of ^{235}U or U in a material because of unavoidable inexactness in the measurement of weight, U concentration, or ^{235}U enrichment associated with imperfections in equipment, analyst, environmental conditions, etc.

Measurement variance bounds on ID. A limit of error on an inventory difference (LEID) based solely on a cumulation of measurement variance, to the exclusion of any other form of variance.

Process variance. Variance associated with stated amounts of ^{235}U or U in a material balance area that arises from equipment holdup, bookkeeping errors, unmeasured inventory, etc., that is environmental or human factors beyond basic measurement inexactness.

Random (variance). Random variance is variance that is found to exist but is not linked to a specific cause by statistical analysis.

Raw data. Direct readings taken from instruments used in a particular measurement process, for example, tare weight and gross weight read from a scale in the weighing process.

Reduced data. The calculated final result of a particular measurement process, for example, net weight as the difference gross weight minus tare weight. Other examples are $\bar{X}U$, $\bar{X}^{235}U$ and parts per million (ppm) impurities.

Relative standard deviation. Standard deviation of measurements divided by average of measurements. (The coefficient of variation is the relative standard deviation converted to a percentage through multiplication by 100.)

Removal (R). A transaction where material leaves a material balance area sometime between the beginning and ending inventories. (Also shipment.)

Sampling (variance). Sampling variance is variance that is linked to the specific act of using only a sampled part of a material to analytically assess U concentration or ^{235}U enrichment in the whole, for example, doing lab analysis on a small wafer from a large ingot, and attributing the analytical result to the whole of the material.

Standard deviation. A statistical measure of the spread of a group of measurements around their central (average) value, mathematically determined as the square root of the average squared difference of measurements from the average. (Also square root of variance.)

Static material. Material that appears in the material balance area as both a beginning inventory or addition and a removal or ending inventory

during a material accounting period without remeasurement. Such material cannot impact the inventory difference and should play no part in determining the limit of error on the inventory difference.

Throughput (T). The addition of the beginning inventory and addition transactions, or $T = BI + A$.

Total variance bounds on ID. A limit of error on an inventory difference (LEID) based on the cumulation of both measurement variance and process variance. This LEID will be at least as large as the LEID based solely on measurement variance.

Variance. A statistical measure of the spread of a group of measurements around their central (average) value, mathematically determined as the average squared difference of measurements from the average. More generally, a measure of uncertainty around a supposed hypothetical value, such as the supposed hypothetical ID of zero.

Variance components. Different parts of an overall variance that have been linked to specific sources, for example, the random weighing, random uranium analysis, uranium sampling, etc., components of an overall measurement variance.

APPENDIX B

Variance Approximation by Taylor Series Expansion

Variance Approximation By Taylor Series Expansion

A quantity of interest, say Q , which is a function of a number of variables $X_1, X_2, \dots, X_m = \underline{X}$, say $f(\underline{X})$, may be represented in a Taylor Series expansion around the means of $X_1, X_2, \dots, X_m$, denoted $\mu_1, \mu_2, \dots, \mu_m = \underline{\mu}$ as

$$f(\underline{X}) = f(\underline{\mu}) + \sum_{j=1}^m (X_j - \mu_j) \left[\frac{\partial f}{\partial X_j} \Big|_{\underline{\mu}} \right] + \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m (X_i - \mu_i)(X_j - \mu_j) \left[\frac{\partial^2 f}{\partial X_i \partial X_j} \Big|_{\underline{\mu}} \right] + R \quad (B1)$$

If one assumes the absence of covariance between the X 's, it is clear that the mean $f(\underline{X})$ can be approximated as

$$E[f(\underline{X})] \doteq f(\underline{\mu}) \quad (B2)$$

since $E[(X_j - \mu_j)] = 0$ and $E[(X_i - \mu_i)(X_j - \mu_j)] = 0$ by assumption.

The variance of $f(\underline{X})$ is definitionally the expectation $E\{f(\underline{X}) - E[f(\underline{X})]\}^2$, or $E\{f(\underline{X}) - f(\underline{\mu})\}^2$, given (B2). Using terms in (B1) only through first partial derivatives, one can approximate the variance of $Q = f(\underline{X})$, say σ_Q^2 , by

$$\sigma_Q^2 \doteq E\{f(\underline{X}) - f(\underline{\mu})\}^2 \doteq E\left\{ \sum_{j=1}^m (X_j - \mu_j) \left[\frac{\partial f}{\partial X_j} \Big|_{\underline{\mu}} \right] \right\}^2 \quad (B3)$$

The first partial derivatives evaluated at $\underline{\mu}$ are fixed with respect to the expectation operator, so that the operative expectation becomes $E(X_j - \mu_j)^2 = \sigma_{X_j}^2$, the variance of X_j . One sees then, assuming absence of covariance between the X 's, that

$$\sigma_Q^2 \doteq \sum_{j=1}^m \left[\frac{\partial f}{\partial X_j} \Big|_{\underline{\mu}} \right]^2 \sigma_{X_j}^2, \quad (B4)$$

as in the paper's equation (1).

For the paper's example $Q = f(\underline{X}) = X_1 X_2$, the difference between the approximate equation (2) result based on (B4) and the exact equation (3) result is the term $\sigma_{X_1}^2 \sigma_{X_2}^2$. This difference is caused by ignoring the second partial derivatives in (B1) for $i = 1, j = 2$ and $i = 2, j = 1$, which are both 1. A typical result of ignoring these terms in (B1) will be to ignore terms which are squared products of standard deviations, while terms resulting from the first partials which are squared products of a mean and a standard deviation are retained. Thus the approximations should be adequate when σ_{X_j} is small relative to μ_j across $j = 1, 2, \dots, m$.

Certain $Q = f(\underline{X})$ permit the sequential application of (B4) in the variance approximation. Consider $Q = f(\underline{X}) = X_1 X_2 X_3$. One may look at this Q sequentially as

$$\begin{aligned} g &= X_1 X_2 \\ Q &= g X_3 \end{aligned} \quad (B5)$$

Approximating σ_g^2 via (B4), one finds

$$\sigma_g^2 \doteq \mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2. \quad (B6)$$

Approximating σ_Q^2 via (B4) from the form $Q = g X_3$, one finds

$$\sigma_Q^2 \doteq \mu_g^2 \sigma_3^2 + \mu_3^2 \sigma_g^2. \quad (B7)$$

Substituting for σ_g^2 from (B6) and noting that $\mu_g^2 \doteq \mu_1^2 \mu_2^2$, (B7) is equivalently

$$\sigma_Q^2 = \mu_1^2 \mu_2^2 \sigma_3^2 + \mu_1^2 \mu_3^2 \sigma_2^2 + \mu_2^2 \mu_3^2 \sigma_1^2 \quad (B8)$$

This is exactly the same result one obtains by direct application of (B4) to the form $Q = X_1 X_2 X_3$.

Sequential application of (B4) is inappropriate for certain other forms $Q = f(\underline{X})$. Consider $Q = f(\underline{X}) = (X_3 - X_2)/(X_1 - X_2)$. One may look at this Q sequentially as

$$\begin{aligned} g &= X_3 - X_2 \\ h &= X_1 - X_2 \\ Q &= g/h \end{aligned} \quad (B9)$$

Using (B4) sequentially on g , h , and Q , approximate variances are

$$\begin{aligned} \sigma_g^2 &= \sigma_3^2 + \sigma_2^2 \\ \sigma_h^2 &= \sigma_1^2 + \sigma_2^2 \\ \sigma_Q^2 &= \frac{\sigma_g^2}{\mu_h^2} + \frac{\sigma_h^2 \mu_g^2}{\mu_h^4} \end{aligned} \quad (B10)$$

and substituting for σ_g^2 , σ_h^2 , $\mu_g = \mu_3 - \mu_2$, and $\mu_h = \mu_1 - \mu_2$ in σ_Q^2 ,

$$\sigma_Q^2 = \frac{\sigma_3^2 + \sigma_2^2}{(\mu_1 - \mu_2)^2} + \frac{(\sigma_1^2 + \sigma_2^2)(\mu_3 - \mu_2)^2}{(\mu_1 - \mu_2)^4} \quad (B11)$$

The direct application of (B4) to the form $Q = (X_3 - X_2)/(X_1 - X_2)$ yields terms in σ_1^2 and σ_3^2 which are the same as those in (B11). However, the term in σ_2^2 is not the same as that in (B11). The involvement of X_2 in both g and h in (B9) results in the failure of the sequential application for this Q form.

APPENDIX C

Measurement Variance Aggregation Equations

Measurement Variance Aggregation Equations

Jacek's (1973) Chapter 6 discussion of variance aggregation by uncorrelated primary error source provides the blueprint for a process of measurement variance aggregation. The uncorrelated primary error sources are weighing, analysis and sampling for element (uranium), and analysis and sampling for isotope (^{235}U).

Let us focus on measured weight ^{235}U . For individual item i , define

ω_i = true net weight.

W_{ih} = measured net weight using scale h .

π_i = true uranium proportion.

P_{im} = measured uranium proportion using analytical method m .

f_i = true ^{235}U enrichment.

R_{it} = measured ^{235}U enrichment using analytical method t .

ω_i^{235} = true weight ^{235}U .

W_i^{235} = measured weight ^{235}U .

From these definitions, it follows that

$$\omega_i^{235} = \omega_i \pi_i f_i \quad (C1)$$

$$W_i^{235} = W_{ih} P_{im} R_{it}$$

The measurements W_{ih} , P_{im} , and R_{it} , when representative of actual direct measurements, are conceived of as random variables produced by a multiplicative function of the respective true value, one or more effects, and random error, where the effects and random error are mean 1 random variables. The measured net weight is

$$W_{ih} = \omega_i \prod_j \lambda_{hjp} \varepsilon_{\omega ih} \quad (C2)$$

where λ_{hjp} represents level p of effect j for scale h and $\epsilon_{\omega ih}$ represents random weighing error in weighing item i on scale h . The measured uranium proportion is

$$P_{im} = \pi_i \prod_k \phi_{mkq} \eta_{\pi s} \epsilon_{\pi im} , \quad (C3)$$

where ϕ_{mkq} represents level q of effect k for analytical uranium measurement method m , $\eta_{\pi s}$ represents sampling random error associated with basing the π measurement on sample s , and $\epsilon_{\pi im}$ represents analytical random error in analyzing uranium proportion in item i using method m . The measured ^{235}U enrichment is

$$R_{it} = \int_i \prod_{\ell} \psi_{t\ell r} \eta_{fs} \epsilon_{fit} , \quad (C4)$$

where $\psi_{t\ell r}$ represents level r of effect ℓ for analytical ^{235}U enrichment method t , η_{fs} represents sampling random error associated with basing the measurement on sample s , and ϵ_{fit} represents analytical random error in analyzing ^{235}U enrichment in item i using method t .

The measurements P_{im} , and R_{it} , when representative of historical or assumed indirect measurements, are conceived of as random variables produced by a multiplicative function of the respective true value and what is essentially an effect associated with the use of this fixed historical or assumed value for material presumed equivalent to that in item i . The "measured" uranium proportion is

$$P_{im} = \pi_i f_{\pi n} , \quad (C5)$$

where $f_{\pi n}$ represents the effect of using assumed uranium value n (uranium factor n). The "measured" ^{235}U enrichment is

$$R_{it} = f_i f_{fg} \quad , \quad (C6)$$

where f_{fg} represents the effect of using assumed ^{235}U value g (^{235}U origin or source g).

The measured w_i^{235} in (C1) then is the product of equation (C2) with equation (C3) or (C5), and equation (C4) or (C6). The effect and random error random variables involved are λ_{hjp} , ε_{wih} , ϕ_{mkq} , $\eta_{\pi s}$, $\varepsilon_{\pi im}$, ψ_{tlr} , η_{fs} , ε_{fit} , $f_{\pi n}$, and f_{fg} , with assumed means of 1 and relative standard deviations denoted by $\sigma_{\lambda hj}$, $\sigma_{\varepsilon wh}$, $\sigma_{\phi mk}$, $\sigma_{\eta \pi s}$, $\sigma_{\varepsilon \pi m}$, $\sigma_{\psi tl}$, $\sigma_{\eta fs}$, $\sigma_{\varepsilon ft}$, $\sigma_{f \pi n}$, $\sigma_{f fg}$.

Aggregation and Variance Approximation

The ^{235}U inventory difference for a given MBA is cumulation over many items.

$$ID = \sum_i C_i w_i^{235} \quad , \quad (C7)$$

where $C_i = +1$ for items i in beginning inventory or additions and $C_i = -1$ for items i in removals or ending inventory.

Consider approximating the variance of ID by Taylor Series expansion as discussed with equation (1). One can look upon the ID in (C7) as a quantity of interest $Q = f(\underline{X})$ where $\underline{X} = (\lambda_{hjp}, \varepsilon_{wih}, \phi_{mkq}, \eta_{\pi s}, \varepsilon_{\pi im}, \psi_{tlr}, \eta_{fs}, \varepsilon_{fit}, f_{\pi n}, f_{fg})$. Since different elements of $\underline{X}$ are related to presumably uncorrelated error sources in various measurements (weight, uranium proportion, ^{235}U enrichment), it is reasonable to suppose no covariance among elements of $\underline{X}$ and apply (1) to approximate the variance of Q , that is, of the ID. One would label this a process of variance aggregation by uncorrelated primary error sources.

Note that in this context, the quantities in equation (1) would have the following forms:

- $\left[\frac{\partial f}{\partial X_j} \mid \underline{\mu} \right]$ would be the sum over one or more i of $C_i \omega_i^{235}$, since $\underline{\mu} = \underline{1}$, and $\omega_i \pi_i^f = \omega_i^{235}$ will be present. One would be forced to estimate ω_i^{235} by W_i^{235} .
- σ_{X_j} would be one of the relative standard deviations $\sigma_{\lambda hj}$, $\sigma_{\epsilon \omega h}$, $\sigma_{\phi mk}$, etc.

One can summarize what is added into the measurement variance aggregation by the different elements of $\underline{X}$ as follows:

- Weighing effects (λ_{hjp}). $(\sum_i C_i W_i^{235})^2 \sigma_{\lambda hj}^2$ for each hjp , where the items i included are all items weighed on scale h with level p of effect j .
- Weighing random variance ($\epsilon_{\omega ih}$). $(W_i^{235})^2 \sigma_{\epsilon \omega h}^2$ for each h , where the single item i included is the item weighed on scale h with $\epsilon_{\omega ih}$ weighing random error.
- Uranium proportion effects (ϕ_{mkq}). $(\sum_i C_i W_i^{235})^2 \sigma_{\phi mk}^2$ for each mkq , where the items i included are all items with uranium proportion measured by analytical method m with level q of effect k .
- Uranium proportion sampling random variance ($\eta_{\pi s}$). $(\sum_i W_i^{235})^2 \sigma_{\eta \pi s}^2$ for each s , where the items i included are all items assigned a measured value based on the same sample s . This may be a single item (for example, an ingot), or all items in a lot (for example, cans of green salt) when lot-wide samples are taken. (The C_i may be ignored given that they will all have the same sign when they are in the same lot.) A further aggregation over s to specific material types is made in tabulated results (for example, Table 10).

- . Uranium proportion analytical random variance ($\epsilon_{\pi m}$). $(W_i^{235})^2 \sigma_{\epsilon_{\pi m}}^2$ for each m , where the single item i included is the item with uranium proportion measured by analytical method m with $\epsilon_{\pi m}$ analytical random error.
- . ^{235}U enrichment effects ($\psi_{t\ell r}$). $(\sum_i C_i W_i^{235})^2 \sigma_{\psi_{t\ell r}}^2$ for each $t\ell r$, where the items i included are all items with ^{235}U enrichment measured by analytical method t with level r of effect ℓ .
- . ^{235}U enrichment sampling random variance (η_{fs}). $(\sum_i W_i^{235})^2 \sigma_{\eta_{fs}}^2$ for each s , where the items i included are all items assigned a measured value based on the same sample s . This may be a single item, or all items in a lot when lot-wide samples are taken.
- . ^{235}U enrichment analytical random variance (ϵ_{fit}). $(W_i^{235})^2 \sigma_{\epsilon_{fit}}^2$ for each t , where the single item i included is the item with ^{235}U enrichment measured by analytical method t with ϵ_{fit} analytical random error.
- . Indirect uranium proportion measurement effect ($f_{\pi n}$). $(\sum_i C_i W_i^{235})^2 \sigma_{f_{\pi n}}^2$ for each n , where the items i included are all items for which uranium factor n is used as a supposed measured P_{im} via (C5).
- . Indirect ^{235}U enrichment measurement effect (f_{fg}). $(\sum_i C_i W_i^{235})^2 \sigma_{f_{fg}}^2$ for each g , where the items i included are all items for which ^{235}U origin or source g is used as a supposed measured R_{it} via (C6).

Notes

1. The discussion for measured weight uranium is a subset of the preceding discussion, simply ignoring any reference to true or measured ^{235}U enrichment f_i or R_{it} . All logic and aggregation

patterns for an approximate variance for a uranium inventory difference follow in the same manner.

2. The relative simplicity of the aggregation rules here compared to Jaech's (1973) Table 6.2 - 6.3 results from two factors. First, the present rules are for one-sample, one-analysis measurement practices such as were employed in the NLO exercise data; Jaech's rules include possible multiple-sample, multiple-analysis measurement practices. Second, Jaech maintains the long-term systematic error, short-term systematic error dichotomy which is collapsed into the single category "effects" here.
3. The various relative standard deviations appear in this report as follows:

- $\sigma_{\lambda h j}$ - Would be in Table 1 (not significant).
- $\sigma_{\epsilon \omega h}$ - Table 1.
- $\sigma_{\phi m k}$ - Would be in Table 2 (not significant).
- $\sigma_{\eta \pi s}$ - Table 4.
- $\sigma_{\epsilon \pi m}$ - Table 2.
- $\sigma_{\psi t l}$ - Would be in Table 3 (not significant).
- $\sigma_{n f s}$ - Table 4 (all zero).
- $\sigma_{\epsilon f t}$ - Table 3.
- $\sigma_{f \pi n}$ - Appendix G (divide factor uncertainty by factor).
- $\sigma_{f f g}$ - Page 54 (three subsets within g described).

APPENDIX D

Process Variance Estimation

Process Variance Estimation

NUSAC (1981) provides methodology for estimating the process variance associated with process error, assuming it to be constant over time. The estimation requires as data a sequence of historical inventory differences, propagated measurement variance totals in each inventory difference period, and propagated measurement covariance totals between inventory difference periods.

Consider a sequence of inventory differences $Y_1, Y_2, \dots, Y_n$ for a given material balance area. Assuming no diversion, Y_i can be modeled as

$$Y_i = X_i + e_i \quad , \quad (D1)$$

where e_i represents the measurement error contribution and X_i represents unmeasured inventory, including holdup, bookkeeping errors, etc. We assume

$$E(e_i) = 0 \text{ for all } i$$

$$\sigma_{e_i}^2 = V(e_i)$$

$$\sigma_{e_j e_k} = \text{COV}(e_j, e_k)$$

$$E(Y_j) = E(X_i) = b \quad (D2)$$

$$\sigma_{X_i}^2 = V(X) \text{ for all } i$$

$$\sigma_{X_j X_k} = \text{COV}(X_j, X_k) = \begin{cases} \text{COV}(X_{+1}) & \text{all } j = k - 1 \\ 0 & \text{all } j < k - 1 \end{cases}$$

$$\sigma_{X_j e_k} = 0 \text{ for all } j \text{ and } k$$

Given (D1) and (D2),

$$V(Y_i) = V(X) + V(e_i) \quad . \quad (D3)$$

$V(e_i)$ is a result of the process of error propagation of measurement errors. If we can estimate process variance $V(X)$, say as $\widehat{V(X)}$, then clearly we can estimate $V(Y_i)$ and produce LEIDs on the observed inventory difference, y_i .

The sample variance of a sequence of observed inventory differences $y_1, y_2, \dots, y_n$ is

$$s_y^2 = \frac{\sum_{j=1}^n y_j^2 - \left[\left(\sum_{j=1}^n y_j \right)^2 / n \right]}{n - 1} \quad , \quad (D4)$$

equivalently written

$$s_y^2 = \frac{\sum_{j=1}^n y_j^2}{n} - \frac{2}{n(n-1)} \sum_{j < k} y_j y_k \quad . \quad (D5)$$

Note from (D1) that the general product $y_j y_k$ is

$$y_j y_k = x_j x_k + x_j e_k + e_j x_k + e_j e_k \quad . \quad (D6)$$

The expectation $E(y_j y_k)$ for various j and k combinations is

$$E(y_j y_k) = \begin{cases} V(X) + b^2 + V(e_j) & j = k \\ \text{COV}(X_{+1}) + b^2 + \text{COV}(e_j, e_k) & j = k - 1 \\ b^2 + \text{COV}(e_j, e_k) & j < k - 1 \end{cases} \quad (D7)$$

Using (D7), the expectation of s_y^2 , $E(s_y^2)$, as expressed in (D5) is then seen to be

$$E(s_y^2) = V(X) + \sum_{j=1}^n \frac{V(e_j)}{n} - \frac{2}{n} \text{COV}(X_{+1}) - \frac{2}{n(n-1)} \sum_{j < k} \text{COV}(e_j, e_k) \quad (D8)$$

The $V(e_j)$ and $\text{COV}(e_j, e_k)$ are presumed results of the error propagation as executed by NUSAC (1981). Given s_y^2 as an estimate of $E(s_y^2)$, one could estimate $V(X)$, except for the fact that $\text{COV}(X_{+1})$ is also unknown.

Next consider the sample covariance between successive y_j 's, denoted $s_{j,j+1}$ and defined as

$$s_{j,j+1} = \sum_{j=1}^{n-1} \frac{y_j y_{j+1}}{n-1} - \frac{\left(\sum_{j=1}^n y_j \right)^2}{n^2} \quad (\text{D9})$$

This can also be written as

$$s_{j,j+1} = \frac{(n^2 - 2n + 2)}{n^2(n-1)} \sum_{j=1}^{n-1} y_j y_{j+1} - \frac{\sum_{j=1}^n y_j^2}{n^2} - \frac{2}{n^2} \sum_{j=1}^{n-2} \sum_{k=j+2}^n y_j y_k \quad (\text{D10})$$

One may evaluate the expected value $E(s_{j,j+1})$ using the general results of (D7) in the same pattern as was used for $E(s_y^2)$. This expectation is

$$\begin{aligned} E(s_{j,j+1}) &= \frac{(n^2 - 2n + 2)}{n^2} \left[\text{COV}(X_{+1}) + \sum_{j=1}^{n-1} \frac{\text{COV}(e_j, e_{j+1})}{n-1} \right] \\ &\quad - \frac{V(X)}{n} - \sum_{j=1}^n \frac{V(e_j)}{n^2} - \frac{2}{n^2} \sum_{j=1}^{n-2} \sum_{k=j+2}^n \text{COV}(e_j, e_k) \end{aligned} \quad (\text{D11})$$

Equations (D8) and (D11) both contain the two unknowns $V(X)$ and $\text{COV}(X_{+1})$, and may be used jointly, substituting estimates s_y^2 and $s_{j,j+1}$ for the expectations, to solve for these unknowns. [Note that the $\text{COV}(e_j, e_k)$ summation in (D8) is the sum of the separate e COV summations in (D11).] Substituting s_y^2 and $s_{j,j+1}$ for the expectations and adding n times equation (D11) to equation (D8), $V(X)$ vanishes and one may solve for

$$\widehat{\text{COV}}(X_{+1}) = \frac{s_y^2 + ns_{j,j+1}}{n-2} + \frac{2}{(n-1)(n-2)} \sum_{j=1}^{n-2} \sum_{k=j+2}^n \text{COV}(e_j, e_k) \quad (\text{D12})$$

$$- \frac{1}{n-1} \sum_{j=1}^{n-1} \text{COV}(e_j, e_{j+1})$$

Substituting $\widehat{\text{COV}}(X_{+1})$ in equation (D8) and solving for the estimated process variance $\widehat{V}(X)$, one obtains

$$\widehat{V}(X) = s_y^2 - \sum_{j=1}^n \frac{V(e_j)}{n} + \frac{2}{n} \widehat{\text{COV}}(X_{+1}) \quad (\text{D13})$$

$$+ \frac{2}{n(n-1)} \sum_{j < k} \text{COV}(e_j, e_k)$$

As was noted in the Applied Methodology section of the main body of this report, none of the historical information required to compute $\widehat{V}(X)$ via equation (D13) was available in the context of the NLO exercise. The calculation attempted in the computer program SUBROUTINE PROCESS does the following:

- . Uses a sequence of $n = 9$ observed inventory differences from a historical NLO MBA similar to the NLO exercise MBA.
- . Approximates historical propagated measurement error, $V(e_j)$, as proportional to that in the exercise period.
- . Assumes the summation in $\text{COV}(e_j, e_k)$ is zero.

APPENDIX E
Measurement Methods Summary

Measurement Methods Summary

The following table summarizes the measurement methods applied to the NLO exercise materials, indicating the raw measurements recorded, the reduced measurement desired as a final result, and how equation (1) was used to propagate reduced data variances when the propagation was started from the raw data level.

Five of the measurement method reduced results directly relate to net weight, proportion of uranium, and proportion of ^{235}U . The other five measurement method reduced results are impurities amounts which are used as follows:

- . Subtract atomic absorption impurities from gravimetric uranium to get final proportion of uranium in green salt (UF_4) material.
- . Subtract sum of colorimetric analysis, emission spectrometry, JECO carbon analysis, and micro-kjeldahl nitrogen analysis impurities from 1 to get final proportion of uranium in ingots.

Note that where the table indicates sequential use of equation (1), the propagation from raw to reduced was accomplished with the computer program SUBROUTINE VPROP.

Measurement Method Summary by Raw and Reduced Data and Equation (1) Use

Measurement	Raw Data	Reduced Data	Reduced Data Equation	Equation (1) Use
Weighting	R(1):Tare weight lbs. R(2):Gross weight lbs.	Net weight lbs.	$R(2)-R(1)$	Sequential (one step)
Volumetric uranium assay	R(1):Calib. factor gU/ml R(2):Sample weight g R(3):Initial dilution R(4):Final dilution R(5):Volume titrant ml	Proportion of uranium	$R(1)R(3)R(4)R(5)/R(2)$	Sequential
Gravimetric uranium assay	R(1):Boat plus sample weight g R(2):Boat weight g R(3):After ignition weight g	Proportion of uranium	$\frac{.84779[R(3)-R(2)]}{[R(1)-R(2)]}$	Direct
Atomic absorption	R(1):ppm Ni R(2):ppm Fe R(3):ppm Cr R(4):ppm Cu	Total ppm impurities	$R(1)+R(2)+R(3)+R(4)$	Sequential
Colorimetric analysis	R(1):ppm Fe R(2):ppm Al	Total ppm impurities	$R(1)+R(2)$	Sequential (one step)
Emission spectrometry	R(1):ppm Ni R(2):ppm Cu R(3):ppm Si R(4):ppm Cd R(5):ppm Mg R(6):ppm Cr R(7):ppm Be R(8):ppm Mn R(9):ppm B R(10):ppm Zr	Total ppm impurities	$R(1)+R(2)+R(3)+R(4)+R(5)+R(6)+R(7)+R(8)+R(9)+R(10)$	Sequential
LECO carbon analysis	R(1):%C	Percent carbon impurities	$R(1)$	None (reduced = raw)
Micro-Kjeldahl nitrogen analysis	R(1):ppm N_2	Total ppm impurities	$R(1)$	None (reduced = raw)
Gas mass spectrometry	R(1): SA_1 R(2): X_1 R(3): SB_1 R(4): SB_2 R(5): X_2 R(6): SA_2 R(7): h_b R(8): h_a	Proportion of ^{235}U	$\frac{MX}{(100+MX)}$ $MX = R(8) + \frac{[R(7)-R(8)][R(5)-R(6)]}{(R(5)-R(6))}$ $RX = R(2) + R(5)$ $RA = R(1) + R(6)$ $RB = R(3) + R(4)$	Direct
Thermal mass spectrometry	R(1): $^{234}U/^{238}U$ R(2): $^{235}U/^{238}U$ R(3): $^{236}U/^{238}U$	Proportion of ^{235}U	$\frac{235.04R(2)}{238.05+234.05R(1)+235.04R(2)+236.05R(3)}$	Direct

APPENDIX F

Random Effects ANOVA Models and Reduced/Raw Data Measurement Variance Estimation

Random Effects ANOVA Models and Reduced/Raw Data Measurement Variance Estimation

This appendix has two major parts. The first part introduces the concept of estimating variance components using random effects ANOVA models and indicates how the estimation is done by way of examples. The second part contains tabular data used for variance components estimation in the NLO exercise. The first part of the appendix is not a substitute for a statistical text on variance components estimation. Those wanting a more thorough understanding should consult Searle (1971) or Scheffe' (1959).

Estimating Variance components - No Effects Case

The simplest situation is that where no effects are present and we simply desire to estimate the random error variance associated with the measurement. We can represent the measurement, y_j , as being composed of a true mean value, μ , and a random error component, ϵ_j . Thus, for n measurements,

$$y_j = \mu + \epsilon_j \quad j = 1, 2, \dots, n \quad . \quad (F1)$$

In order to estimate the random error variance, we assume the mean value of ϵ_j is zero, the variance of ϵ_j is σ_ϵ^2 , constant over j , and ϵ_i and ϵ_j are independent for all $i \neq j$.

Under these assumptions, the estimators for μ and σ_ϵ^2 are

$$\hat{\mu} = \bar{y} = \frac{1}{n} \sum_{j=1}^n y_j = \text{sample average} \quad (F2)$$

$$\hat{\sigma}_\epsilon^2 = s^2 = \frac{1}{n-1} \sum_{j=1}^n (y_j - \bar{y})^2 = \text{sample variance} \quad .$$

For example, given $n = 10$ observed values of ppm copper (Cu) impurities as raw data from an emission spectrometry measurement of 25, 26, 26, 26, 27, 24, 26, 27, 25, 26, one finds $\hat{\mu} = \bar{y} = 25.8$ and $\hat{\sigma}_E^2 = s^2 = .8444$.

Tables 1-4 in the main text of this report reflect estimation of random error variance in a no effects case. However, the results are stated in terms of relative standard deviations rather than variances. This statistic is readily defined in terms of (F2) as

$$\text{Relative standard deviation} = \frac{s}{\bar{y}} \quad (\text{F3})$$

In the above example, the relative standard deviation is $\sqrt{.8444}/25.8 = .0356$. Relative standard deviation is closely related to another statistic, coefficient of variation, simply the relative standard deviation in percentage terms, 3.56% in the above example. Use of the relative standard deviation removes the influence of data scale on the perceived variability. For example, if total ppm impurities for five-elements from an emission spectrometry measurement in $n = 10$ observation were 173, 182, 177, 169, 191, 178, 171, 175, 181, 167, one could calculate $\hat{\mu} = \bar{y} = 176.4$ and $\hat{\sigma}_E^2 = 50.49$. The comparison of the 50.49 five-element variance to the .8444 one-element variance is misleading, both because of the different data scales and the squared units (ppm^2) involved. However, the five-element relative standard deviation is $\sqrt{50.49}/176.4 = .0403$, quite comparable to the one-element .0356, indicating similar levels of measurement accuracy in the one-element and five-element ppm measurement.

Estimating Variance Components - Single Effect Case

In the single effect case, there is one potential source of variation beyond random error variation that one wants to investigate. Some typical

examples are instrument, technician, analytical method. The model is

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij} \quad , \quad \begin{array}{l} i = 1, 2, \dots, a \\ j = 1, 2, \dots, n \end{array} \quad (F4)$$

where y_{ij} is the j^{th} observation on the i^{th} level of the random effect α_i , μ is the overall mean, and ϵ_{ij} is the random error component. We assume ϵ_{ij} has mean value zero, constant variance σ_ϵ^2 over all i and j , is independent of α_i for all i and j , and is independent of ϵ_{lm} for $i \neq l$ or $j \neq m$. The error associated with the effect of interest, α_i , is assumed to have mean zero and variance σ_α^2 , with α_i and α_j independent for $i \neq j$. Interest centers on estimating the unknown parameters μ , σ_α^2 , and σ_ϵ^2 . We assume that the same number, n , of observations have been taken at each of the a levels of the effect of interest. For example, if the interest was in technicians, we might run an experiment where each of $a = 3$ technicians analyzed five aliquots of the same sample of material, giving 15 total observations, five at each level of the effect "technician".

It can be shown [see Searle (1971)] that the required estimators are given by

$$\hat{\mu} = \frac{1}{na} \sum_{i=1}^a \sum_{j=1}^n y_{ij}$$

$$\hat{\sigma}_\epsilon^2 = \frac{1}{a(n-1)} \sum_{i=1}^a \sum_{j=1}^n (y_{ij} - \bar{y}_{i.})^2 \quad (F5)$$

$$\hat{\sigma}_\alpha^2 = \frac{1}{n} \left[\frac{1}{(a-1)} \sum_{i=1}^a (\bar{y}_{i.} - \bar{y}_{..})^2 - \hat{\sigma}_\epsilon^2 \right] \quad ,$$

where $\bar{y}_{i.}$ denotes the mean of the observations at the i^{th} level of the effect and $\bar{y}_{..}$ denotes the overall sample mean.

As an example, suppose that one is interested in the possible variation between three technicians when measuring the percent ^{235}U using the mass spectrometer. Each technician is given five samples of the same material and is asked to analyze them. The results in percent by weight are

- . Technician 1 - .994, .847, .992, .845, .985
- . Technician 2 - .998, 1.006, .980, .975, .897
- . Technician 3 - .921, .919, .890, .851, .898 .

The parameter estimates are $\hat{\mu} = .933$, $\hat{\sigma}_e^2 = .002983$, and $\hat{\sigma}_\alpha^2 = .000825$.

Had the above example been a real part of the NLO exercise on one of the mass spectrometers in Table 3, $\sqrt{.002983}/.933 = .05854$ would be seen in that table as a reduced data relative standard deviation, while $\sqrt{.000825}/.933 = .03079$ would be seen in that table as an effect relative standard deviation associated with technician.

Estimating Variance components - More Complicated Cases

Examples of variance component estimation for two or more effects are given in Searle (1971). Note that the formulas for estimators such as those in (F5) for $\hat{\sigma}_\alpha^2$ assume equal numbers of observations at each effect level. Formulas for the unequal observations case are, however, well known and available.

Tabular Data for Variance Components Estimation in the NLO Exercise

Tables F1 through F10 contain the recycle data used in the variance components estimations leading to most of the relative standard deviations in Tables 2 and 3 in the main body of this report. The R(j) column headings in the tables refer to the Appendix E raw data definitions. Similar data (not included here) and analysis led to the relative standard

deviations of Tables 1 and 4. Note that the reported numbers all result from the no effects case, since analysis for possible effects revealed none, as seen in the blank columns labelled "Effects" in Tables 1-4.

Table F1. Volumetric uranium assay recycle data

R(1)	R(2)	R(3)	R(4)	R(5)
0.0032090	0.30267	1.0	1.0	79.92
0.0032090	0.30202	1.0	1.0	79.69
0.0030290	0.30401	1.0	1.0	80.27
0.0032352	0.30899	1.0	1.0	81.01
0.0032032	0.30204	1.0	1.0	79.94
0.0031773	0.30193	1.0	1.0	80.56
0.0031773	0.30064	1.0	1.0	80.15
0.0031773	0.30655	1.0	1.0	81.78
0.0031773	0.31131	1.0	1.0	83.05
0.0031773	0.30627	1.0	1.0	81.70
0.0031925	0.30418	1.0	1.0	80.67
0.0031925	0.30275	1.0	1.0	80.34
0.0031995	0.30231	1.0	1.0	80.21
0.0031925	0.30527	1.0	1.0	81.00
0.0031925	0.31216	1.0	1.0	82.85
0.0031620	0.30904	1.0	1.0	82.87
0.0031679	0.30414	1.0	1.0	81.29
0.0031620	0.30698	1.0	1.0	82.32
0.0031620	0.30325	1.0	1.0	81.25
0.0030981	0.30482	1.0	1.0	83.34
0.0030950	0.30928	1.0	1.0	84.64
0.0030969	0.30392	1.0	1.0	83.12
0.0030969	0.30142	1.0	1.0	82.46
0.0030960	0.30150	1.0	1.0	82.47

Table F2. Gravimetric uranium assay recycle data

R(1)	R(2)	R(3)
6.2198	5.4300	6.1361
6.67094	5.43085	6.53963
6.72087	5.40660	6.5816
6.72786	5.40853	6.58815
6.84517	5.35546	6.68724
6.53769	5.38448	6.41551
6.6107	5.4395	6.4867
6.92630	5.44282	6.76902
7.07952	5.27781	6.88819
6.83630	5.03730	6.64548
6.77691	5.40708	6.63191
6.96124	5.40590	6.79663
7.07060	5.32788	6.88600
6.84471	5.33348	6.68443
6.87000	5.32790	6.70654
6.98637	5.43683	6.82203
6.98290	5.43761	6.81910
6.98850	5.38066	6.81797
6.82176	5.39055	6.67013
7.1122	5.6040	6.9523
6.82658	5.32904	6.66776
6.33813	5.26505	6.22432
6.3000	5.2452	6.1887
6.94747	5.42891	6.78669
6.85603	5.33149	6.70329
6.37658	5.26454	6.25884
6.4021	5.3915	6.2950
6.3546	5.3579	6.2490
6.96192	5.32861	6.78901
6.44492	5.26460	6.32000
6.2939	5.2494	6.1832
5.47360	5.18790	5.44330
6.93467	5.60496	6.79368
6.33268	5.29499	6.22269
6.30995	5.29502	6.20234
6.32292	5.29526	6.21401
6.21465	5.38326	6.12652
6.82649	5.29570	6.66432
6.83180	5.18808	6.65760
6.90334	5.35992	6.73981
6.66270	5.43705	6.53295
6.82372	5.27387	6.65952
6.85956	5.35369	6.69990
6.47918	5.38310	6.36307
6.60095	5.40619	6.47442
6.89679	5.38979	6.73715
7.13629	5.60411	6.97382
6.79956	5.27316	6.63784
6.40447	5.26333	6.28356
6.06457	5.11352	5.96376
6.52966	5.03625	6.37155
6.27566	5.26405	6.16839
6.52469	5.43812	6.40952
6.18214	5.38068	6.09716
6.76919	5.40650	6.62471
6.09617	5.25112	6.00664
6.30637	5.18868	6.18800
6.42848	5.21800	6.30032
6.97964	5.30360	6.80201
6.55085	5.40631	6.42900
6.88303	5.30695	6.71615
6.62801	5.43681	6.50200
6.87959	5.39057	6.72195
6.43659	5.36415	6.32320

Table F3. Atomic absorption recyle data

Standard C				Standard D			
R(1)	R(2)	R(3)	R(4)	R(1)	R(2)	R(3)	R(4)
26	46	12	5	22	33	10	4
25	54	12	5	21	36	10	4
25	54	14	4	22	35	8	4
24	49	14	5	27	52	20	5
26	43	15	5	16	37	13	4
28	53	22	7	16	30	14	4
23	44	13	6	19	30	10	5
30	57	12	5	24	31	6	8
25	55	14	8	20	33	11	4
35	48	13	5	21	36	9	3
22	46	13	6	20	40	8	4
22	40	10	5	17	31	8	4
29	46	13	4	17	38	8	5
22	37	12	4	21	34	6	4
				20	37	8	4

Table F4. Colorimetric analysis recycle data

R(1)	R(2)	R(1)	R(2)
336	798	332	792
336	796	331	772
338	806	333	797
334	781	332	708
338	796	330	784
334	800	330	799
336	806	334	796
337	813	331	796
338	798	330	794
337	782	332	790
336	796	331	793
336	795	330	782
336	794	332	783
340	794	330	793
332	799	330	790
334	797	330	808
338	793	329	814
336	791	330	796
336	806	330	782
332	794	332	786
332	790	332	786
334	796	330	790
332	790	334	786
332	807	336	796
332	802		

Table F5. Emission spectrometry recycle data

R(1)	R(2)	R(3)	R(6)	R(8)
39	25	82	16	11
39	26	89	17	11
39	26	84	17	11
38	26	80	15	10
42	27	91	19	12
40	27	83	17	11
37	24	82	17	11
39	26	82	17	11
42	27	81	19	12
35	25	81	16	10
40	26	79	18	12
40	27	84	18	12
38	26	79	16	11
37	25	80	17	10
39	25	85	17	10
37	25	79	16	10
38	26	85	16	10
39	25	87	16	10
37	24	79	16	10
39	27	84	16	11
38	25	76	17	11
36	25	82	15	10

Table F6. LECO carbon analysis recycle data

R(1)	R(1)	R(1)	R(1)	R(1)
623	622	611	609	601
601	606	596	596	600
604	598	587	595	594
609	616	603	607	595
614	595	596	599	593
614	605	593	588	607
599	595	606	595	612
607	604	593	603	600
597	597	590	600	608
601	608	606	599	

Table F7. Micro-Kj nitrogen analysis recycle data

R(1)	R(1)
46	49
49	43
42	49
46	50
56	44
47	30
42	34
50	45
	54

Table F8. Gas mass spectrometer 1 recycle data

R(1)	R(2)	R(3)	R(4)	R(5)	R(6)	R(7)	R(8)
65930	80460	95845	96200	81120	66100	1.0693	.70457
65750	80340	95710	96060	80985	66060	1.0693	.70457
66070	80910	96500	96750	81390	66250	1.0693	.70457
65100	80070	95740	95920	80490	65310	1.0693	.70457
64815	79720	95260	95495	80200	65165	1.0693	.70457
66025	80800	96400	96750	81480	66410	1.0693	.70457
66045	80420	95630	96051	81200	66474	1.0693	.70457
66464	82029	98305	98532	82412	66627	1.0693	.70457
66367	81914	98174	98388	82313	66538	1.0693	.70457
66450	80680	95820	96250	81430	66695	1.0693	.70457
65050	80060	95710	95890	80455	65300	1.0693	.70457
65400	80470	96115	96245	80755	65610	1.0693	.70457
65065	80095	95750	95940	80460	65262	1.0693	.70457
65015	79800	95310	95475	80230	65240	1.0693	.70457
65080	80025	95575	95750	80325	65225	1.0693	.70457
65138	80035	95522	95735	80380	65335	1.0693	.70457
64990	79968	95545	95710	80390	65305	1.0693	.70457
65110	80020	95550	95725	80370	65290	1.0693	.70457
65155	80050	95625	95830	80445	65360	1.0693	.70457
65110	79985	95622	95835	80430	65315	1.0693	.70457
65058	79830	95250	95430	80195	65272	1.0693	.70457
65042	79710	95090	95335	80225	65305	1.0693	.70457
65755	81215	97350	97480	81485	65850	1.0693	.70457

Table F9. Gass mass spectrometer 2 recycle data

R(1)	R(2)	R(3)	R(4)	R(5)	R(6)	R(7)	R(8)
18065	12418	14118	14185	12539	10925	1.4401	1.0693
10928	12482	14185	14250	12608	10985	1.4401	1.0693
10925	12485	14195	14258	12605	10991	1.4401	1.0693
10893	12570	14378	14410	12643	10943	1.4401	1.0693
10910	12573	14369	14403	12650	10955	1.4401	1.0693
10600	11905	13390	13485	12088	10680	1.4401	1.0593
10553	11870	13370	13439	12050	10646	1.4401	1.0693
10822	12325	14002	14095	12500	10890	1.4401	1.0693
10903	12355	13960	14075	12535	10980	1.4401	1.0693
10910	12360	13980	14073	12538	10990	1.4401	1.0693
10873	12420	14122	14183	12545	10930	1.4401	1.0693
10928	12498	14223	14293	12635	10993	1.4401	1.0693
10598	11915	13400	13478	12080	10675	1.4401	1.0693
10498	11800	13275	13370	11985	10595	1.4401	1.0693
10615	11940	13435	13515	12120	10735	1.4401	1.0693
10605	11930	13442	13520	12110	10695	1.4401	1.0693
10765	12325	14050	14145	12500	10885	1.4401	1.0693
10822	12365	10475	14170	12528	10905	1.4401	1.0693
10810	12282	13895	13985	12430	10875	1.4401	1.0693
10800	12325	13993	14055	12472	10905	1.4401	1.0693
10828	12330	13985	14065	12478	10909	1.4401	1.0693
10895	12390	14040	14130	12550	11000	1.4401	1.0693
10784	12296	13990	14083	12499	10895	1.4401	1.0693
10717	12300	14010	14145	12505	10865	1.4401	1.0693
10790	12340	14060	14140	12510	10885	1.4401	1.0693
10840	12382	14100	14190	12565	10940	1.4401	1.0693
10795	12343	14045	14140	12520	10905	1.4401	1.0693
10825	12370	14070	14160	12540	10915	1.4401	1.0693
10850	12354	14020	14090	12480	10905	1.4401	1.0693
10775	12327	14000	14085	12470	10865	1.4401	1.0693
10775	12320	14010	14097	12455	10860	1.4401	1.0693
10800	12330	14007	14090	12475	10850	1.4401	1.0693

Table F10. Gas mass spectrometer 7 recycle data

R(1)	R(2)	R(3)	R(4)	R(5)	R(6)	R(7)	R(8)
90210	90950	91735	91810	91060	90245	.96215	.94283
90450	91230	91970	92035	91265	90480	.96215	.94283
90030	90790	91560	91610	90875	90035	.96215	.94283
90182	90940	91712	91755	91025	90175	.96215	.94283
90240	91000	91670	91785	91060	90230	.96215	.94283
90765	91555	92360	92375	91605	90785	.96215	.94283
90420	91270	92085	92090	91320	90460	.96215	.94283
81675	87010	87690	87745	87080	86295	.96215	.94283
86273	86995	87755	87795	87090	86280	.96215	.94283
90605	91438	92270	92285	91470	90605	.96215	.94283
90675	91515	92330	92350	91529	90650	.96215	.94283
90705	91520	92330	92370	91570	90705	.96215	.94283
90765	91590	92415	92435	91645	90750	.96215	.94283
90580	91360	92175	92190	91410	90585	.96215	.94283
90665	91465	92255	92285	91475	90615	.96215	.94283
90855	91635	92460	92477	91653	90840	.96215	.94283
90805	91570	92325	92382	91593	90760	.96215	.94283
90225	91020	91850	91905	91145	90295	.96215	.94283
90135	90915	91650	91690	90975	90140	.96215	.94283
90095	90855	91645	91685	90960	90145	.96215	.94283
90385	91115	91875	91925	91220	90410	.96215	.94283
90105	90862	91638	91670	90955	90115	.96215	.94283
90270	91030	91830	91850	91115	90312	.96215	.94283
90605	91390	92185	92210	91440	90620	.96215	.94283
90265	91060	91855	91890	91125	90295	.96215	.94283
86342	87050	87795	87835	87145	86390	.96215	.94283
85700	86515	87335	87380	86585	85765	.96215	.94283
85750	86490	87295	87320	86585	85745	.96215	.94283
90650	91485	92293	92310	91520	90665	.96215	.94283
90665	91475	92285	92300	91515	90650	.96215	.94283
90620	91450	92280	92295	91495	90640	.96215	.94283
90494	91320	92160	92155	91352	90496	.96215	.94283
90460	91275	92060	92110	91330	90505	.96215	.94283
90465	91260	92065	92070	91325	90490	.96215	.94283
90450	91265	92060	92075	91310	90460	.96215	.94283
90675	91475	92290	92310	91525	90665	.96215	.94283
90650	91470	92290	92320	91490	90620	.96215	.94283
90275	91070	91885	91910	91130	90295	.96215	.94283
90410	91190	92005	92025	91225	90385	.96215	.94283
90440	91260	92070	92080	91290	90430	.96215	.94283
90570	91440	92255	92280	91475	90510	.96215	.94283
90570	91390	92170	92220	91440	90575	.96215	.94283
90540	91320	92155	92190	91410	90560	.96215	.94283
90635	91450	92295	92325	91510	90635	.96215	.94283
90615	91430	92245	92280	91480	90630	.96215	.94283
90495	91300	92120	92150	91355	90460	.96215	.94283
90720	91540	92330	92335	91570	90720	.96215	.94283
90096	90850	91625	91695	90962	90140	.96215	.94283
90025	90790	91580	91635	90890	90070	.96215	.94283
90045	90770	91505	91605	90855	90040	.96215	.94283
89865	90650	91450	91495	90730	89876	.96215	.94283
90585	91395	92220	92245	91480	90620	.96215	.94283
90615	91400	92230	92260	91440	90610	.96215	.94283
90580	91370	92240	92300	91490	90650	.96215	.94283
89790	90555	91340	91395	90660	89820	.96215	.94283
89580	90350	91140	91210	90460	89625	.96215	.94283
84965	85760	86535	86600	85865	85085	.96215	.94283
90125	90875	91670	91730	90960	90130	.96215	.94283
90125	90875	91670	91730	90960	90130	.96215	.94283
90120	90990	91700	91720	91000	90180	.96215	.94283
90180	90955	91710	91750	91025	90190	.96215	.94283
90230	90930	91745	91790	91020	90250	.96215	.94283
90045	90840	91655	91680	90915	90130	.96215	.94283
90165	90935	91735	91745	90990	90160	.96215	.94283
90190	90965	91785	91805	91030	90210	.96215	.94283
90195	91020	91795	91815	91045	90220	.96215	.94283

APPENDIX G

Material List with Uranium Factors and Uncertainties

Material List with Uranium Factors and Uncertainties

Material Description Code	Source Code	Class Code	Uranium Factor (%U)	Factor Uncertainty	Material Name
011	530	H	0.50	0.2	Contaminated Soil, Rock, Sand, etc.
011	530	M	0.50	0.1	
011	927	H	3.00	0.5	
017	530	H	3.00	0.5	Contaminated Uncrushed Graphite
017	530	M	3.00	1.0	
017	920	H	3.00	0.5	
017	920	M	3.00	0.5	
019	510	0	10.00	0.2	Contaminated Magnesium
019	510	5	10.00	0.2	
028	900	0	0.50	0.1	Contaminated Asbestos, Polyethylene, etc.
029	333	4	21.00	1.0	Dust Collector Bags
029	333	5	21.00	1.0	
029	346	5	13.00	0.5	
029	512	5	12.00	0.5	
029	513	5	3.00	0.2	
029	520	0	3.60	0.2	
029	520	5	3.60	0.2	
029	530	3	3.60	0.2	
029	533	5	46.00	2.0	
029	535	5	79.00	5.0	
029	827	5	39.00	3.0	
029	920	0	70.00	10.0	
029	926	5	70.00	5.0	
029	927	H	70.00	5.0	
030	530	H	0.25	0.2	Magnesium Oxide and Zirconate
034	513	0	2.37	0.2	MGF ₂ for Milling
034	518	0	2.15	0.5	
035	112	0	2.00	0.5	MGF ₂ or CAF ₂ Good Liner Material
035	512	0	1.60	0.5	
035	513	5	3.60	2.0	
038	518	0	5.00	0.5	MGF ₂ + 20 Mesh

Material List with Uranium Factors and Uncertainties (Cont'd.)

Material Description Code	Source Code	Class Code	Uranium Factor (ZU)	Factor Uncertainty	Material Name
046	510	0	13.10	2.0	Non-Oily Sludges for Oxidation
046	510	5	13.10	2.0	
046	530	0	26.40	3.0	
046	530	4	52.80	5.0	
046	530	5	52.80	5.0	
057	518	0	8.00	1.0	Wet Crushed Slag
062	512	0	20.73	0.2	High Fluoride Dust Collector Residues
062	512	2	20.73	0.2	
062	512	4	25.12	5.0	
062	520	0	4.80	0.5	
062	523	0	3.21	0.2	
065	514	0	65.00	5.0	High Fluoride Scrap Salts
070	516	0	90.00	3.0	Rockwell Spills
070	516	4	90.00	3.0	
070	516	5	90.00	3.0	
070	518	5	90.00	3.0	
071	516	0	9.72	2.0	Rockwell Cleanings
071	516	5	33.25	5.0	
071	518	0	9.72	0.2	
077	518	0	1.40	0.5	Dry Crushed Slag
079	510	5	47.20	5.0	Unfired Reduction Charges Plus MGF2
079	514	0	40.00	5.0	
079	514	2	35.00	2.0	
101	534	H	78.90	2.0	High Fluoride Scrap U308 or TH02
101	534	M	78.90	2.0	
101	920	M	80.72	2.0	
101	927	H	71.58	2.0	
101	927	M	80.72	2.0	
104	510	H	97.30	1.0	Metal Spills and Extrusion Ends
104	530	H	97.30	0.5	
104	550	M	100.00	0.2	

Material List with Uranium Factors and Uncertainties (Cont'd.)

Material Description Code	Source Code	Class Code	Uranium Factor (ZU)	Factor Uncertainty	Material Name
129	112	H	85.50	1.3	Dirty Prill, Code 5 Derbies, etc.
129	112	0	85.50	1.3	
129	112	4	91.30	1.0	
129	112	5	91.30	1.0	
129	518	0	4.00	2.0	
129	518	4	10.00	0.5	
129	518	5	81.60	1.0	
132	535	H	42.75	5.0	Low Fluoride Dust Collector Residues
132	535	M	74.20	5.0	
135	533	H	12.16	2.0	High Fluoride Dust Collector Residues (>20%)
210	440	0	75.80	2.0	UF ₄ or 1HF ₄
210	510	5	75.80	2.0	
212	440	2	75.80	2.0	UF ₄ from Hanford UO ₃
216	515	5	75.80	5.0	Charged UF ₄ Pots
216	517	5	75.80	5.0	
216	518	5	75.80	5.0	
218	518	0	95.30	0.5	Clean Prill for Double Melting
218	518	2	95.30	0.5	
218	518	4	95.30	0.5	
218	518	5	95.30	0.2	
219	530	H	99.50	0.5	Metal from Spills for Double Melting
219	535	M	99.50	0.2	
219	550	H	99.50	0.2	
219	920	H	99.50	0.5	
219	920	M	99.50	0.5	
220	518	0	99.10	0.2	Code 2 Derbies for Double Melting, etc.
220	518	4	98.10	0.2	
220	518	5	97.30	0.2	
224	CCP	0	100.00	0.2	Solid Unpickled Metal Other than Spills and Top Crops for Double Melting
224	CCP	1	100.00	0.2	
224	DZA	1	99.27	0.2	
224	HXA	1	100.00	0.2	
224	530	H	100.00	0.2	
224	620	3	99.80	0.2	

Material List with Uranium Factors and Uncertainties (Cont'd.)

Material Description Code	Source Code	Class Code	Uranium Factor (ZU)	Factor Uncertainty	Material Name
227	732	H	99.50	0.5	Melted Samples for Double Melting
227	732	M	99.50	0.4	
227	732	0	99.50	0.4	
227	732	1	99.50	0.2	
227	732	3	99.50	0.2	
227	732	4	99.50	0.4	
227	732	5	99.50	0.4	
227	920	H	99.50	0.5	
227	920	M	99.50	0.5	
227	920	3	99.50	0.2	
228	DZA	1	100.00	0.2	Solid Metals to be Pickled
229	530	5	99.50	0.4	First Generation Top Crops from Product Ingots
229	550	H	99.50	0.4	
229	550	3	99.50	0.2	
229	550	5	99.50	0.4	
229	920	H	99.50	0.5	
229	920	M	99.90	0.1	
230	920	H	99.80	0.1	Sawed Primary Ingot Sections Containing Top Crops
230	920	M	99.80	0.1	
231	920	M	99.80	0.1	Sawed Primary Ingot Sections with No Top Crops
231	920	3	99.80	0.1	
240	530	H	99.80	0.1	Double Melt Ingots to be Sawed and Pickled
241	530	3	99.80	0.1	Double Melt Ingots to be Sawed but not Pickled
252	645	H	99.50	0.5	High Impurity Briquettes
252	645	M	99.00	0.2	
252	645	5	99.00	0.5	
300	FZB	1	99.80	0.2	Derbies, Code 1 and Code 3
300	330	0	99.72	0.2	
300	330	4	99.72	0.2	
300	518	0	99.12	0.2	
300	518	4	99.10	0.2	
300	518	5	99.30	0.2	
300	620	3	99.80	0.2	

Material List with Uranium Factors and Uncertainties (Cont'd.)

Material Description Code	Source Code	Class Code	Uranium Factor (%U)	Factor Uncertainty	Material Name
302	645	H	98.20	0.4	Briquettes
302	645	M	98.20	0.4	
302	645	O	98.20	0.4	
302	645	3	99.80	0.1	
302	645	5	98.20	0.4	
304	920	H	100.00	0.2	Low Impurity Solid Remelted Metal
304	920	M	100.00	0.2	
307	530	H	100.00	0.2	Zirconium Product
307	660	H	100.00	0.2	
307	663	H	100.00	0.2	
307	980	H	100.00	0.2	
307	980	M	100.00	0.2	
307	980	9	100.00	0.2	
311	FTA	H	100.00	0.2	SR Standard Solid Metal
311	980	3	99.80	0.1	
313	FTA	H	100.00	0.2	Pickled Crops from HW Metal
313	FTA	M	99.80	0.2	
313	FTA	3	99.80	0.1	
313	621	3	99.80	0.1	
313	920	H	100.00	0.2	
313	930	H	100.00	0.2	
313	951	H	100.00	0.2	
313	951	M	100.00	0.2	
313	951	O	99.80	0.1	
313	951	3	99.80	0.1	
314	550	3	99.80	0.1	Pickled Primary Ingot Sections Containing Top Crops
314	920	H	100.00	0.2	
314	920	M	100.00	0.2	
314	920	3	99.80	0.1	
314	930	M	100.00	0.2	
314	980	H	100.00	0.2	
314	980	M	100.00	0.2	
315	920	H	100.00	0.2	Pickled Primary Ingot Sections with no Top Crops
315	920	M	100.00	0.2	
315	920	3	99.80	0.1	
315	930	M	100.00	0.2	
315	940	M	100.00	0.2	
315	980	M	100.00	0.2	

Material List with Uranium Factors and Uncertainties (Cont'd.)

Material Description Code	Source Code	Class Code	Uranium Factor (ZU)	Factor Uncertainty	Material Name
324	665	3	99.80	0.1	Inner Reject Elements
327	920	3	100.00	0.2	Pickled Reject Billets or Billet Sections
331	920	H	100.00	0.2	Unpickled Primary Ingot Sections with no Top Crops
333	550	3	99.80	0.1	Pickled Chemical Reject Crops
333	920	H	100.00	0.2	
333	920	M	99.80	0.1	
333	951	H	100.00	0.2	
333	951	M	99.80	0.1	
333	951	3	99.80	0.1	
335	621	3	99.80	0.1	Crushed Tubular Elements
335	665	3	99.80	0.1	
336	FTA	H	100.00	0.2	Pickled Extrusion Butts
336	FTA	M	100.00	0.2	
336	FTA	3	99.80	0.1	
337	980	0	100.00	0.2	Decad Metal Other Than Zirnlo

APPENDIX H

Error Propagation Computer Code

Error Propagation Computer Code

The microfiche attached on the inside back cover of this report contains the commented computer code listing for the NLO error propagation exercise computer program. A brief description of the general characteristics of this computer code is given at the end of Section III of the main body of this report.

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