

July 14, 2000

To be published in Summary  
*TRANSACTIONS*

Computational Physics and Engineering Division (10)

**PROTOTYPIC APPLICATIONS OF SENSITIVITY AND UNCERTAINTY  
ANALYSIS FOR EXPERIMENT NEEDS**

B. T. Rearden, C. M. Hopper, K. R. Elam, B. L. Broadhead, and P. B. Fox

Oak Ridge National Laboratory,\*  
P. O. Box 2008,  
Oak Ridge, TN 37831-6370  
(865) 574-6085

Submitted to the  
American Nuclear Society  
ANS/ENS 2000 International Winter Meeting and Embedded Topical Meetings,  
November 12–16, 2000,  
Washington, D.C.

The submitted manuscript has been authored by a contractor of the U.S. Government under contract No. DE-AC05-00OR22725. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

---

\*Managed by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy.

# **PROTOTYPIC APPLICATIONS OF SENSITIVITY AND UNCERTAINTY ANALYSIS FOR EXPERIMENT NEEDS**

B. T. Rearden, C. M. Hopper, K. R. Elam, B. L. Broadhead, and P. B. Fox

Oak Ridge National Laboratory  
P. O. Box 2008,  
Oak Ridge, TN 37831-6370  
(865) 574-6085

## **INTRODUCTION**

The Idaho National Engineering and Environmental Laboratory (INEEL) requested that the Oak Ridge National Laboratory (ORNL) apply new prototypical Sensitivity and Uncertainty (S/U) analysis tools to determine if a series of proposed critical experiments would add new information for the validation of codes and estimation of computational biases for storage and transport applications of DOE-owned spent nuclear fuel. For this analysis, the S/U techniques were applied to a series of proposed critical experiments, a prototypic highly enriched spent fuel shipping cask model, and numerous existing benchmark critical experiments. First, the S/U techniques were used to determine the uniqueness of the data provided by the proposed experiments as compared to existing experimental data. Next, various experimental data sets were tested for applicability to a theoretical design of a prototypic shipping cask. Finally, the computational bias for this shipping cask was estimated using the Generalized Linear Least Squares Methodology (GLLSM).

## **ANALYSIS OF PROPOSED EXPERIMENTS**

A series of critical experiments are being considered by INEEL to validate criticality safety analysis codes for new applications involving the storage and transport of DOE-owned spent nuclear fuel. The preliminary designs of these experiments were provided to ORNL in the

form of an unpublished draft document. Because of the preliminary status of these experiment designs, the description included here is intentionally vague. However, it can be stated that these proposed experiments consist of arrays of highly-enriched uranium fuel elements, with aluminum cladding, separated by stainless steel plates. In the 45 cases provided to ORNL, the spacing between the fuel-rod arrays was varied, and the thickness of the stainless steel plates was varied. In some cases, a lead reflector surrounded the array.

The experiments were organized into five series. The first series consisted of five experimental configurations with a small water gap between the assemblies. The thickness of the stainless steel divider plates was varied from the base case with no plate up to the fifth case with a thick plate. The next three series were identical to this one, except for the thickness of the water gap, which was increased for each successive series. The fifth series consisted of a single experiment with a large water gap and no divider plate. The first, third, and fifth case of series one and four were each repeated with four lead reflectors of increasing thickness. Each of these models was analyzed with the SEN3 sequence (described in a previous paper in this session<sup>1</sup>) to produce the sensitivity coefficients necessary for the S/U analysis.

## **DEVELOPMENT OF CASK MODEL**

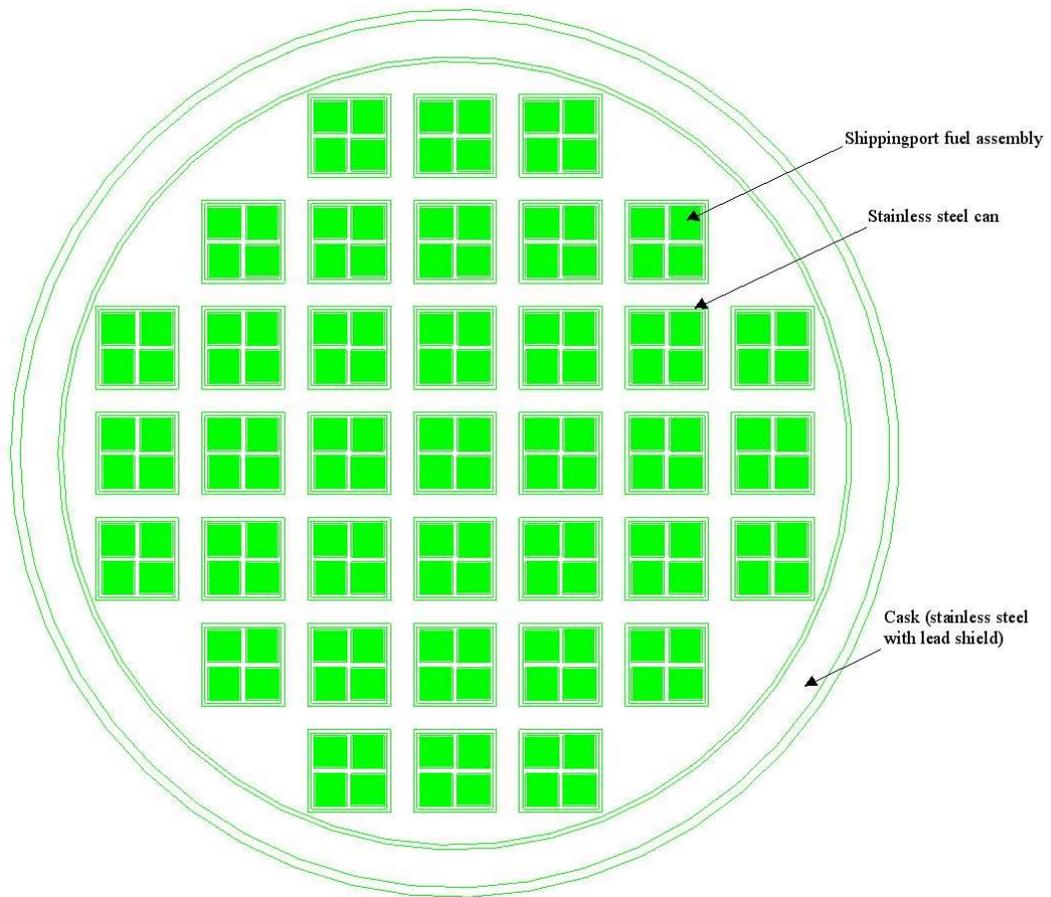
For this preliminary work, a generic shipping cask model was produced based on Shippingport PWR fuel housed in square-pitched stainless steel canisters and placed in a lead-shielded cask. The model used for this application is based on information available in open literature, and may not be representative of any design proposed by INEEL. The physical description of the criticality model input for the Shippingport PWR fuel elements was the same as that used in a previous criticality evaluation performed at Sandia National Laboratories (SNL).<sup>2</sup> These fuel elements are 93% enriched in <sup>235</sup>U and are clad in Zircalloy-2. The fuel

elements were explicitly modeled in the x-y plane. For the axial direction, the fuel region properties were extended to a height of 600 cm. No structural components were modeled above or below the fueled region.

The shipping cask is designed to contain 37 of the Shippingport assemblies in a can-in-cask configuration. Each assembly is contained in a stainless steel can with 20-cm inner width. The can thickness is 0.9525 cm (3/8") on all sides (including top and bottom). The pitch of the assemblies is 28 cm. The cask inner diameter is 207.2634 cm with a stainless steel liner of 1.25-cm thickness. A 30-cm-thick lead shield surrounds this liner. The cask has an outer stainless steel shell of 2.5-cm thickness. All outer cask materials are also present on top and bottom of cask with the same thicknesses. The cask is fully flooded inside and surrounded by a thick water reflector outside. A criticality calculation using KENO V.a in the CSAS25 sequence of SCALE with the 44-group ENDF/B-V library produced a  $k_{eff}$  value of  $0.9400 \pm 0.0004$ . A cross-section view of the cask is shown in Figure 1. This model was analyzed with the SEN3 sequence to produce the sensitivity coefficients necessary for the S/U analysis.

## **EXPERIMENTAL BENCHMARKS**

A suite of 122 experimental benchmarks from 10 benchmark sets from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (IHECSBE)<sup>3</sup> was compiled by INEEL for use in this project. These experimental benchmarks consisted of assemblies of HEU and LEU fuels with various divider materials separating the assemblies. Each of the 122 experimental configurations from the benchmark sets was analyzed with the SEN3 sequence. The sensitivity data was saved for further analysis with the S/U techniques.



**Figure 1. Cross-Section View of Shippingport PWR Fuel Elements in Shipping Cask**

## **FURTHER BENCHMARK EXPERIMENTS**

A suite of further benchmark experiment sensitivity data was also used in this analysis. This suite was compiled from other projects and includes sensitivity evaluations of 425 experimental configurations. In this suite, there are 168 LEU experiments, including solution systems, fuel pin lattices, and solid oxide and fluoride systems moderated by water, paraffin or sterotex.

Seventy-five HEU experiments including solution systems, metal systems, and uranium hydride systems. There are twenty experiments with an intermediate  $^{235}\text{U}$  enrichment including eleven systems with uranium metal and 9 systems with either  $\text{UO}_2$  or  $\text{UF}_4$ . Seventy-eight

plutonium critical experiments consisting of solution systems, metal systems, and oxide systems are included. Seventy-six mixed plutonium and uranium systems involving solution systems, fuel pin lattices, solid mixed-oxide systems moderated by polystyrene and one mixed metal sphere are included in this set of benchmarks. Two experiments fuel by  $^{233}\text{U}$  are included. Six  $^{235}\text{U}$  systems including  $\text{SiO}_2$  in the core or reflector are also included. These experiments cover a broad range of criticality safety applications. Each of these experiments was analyzed with either the SEN1<sup>1</sup> or SEN3 sensitivity analysis sequence.

## **SENSITIVITY AND UNCERTAINTY ANALYSIS**

### **Integral Parameter Results**

The integral parameter techniques invoked in the CANDE code, described in previous papers in this session,<sup>1,4</sup> were applied to the aforementioned criticality models. First the proposed set of 45 critical benchmark experiments was used as the “applications” and the suites of 122 new IHECSBE cases and the 425 previously analyzed benchmark cases were used as the experimental database. The purpose of this exercise was the determination of the uniqueness of the proposed experimental set. If a significant number of the existing experiments were found to match the new experiments for all nuclide-reaction pairs, then no new data would be gained by performing the new experiments.

For brevity in this initial evaluation, only series 1 and 4 with and without lead reflectors were analyzed with the integral parameter techniques. A summary of the results of this analysis is shown below in Table I. In this table, summary values for each experimental series are given. These summary values denote the approximate number of benchmark experiments that had a dE value within 5% of the application for a given nuclide-reaction. Two columns are presented for

each case. The column denoted “122 exp” shows the summary value for the case series compared to the 122 critical experiments from the IHECSBE. The column denoted “547 exp” includes the 122 experiments plus the 425 experiments previously evaluated with sensitivity techniques. An entry of “-” means that the particular application did not meet a sensitivity threshold for this particular nuclide-reaction, or that the nuclide was not present in the model. That is, regardless of the similarities of this application to the experiments, this nuclide-reaction has such a small contribution to  $k_{eff}$  as to be ignored. A value of “0” denotes that the nuclide-reaction was important in the application, but that no experiments met the criterion for this case. For entries with a data range (e.g., “0-10”) there were some cases with a low value, and some with a high value, but few in between.

**Table I. Summary of “dE” Tallies for Proposed Experiments**

	Series 1		Series 4		Series 1 w/ Pb		Series 4 w/ Pb	
	122 exp	547 exp	122 exp	547 exp	122 exp	547 exp	122 exp	547 exp
<b>H-1 Capture</b>	100	300	50	140	90	260	45	150
<b>H-1 Scatter</b>	86	220	35	60	85	220	45	95
<b>O-16 scatter</b>	19	200	24	220	28	230	70	350
<b>Al-27 capture</b>	0	2	0	4	0	2	0	4
<b>Al-27 scatter</b>	0	0	0	0	0	0	0	0
<b>Cr capture</b>	9	24	-	-	9	27	-	-
<b>Fe capture</b>	9	30	9	35	9	30	9	32
<b>Fe scatter</b>	35	50	-	-	33	46	-	-
<b>Zr scatter</b>	7	12	7	18	7	14	7	18
<b>Pb scatter</b>	-	-	-	-	0-10	0-11	0	0
<b>U-235 fission</b>	7	1-21	26	85	7	20	15	60
<b>U-235 capture</b>	0	3-15	5-34	22-94	2	3-16	2-31	15-92
<b>U-238 capture</b>	115	340	390	390	115	350	118	380

An analysis of Table I reveals that very few of the experimental benchmarks met the similarity criterion for either of the Al reactions. It can be concluded from this analysis, that the proposed experiments may validate Al cross sections for high-enriched, water-moderated uranium systems better than other experiments in the database. It is also apparent that this series

of proposed experiments may provide additional validation of  $^{235}\text{U}$  capture relative to the suite of 122 experiments. The complete suite of 547 experiments does appear to have many systems that validate  $^{235}\text{U}$  for this particular situation as well as the proposed experiments. In addition, the proposed experiments provide unique validation of Pb scattering for most cases. It appears that numerous other systems have similar sensitivities to the proposed experiments for all other nuclide-reactions.

Table II shows the summary dE tallies for the prototypic shipping cask application. The CANDE code was used to analyze this cask against four different benchmark data sets. The “122 exp” set is the newly analyzed set from the IHECSBE. The “167 exp” set is the “122 exp” set plus the 45 proposed experiments. The “547 exp” set is the “122 exp” set plus the 425 previously analyzed benchmarks. The “592 exp” set is the “547 exp” set plus the 45 proposed experiments. The “sensitivity” column shows the sensitivity of  $k_{eff}$  for the cask application to the particular nuclide-reaction.

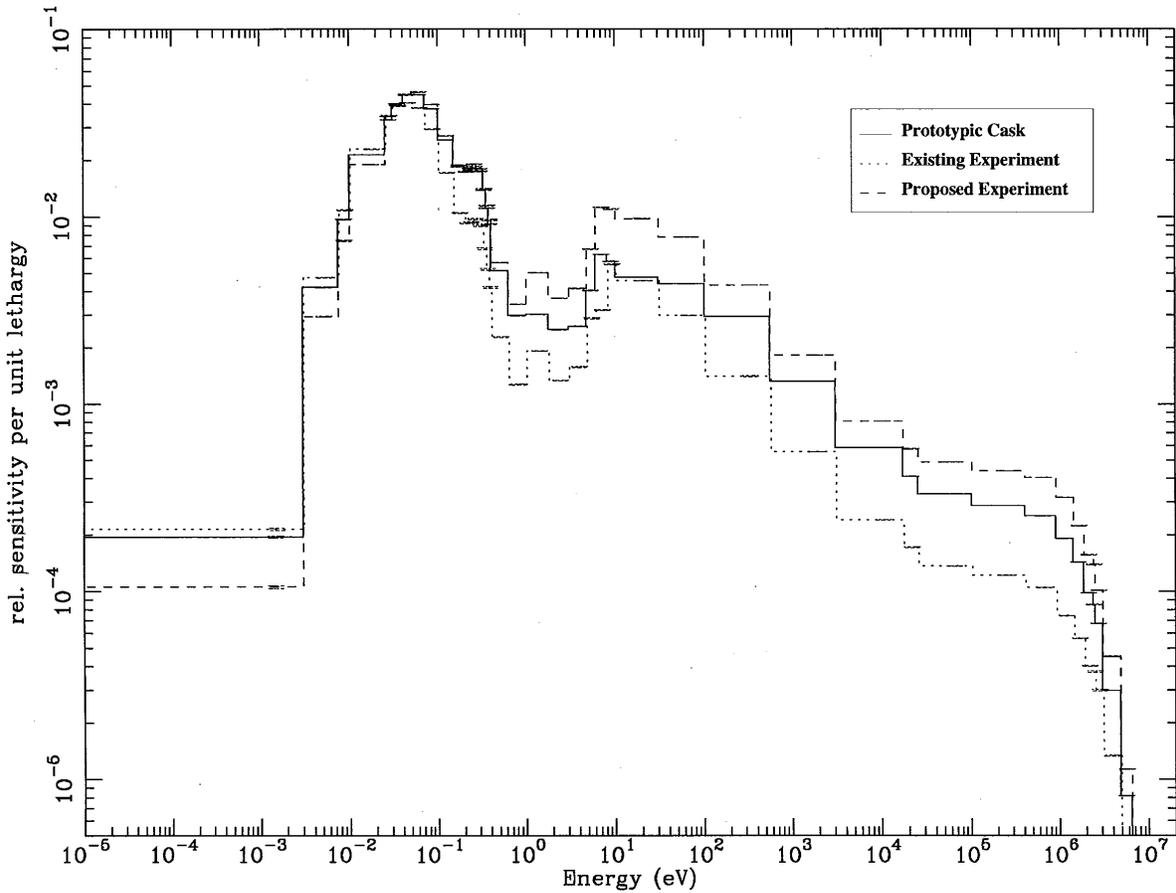
**Table II. “dE” Tallies for Prototypic Cask**

	sensitivity	122 exp	167 exp	547 exp	592 exp
<b>H-1 Capture</b>	-0.1224	54	70	166	182
<b>H-1 Scatter</b>	0.2106	0	1	0	1
<b>O-16 scatter</b>	0.0169	122	167	428	473
<b>Cr capture</b>	-0.0179	9	9	11	11
<b>Fe capture</b>	-0.0495	9	9	10	10
<b>Fe scatter</b>	0.0000	-	-	-	-
<b>Ni capture</b>	-0.0119	9	9	14	14
<b>Zr capture</b>	-0.0241	0	0	0	0
<b>Zr scatter</b>	0.0222	0	0	0	0
<b>Pb scatter</b>	0.0001	-	-	-	-
<b>U-235 fission</b>	0.2764	119	145	253	279
<b>U-235 capture</b>	-0.1423	7	44	35	72
<b>U-238 capture</b>	-0.0035	-	-	-	-

An analysis of the data for the Shippingport cask reveals several points. None of the experiments in any database are as sensitive to the Zr reactions as the designed cask. Also, only

one of the proposed experiments is as sensitive to  $^1\text{H}$  scattering as the cask. Investigation of  $^1\text{H}$  scattering revealed that a large number of systems were only slightly outside the criterion. Thus, this result indicates a possible need for modification of the criterion rather than an inadequacy of the benchmarks. The proposed experiments do offer similar sensitivities to  $^{235}\text{U}$  capture in the cask. The proposed experiments do not have similar sensitivities to the components of stainless steel in the cask, however other experiments in the 122-benchmark suite have similar sensitivities to these elements. Although well validated by other benchmarks, the proposed experiments offer additional validation for  $^{16}\text{O}$  scattering and  $^{235}\text{U}$  fission.

The sensitivity profiles for  $^{235}\text{U}$  capture for the prototypic shipping cask, a sample existing critical experiment and a typical proposed critical experiment are shown in Figure 2. It is evident that the prototypic cask application is more sensitive to  $^{235}\text{U}$  capture than the existing experiment. However, the proposed experiment is more sensitive to  $^{235}\text{U}$  capture than the prototypic cask. The integral parameter techniques indicated that the proposed experiment could be used in the validation of the prototypic cask. However, the same techniques indicated that the existing experiment was not applicable to code validation for this application. This is because the integral parameter techniques require an experiment to be at least as sensitive to the particular nuclide-reaction as is the application it is intended to validate.



**Figure 2.  $^{235}\text{U}$  Capture Sensitivity Profiles for Prototypic Cask, Sample Existing Critical Experiment and a Typical Proposed Critical Experiment**

A further analysis was performed using the  $c_k$  and  $E_{\text{sum}}$  parameters described in previous papers in this session.<sup>4,5</sup> Previously developed guidance<sup>6</sup> states that a benchmark set provides adequate validation for an experiment if 20 or more benchmark systems have a  $c_k$  or  $E_{\text{sum}}$  of 0.8 or higher. A system is also well validated if 10 or more benchmark systems have a  $c_k$  of 0.9 or higher. A count of the number of experiments meeting the criteria of  $c_k$  values relative to the prototypic cask of greater than 0.8 and 0.9 was performed. Also, the number of experiments that meet the criteria of  $E_{\text{sum}}$  greater than 0.8 was recorded. These results are shown below in Table III.

**Table III. Number of Experiments with Integral Parameter Results Meeting Certain Criteria with the Prototypic Cask**

	122 exp	167 exp	547 exp	592 exp
$c_k > 0.8$	120	165	311	356
$c_k > 0.9$	50	89	139	178
$E_{sum} > 0.8$	119	164	271	316

For this particular application, each of the benchmark data sets provides adequate validation based on any of these criteria. These results indicate an overall similarity of the systems based on less stringent criteria than that used to generate the results provided in Table II. Although individual nuclide-reactions may not provide an exact match, a number of the existing experiments and nearly all of the proposed experiments meet these criteria and would be applicable for the validation of the prototypical-shipping cask.

### **GLLSM Results**

The GLLSM techniques, defined in a previous paper in this session<sup>7</sup> have been applied to the prototypic cask to predict the computational bias based on the chosen code validation data set. This bias was calculated for the “122 exp”, “167 exp”, and “592 exp” benchmark sets. The predicted computational bias based on each benchmark set is shown in Table IV.

**Table IV. GLLSM Predicted Computational Biases for Generic Casks**

	Shippingport Cask
122 exp	0.4680%
167 exp	0.3641%
592 exp	0.6856%

From this analysis, it is apparent that the addition of the 45 proposed experiments would provide an improved computation bias for these two applications. The addition of the 425 experiments actually increases the bias for this application.

## **CONCLUSIONS**

This paper has demonstrated some of the uses for the S/U analysis techniques, developed at ORNL, relevant to tailoring an experiment design to meet a particular need. Additionally, the use of graded approach to applicability was shown, where measures are available for system-wide relevance as well as isotope-specific benchmark coverage. This preliminary analysis has revealed that new information relevant to code validation and the prediction of computational biases for DOE spent nuclear fuel applications may be gained from the experimental set proposed by INEEL. Further analyses will be conducted in the near future to examine storage pool applications of DOE spent nuclear fuel.

## **REFERENCES**

1. B. T. REARDEN and R. L. CHILDS, "Prototypic Sensitivity and Uncertainty Analysis Codes for Criticality Safety with the SCALE Code System," *ANS/ENS 2000 International Winter Meeting and Embedded Topical Meetings*, November 12–16, 2000, Washington, D.C. *Trans. Am. Nucl. Soc.* (November 2000).
2. RECHARD, R. P. editor, "Performance Assessment of the Direct Disposal in Unsaturated Tuff of Spent Nuclear Fuel and High-Level Waste Owned by U.S. Department of Energy, Volume #2: Methodology and Results," SAND94-2562/2, UC-900, Sandia National Laboratories (1995).

3. *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, Nuclear Energy Agency Nuclear Science Committee of the Organization for Economic Co-operation and Development, NEA/NSC/DOC(95)03, Paris (1999).
4. B. L. BROADHEAD and B. T. REARDEN, “Sensitivity Foundations for S/U Criticality Validation Techniques,” *ANS/ENS 2000 International Winter Meeting and Embedded Topical Meetings*, November 12–16, 2000, Washington, D.C. *Trans. Am. Nucl. Soc.*, (November 2000).
5. B. L. BROADHEAD, “Uncertainty Analysis Methods for S/U Criticality Validation Techniques,” *ANS/ENS 2000 International Winter Meeting and Embedded Topical Meetings*, November 12–16, 2000, Washington, D.C. *Trans. Am. Nucl. Soc.* (November 2000).
6. B. L. BROADHEAD, C. M. HOPPER, R. L. CHILDS, and C. V. PARKS, “Sensitivity and Uncertainty Analyses Applied to Criticality Validation, Volume 1: Methods Development,” NUREG/CR-6655, Vol. 1 (ORNL/TM-13692/V1), U.S. Nuclear Regulatory Commission, Oak Ridge National Laboratory (November 1999).
7. B. L. BROADHEAD, “Illustrative Examples of Least Squares Methods for Criticality Safety,” *ANS/ENS 2000 International Winter Meeting and Embedded Topical Meetings*, November 12–16, 2000, Washington, D.C. . *Trans. Am. Nucl. Soc.* (November 2000).