# Some Innovations of Dr. Mark Williams for the Practical Application of Sensitivity and Uncertainty Analysis to Reactor Analysis and Criticality Safety*

B. T. Rearden

*Oak Ridge National Laboratory, P.O. Box 2008, Bldg. 5700, Oak Ridge, TN 37831-6170, USA* reardenb@ornl.gov

## INTRODUCTION

This paper reviews, in memoriam, some of the influential innovations of Dr. Mark L. Williams that enabled the extension of sensitivity and uncertainty (S/U) analysis methods which have helped researchers gain insights into practical issues in radiation shielding, reactor dosimetry, reactors physics, and nuclear criticality safety. Beginning in the 1970s, Dr. Williams' early work in radiation shielding optimization resulted in the derivation of *contributon theory* as a unique means of computing sensitivity coefficients for fixed-source analysis.[1,2] In the 1980s, his innovations in the calibration of reactor dosimetry analysis are included in the LEPRICON code developed for the Electric Power Research Institute (EPRI).[3] Two key innovations that have proven essential in realizing advanced S/U approaches for reactor physics and criticality safety are (1) the *implicit effect* that captures the impact of resonance self-shielding in multigroup sensitivity analysis and (2) *reactivity differencing S/U analysis*. These two innovations are the focus of this paper.

## IMPLICIT EFFECT OF RESONANCE SELF-SHIELDING CALCULATIONS

The multigroup eigenvalue and reaction rate sensitivity coefficients in the Tools for Sensitivity and Uncertainty Methodology Implementation (TSUNAMI)[4] sequences of the SCALE Code System[5] are calculated using the well-established adjoint-based perturbation theory approach.[6–9] These methods were developed for fast reactor applications in which the effect of resonance self-shielding in the multigroup cross section data is minimal. In the 1990s, Dr. Williams recognized that to provide an accurate estimation of the sensitivity coefficients for systems in which resonance self-shielding is important, the sensitivity coefficients require additional terms to account for the first-order implicit effect of perturbations in the material compositions or nuclear data on the shielded group-wise macroscopic cross section data.[10] For example, in a water-moderated, low-enriched–uranium system, the resonance self-shielded cross section for $^{238}$U(n,γ) is dependent on the moderation of neutrons by $^{1}$H. Thus, the sensitivity of $k_{eff}$ to $^{1}$H elastic scattering has an implicit component introduced by its influence on the resonance self-shielded cross section for $^{238}$U(n,γ), which leads to a change in $k_{eff}$ for the system. Without the implicit effect, sensitivity coefficients are in error relative to the reference direct perturbation results and do not predict the behavior of the true system.

For the cross section data process $y$ of nuclide $j$ in energy group $h$ expressed as $\Sigma^{j}_{y,h}$, which is sensitive to perturbations in process $x$ in energy group $g$ for nuclide $i$ expressed as $\Sigma^{i}_{x,g}$, the complete sensitivity of $k_{eff}$ due to perturbations of $\Sigma^{i}_{x,g}$ can be defined using the chain rule for derivatives as

$$\left(S_{k,\Sigma^{i}_{x,g}}\right)_{complete} = \frac{\Sigma^{i}_{x,g}}{k}\frac{d\,k}{d\Sigma^{i}_{x,g}}$$

$$= \underbrace{\frac{\Sigma^{i}_{x,g}}{k}\frac{\partial k}{\partial \Sigma^{i}_{x,g}}}_{explicit} + \underbrace{\sum_{j}\sum_{h}\frac{\Sigma^{j}_{y,h}}{k}\frac{\partial k}{\partial \Sigma^{j}_{y,h}}\times\frac{\Sigma^{i}_{x,g}}{\Sigma^{j}_{y,h}}\frac{\partial \Sigma^{j}_{y,h}}{\partial \Sigma^{i}_{x,g}}}_{implicit}, \qquad (1)$$

where the partial sensitivity coefficients with respect to $k_{eff}$ are the explicit components computed with typical perturbation theory, and $j$ and $h$ are varied to include all processes influenced by the value of $\Sigma^{i}_{x,g}$.

To realize the implementation of the implicit effect for general purpose calculations, methods evolved over several SCALE releases, including implicit sensitivity versions of the resonance self-shielding codes BONAMI, CENTRM, and PMC.[11,12] To realize the most efficient implementation, Dr. Williams introduced full-range Bondarenko factors in the SCALE multigroup cross section libraries, and implicit terms are computed with a sensitivity version of the BONAMI code, called BONAMIST, with these methods now embedded into the Sensitivity Analysis Module for SCALE (SAMS) in SCALE 6.2. For LATTICECELL calculations, some implicit terms are propagated through the Dancoff factor. In this case, the sensitivities of the Dancoff factors for each zone of the BONAMIST model to each nuclide are computed. Additional details of these approaches are provided in Drs. Rearden and Williams referenced paper from 2011.[4]

When combined with advancements in multigroup eigenvalue perturbation theory in Monte Carlo methods,[13] it became possible, for the first time, to create accurate eigenvalue sensitivity coefficients for complex systems with thermal, intermediate, and fast spectra.

As demonstrated in Rearden and Horwedel's work[12] several sample problems were selected, and the integral sensitivity coefficients were compared to direct perturbation sensitivity values. The direct perturbation values were generated by running several $k_{eff}$ calculations with varied number densities and computing a sensitivity coefficient through central differencing.

The test problems selected for testing the accuracy of the final sensitivity coefficients were critical experiments selected from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*[14] and are identified as follows:

1. HEU-MET-FAST-028 – A model of the Flattop experiment, which consists of a highly enriched uranium core surrounded by a natural uranium reflector
2. LEU-COMP-THERM-033 Case 1 – A well-moderated homogeneous mixture of $U(2)F_4$ and paraffin

At the time of initial publication, the test problems were all run with the SCALE 238-group ENDF/B-VI cross section data library. The results of the direct perturbation calculations and the explicit and complete sensitivities computed by TSUNAMI are shown in Table I. The TSUNAMI explicit sensitivities, which neglect the contributions of the implicit effect, agree well for the fast spectrum system, but they differ from the direct perturbation results by up to 19% for $^{238}U$ for the thermal system. Note that the TSUNAMI complete sensitivity results agree quite well with the direct perturbation results for all cases.

The effect of the implicit sensitivity is further revealed in Fig. 1, where the energy-dependent sensitivity profiles for the sensitivity of $k_{eff}$ to $^{238}U$ total cross section are shown for the explicit and complete sensitivity calculation. The effect of the resonance self-shielding calculation on the resonance-energy sensitivity coefficients is clearly visible in the difference between these two profiles.

**Table I. Comparison of sensitivity results**

| Test problem | Nuclide | Direct perturbation sensitivity | TSUNAMI explicit sensitivity | TSUNAMI complete sensitivity |
|---|---|---|---|---|
| **HEU-MET-FAST-028** | $^{235}U$ in core | 5.8050E-01 | 5.7952E-01 | 5.7952E-01 |
| | $^{238}U$ in reflector | 2.1305E-01 | 2.1648E-01 | 2.1654E-01 |
| | $^{1}H$ | 2.2076E-01 | 2.5154E-01 | 2.2091E-01 |
| **LEU-COMP-THERM-033 Case 1** | $^{238}U$ | -2.0619E-01 | -2.4509E-01 | -2.0718E-01 |

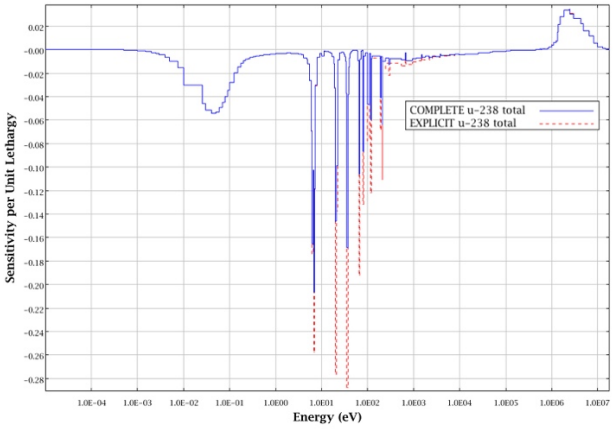


**Figure 1. Energy-dependent explicit and complete sensitivity profiles for $^{238}U$ total cross section from LEU-COMP-THERM-033 Case 1.**

With the innovation of the implicit effect first presented by Dr. Williams,[10] for the first time, multigroup S/U methods could be applied accurately to a wide array of thermal, intermediate, and fast energy systems, opening the door to numerous innovations, including advanced validation approaches[15] that are now part of US Nuclear Regulatory Commission (NRC) guidance,[16] experiment design that has been applied for advanced technologies[17,18], burnup credit for spent nuclear fuel[19], the validation of spent fuel repositories[20], and more. The practical implementation of multigroup approaches in the early 2000s demonstrated the utility of S/U methods for a wide range of applications and led to additional innovations in continuous-energy Monte Carlo approaches that are in wide use today.[21,22,23]

## REACTIVITY SENSITIVITY COEFFICIENTS

Building on the availability of robust eigenvalue S/U methods, Dr. Williams developed an innovative approach to quantify S/U information for the *difference* between two eigenvalue states,[24] leading to the development of the SCALE Tool for Sensitivity Analysis of Reactivity (TSAR). These types of responses are often of interest in reactor physics applications. For example, TSAR can compute data sensitivities and uncertainties of reactivity responses such as control rod worths, fuel and moderator temperature coefficients, and void coefficients for two defined states of a power reactor. Another potential application is in the analysis of critical benchmark experiments for nuclear data testing and validation studies.

Where the relative $k_{eff}$-sensitivity coefficient for an arbitrary data parameter $\alpha$ appearing in the transport equation, including all explicit and implicit effects, is expressed as

$$S_{k,\alpha} = \frac{\partial k/k}{\partial \alpha/\alpha} = -\frac{\partial \lambda/\lambda}{\partial \alpha/\alpha}, \quad (2)$$

an analogous expression defines the relative sensitivity coefficient of the reactivity response:

$$S_{\rho,\alpha} = \frac{\partial \rho_{1\to 2}/\rho_{1\to 2}}{\partial \alpha/\alpha}. \quad (3)$$

Unlike the multiplication factor, the reactivity response can be negative. This can be a source of confusion when interpreting the relative sensitivity coefficient; hence, by convention, TSAR defines sensitivities relative to the *absolute value* of the reactivity; thus,

$$S_{\rho,\alpha} \to \frac{\partial \rho_{1\to 2}/|\rho_{1\to 2}|}{\partial \alpha/\alpha}. \quad (4)$$

In this way, a positive value for the relative sensitivity coefficient means that increasing the value of $\alpha$ always increases the value of the reactivity (i.e., a positive $\rho$ becomes more positive, and a negative $\rho$ becomes less negative). Conversely, a negative relative sensitivity coefficient means that increasing $\alpha$ always decreases the reactivity (i.e., a positive $\rho$ becomes less positive, and a negative $\rho$ becomes more negative). This convention is used in TSAR for all relative quantities involving the reactivity.

These definitions are simplified to the following expression used in TSAR:

$$S_{\rho,\alpha} = \frac{\lambda_2 S_{k_2,\alpha} - \lambda_1 S_{k_1,\alpha}}{|\rho_{1\to 2}|}, \quad (5)$$

where $S_{k_1,\alpha}$ and $S_{k_2,\alpha}$ are the $k$-sensitivities for the two states.

For cases in which the net reactivity change is very small, the denominator of Eq. (5) approaches zero; thus, the relative sensitivity coefficient can increase without bound. The analysis of replacement critical experiments, in which one or more materials are exchanged between configurations but criticality is maintained with other controls, provides $k_{eff}$ values near 1.0 for both $k_1$ and $k_2$. For this reason, TSAR provides an input option to compute *absolute* rather than *relative* sensitivity coefficients.

Prior to executing TSAR, it is necessary to perform TSUNAMI eigenvalue sensitivity calculations for each state—with and without a control rod inserted—in order to generate the relative $k$-sensitivity coefficients. These are written in sensitivity data files (SDFs) and saved for input to TSAR. TSAR reads the two previously prepared files and uses them to evaluate the reactivity sensitivities. The $\rho$-sensitivities are then output to another SDF. Because the complete sensitivities calculated by TSUNAMI include implicit effects associated with resonance self-shielding, the reactivity sensitivities also account for these effects, which can be significant. TSAR also computes the uncertainty in the reactivity difference due to the cross section covariance data.

The development of TSAR was initiated in response to a US NRC request to determine the uncertainty in the coolant void reactivity (CVR) of the ACR-700 reactor design submitted for review by Atomic Energy of Canada, Ltd., in the early 2000s.[25] Dr. Williams led the development of these methods and guided the team that performed the technical assessment for the NRC.[26] A cross section view of the simplified model used in the analysis is shown in Figure 2.

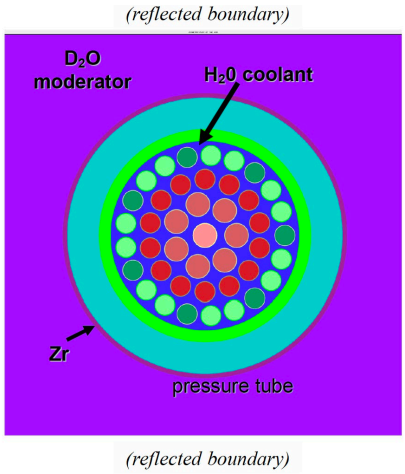


**Figure 2. Cross section view of ACR-700 fuel bundle model.[26]**

The reactor developer had reported a small negative CVR coefficient when voiding the $H_2O$ coolant in the pressure tube while maintaining the $D_2O$ moderator outside the pressure tube. The TSUNAMI and TSAR S/U analysis revealed that, while the uncertainties in a given state due to nuclear data uncertainties are less than 1%, the uncertainty in the CVR was nearly 50%, especially due to the spectral shift induced by the voiding, raising a possible safety issue for this accident scenario and demonstrating the regulatory application of this unique approach.

TSAR has also been applied to the difference in the computed eigenvalues of two benchmarks to establish the sensitivity of the bias trend to various nuclear data used in the calculations. Specifically, S/U methods have been applied in the design and analysis of series of criticality experiments that examine the reactivity of individual structural materials and fission products.[27] Where reactivity experiments are available, the S/U data can be applied in determination of the contribution of individual reaction cross sections in the partial biases of complex

systems, such as fission products in spent nuclear fuel.[28] The application of these methods has served as the technical foundation of NRC's Interim Staff Guidance, *Burnup Credit in the Criticality Safety Analyses of PWR Spent Fuel in Transportation and Storage Casks*.[29]

## CONCLUSIONS

This paper has reviewed the development, implementation, and impact of just two of the many innovations of Dr. Mark Williams that enabled the practical application of S/U methods for reactor physics and criticality safety systems, including design and regulation. Written in memoriam for a session dedicated to Dr. Williams's contributions to the S/U field, this paper cannot possibly capture the vast contributions of our friend and colleague. For those of us who were fortunate enough to work with Mark over many years, his insights and sincere collaborations are greatly missed. Through the inspiration instilled in many of us, his legacy will endure.

## REFERENCES


1. M. L. WILLIAMS, "The Relations Between Various Contributon Variables Used in Spatial Channel Theory," *Nucl. Sci. & Engr.* **64**, pp. 220–222 (1977).
2. M. L. WILLIAMS and H. MANOHARA, "Contributon Slowing Down Theory," *Nucl. Sci. & Engr.* **111**, pp. 345–367 (1992).
3. O. OZER, R. E. MAERKER, M. L. WILLIAMS, B. L. BROADHEAD, J. J. WAGSCHAL and C. Y. FU 1984. "LEPRICON ─ A Systematic Approach to LWR Pressure Vessel Dosimetry," Reactor Physics Topical Meeting of ANS, October 1984, Chicago, IL, pp. 276–285 (1984).
4. B. T. REARDEN, M. L. WILLIAMS, M. A. JESSEE, D. E. MUELLER, and D. A. WIARDA, "Sensitivity and Uncertainty Analysis Capabilities and Data in SCALE," *Nucl. Technol*. **174(2)**, 236–288 (2011).
5. B. T. REARDEN and M. A. JESSEE, Eds., *SCALE Code System*, ORNL/TM-2005/39, Version 6.2.3, UT-Battelle, LLC, Oak Ridge National Laboratory, 2018.
6. E. M. OBLOW, "Sensitivity Theory from a Differential Viewpoint," *Nucl. Sci. Eng.* **59**, 187 (1976).
7. W. M. STACEY, Jr., "Variational Estimates and Generalized Perturbation Theory for the Ratios of Linear and Bilinear Functionals," *J. Math. Phys.* **13**, 1119 (1972); see also W. M. STACEY, Jr., "Variational Estimates of Reactivity Worths and Reaction Rate Ratios in Critical Nuclear Reactors," *Nucl. Sci. Eng.* **48**, 444 (1972).
8. L. N. USACHEV, "Perturbation Theory for the Breeding Ratio and for Other Number Ratios Pertaining to Various Reactor Processes," *J. Nucl. Energy* Pts. A/B, **18**, 571 (1964).
9. A. GANDINI, "A Generalized Perturbation Method for Bilinear Functionals of the Real and Adjoint Neutron Fluxes," *J. Nucl. Energy* **21**, 755 (1967).
10. M. L. WILLIAMS, B. L. BROADHEAD, and C. V. PARKS, "Eigenvalue Sensitivity Theory for Resonance-Shielded Cross Sections," *Nucl. Sci. Eng*. **138**, 177–191 (2001).
11 B. T. REARDEN, M. L. WILLIAMS and J. E. HORWEDEL, "Advances in the TSUNAMI Sensitivity and Uncertainty Analysis Codes Beyond SCALE 5," *Trans. Am. Nucl. Soc.,* **92**, 760–762 (2005).
12 B. T. REARDEN and J. E. HORWEDEL, "Automatic Differentiation with Code Coupling and Applications to SCALE Modules," in *Proc. M&C+SNA 2007*, Monterey, CA, April 15–19, 2007.
13. B. T. REARDEN, "Perturbation Theory Eigenvalue Sensitivity Analysis with Monte Carlo Techniques," Nucl. Sci. Eng. 146, 367–382 (2004).
14. *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 (2005).
15. B. L. BROADHEAD, B. T. REARDEN, C. M. HOPPER, J. J. WAGSCHAL, and C. V. PARKS, "Sensitivity- and Uncertainty-Based Criticality Safety Validation Techniques," *Nucl. Sci. Eng*. **146**, 340–366 (2004).
16. Division of Fuel Cycle Safety and Safeguards, "Justification for Minimum Margin of Subcriticality for Safety," FCSS ISG-10, Rev. 0, US Nuclear Regulatory Commission (2006).
17. B. T. REARDEN, W. J. ANDERSON, and G. A. HARMS, "Use of Sensitivity and Uncertainty Analysis in the Design of Reactor Physics and Criticality Benchmark Experiments for Advanced Nuclear Fuel," *Nucl. Technol*. **151**, 133–158 (2005).
18. N. LECLAIRE, T. IVANOVA, E. LÉTANG, E. GIRAULT, and J. F. THRO, "Fission Product Experimental Program: Validation and Computational Analysis," *Nucl. Sci. Eng.* **161**,188 (2009).
19. J. M. SCAGLIONE, D. E. MUELLER, J. C. WAGNER, and W. J. MARSHALL, *An Approach for Validating Actinide and Fission Product Burnup Credit Criticality Safety Analyses – Criticality ($k_{eff}$) Predictions*, NUREG/CR-7109 (ORNL/TM-2011/514), prepared for the US Nuclear Regulatory Commission by Oak Ridge National Laboratory, Oak Ridge, Tennessee (2012).
20. F. JOHANSSON, "Validation of SCALE 6.2 Using TSUNAMI for Swedish Spent Nuclear Fuel," *Trans. Am. Nucl. Soc.* **119** (2018).

21. B. C. KIEDROWSKI, F. B. Brown, P. P. H. Wilson, "Adjoint-Weighted Tallies for k-Eigenvalue Calculations with Continuous-Energy Monte Carlo," *Nucl. Sci. Eng.* **168**(3), pp. 226–241 (2011).
22. C. M. PERFETTI, B. T. REARDEN, and W. R. MARTIN, "SCALE Continuous-Energy Eigenvalue Sensitivity Coefficient Calculations," *Nucl. Sci. Eng.* **182**(3)**,** 332–353 (2016).
23. A. JINAPHANH, N. LECLAIRE, and B. COCHET, "Continuous-Energy Sensitivity Coefficients in the MORET Code," *Nucl. Sci. Eng.* **184**, 53–68 (2017).
24. M. L. Williams, "Sensitivity and Uncertainty Analysis for Eigenvalue-Difference Responses," *Nucl. Sci. & Eng.* **155**, pp. 18–36 (2007).
25. K. SAPPLE et al, *ACR-700 Technical Description*, 10810-01371-TED-001 Revision 0, Atomic Energy of Canada, Ltd. (2003).
26. M. L. WILLIAMS, J. C. GEHIN and K. T. CLARNO, "Sensitivity Analysis of Reactivity Responses Using One-Dimensional Discrete Ordinates and Three-Dimensional Monte Carlo Methods," *PHYSOR 2006 Topical Reactor Physics Meeting on Advances in Nuclear Analysis and Simulation*, September 2006, Vancouver, Canada, (2006).
27. B. T. REARDEN, I. DUHAMEL, and E. LÉTANG, "New SCALE Sensitivity/Uncertainty Capabilities Applied to Bias Estimation and to Design of MIRTE Reference Experiments," in *Proc. 2009 NCSD Topical Meeting*, Richland, WA, August 14–16 (2009).
28. J. A. ROBERTS, B. T. REARDEN, and P. H. WILSON, "Determination and Application of Partial Biases in Criticality Safety Validation," *Nucl. Sci. Eng.* **173**, 43–57 (2013).
29. Division of Spent Fuel Storage and Transportation, *Burnup Credit in the Criticality Safety Analyses of PWR Spent Fuel in Transportation and Storage Casks*, SFM ISG-8, Rev. 3, US Nuclear Regulatory Commission (2012).