



Standard Guide for Application of Neutron Transport Methods for Reactor Vessel Surveillance, E706 (IID)¹

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1. Scope

1.1 *Need for Neutronics Calculations*—An accurate calculation of the neutron fluence and fluence rate at several locations is essential for the analysis of integral dosimetry measurements and for predicting irradiation damage exposure parameter values in the pressure vessel. Exposure parameter values may be obtained directly from calculations or indirectly from calculations that are adjusted with dosimetry measurements; Guide E944 and Practice E853 define appropriate computational procedures.

1.2 *Methodology*—Neutronics calculations for application to reactor vessel surveillance encompass three essential areas: (1) validation of methods by comparison of calculations with dosimetry measurements in a benchmark experiment, (2) determination of the neutron source distribution in the reactor core, and (3) calculation of neutron fluence rate at the surveillance position and in the pressure vessel.

1.3 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory requirements prior to use.*

2. Referenced Documents

2.1 ASTM Standards:²

E706 Master Matrix for Light-Water Reactor Pressure Vessel Surveillance Standards, E 706(0)

E844 Guide for Sensor Set Design and Irradiation for Reactor Surveillance, E 706(IIC)

E853 Practice for Analysis and Interpretation of Light-Water Reactor Surveillance Results, E706(IA)

E944 Guide for Application of Neutron Spectrum Adjustment Methods in Reactor Surveillance, E 706 (IIA)

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² For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

E1018 Guide for Application of ASTM Evaluated Cross Section Data File, Matrix E706 (IIB)

E2006 Guide for Benchmark Testing of Light Water Reactor Calculations

2.2 Nuclear Regulatory Documents:³

NUREG/CR-1861 LWR Pressure Vessel Surveillance Dosimetry Improvement Program: PCA Experiments and Blind Test

NUREG/CR-3318 LWR Pressure Vessel Surveillance Dosimetry Improvement Program: PCA Experiments, Blind Test, and Physics-Dosimetry Support for the PSF Experiments

NUREG/CR-3319 LWR Pressure Vessel Surveillance Dosimetry Improvement Program: LWR Power Reactor Surveillance Physics-Dosimetry Data Base Compendium

NUREG/CR-5049 Pressure Vessel Fluence Analysis and Neutron Dosimetry

3. Significance and Use

3.1 General:

3.1.1 The methodology recommended in this guide specifies criteria for validating computational methods and outlines procedures applicable to pressure vessel related neutronics calculations for test and power reactors. The material presented herein is useful for validating computational methodology and for performing neutronics calculations that accompany reactor vessel surveillance dosimetry measurements (see Master Matrix E706 and Practice E853). Briefly, the overall methodology involves: (1) methods-validation calculations based on at least one well-documented benchmark problem, and (2) neutronics calculations for the facility of interest. The neutronics calculations of the facility of interest and of the benchmark problem should be performed consistently, with important modeling parameters kept the same or as similar as is feasible. In particular, the same energy group structure and common broad-group microscopic cross sections should be used for both problems. The neutronics calculations involve two tasks: (1) determination of the neutron source distribution in the reactor core by utilizing diffusion theory (or transport theory) calculations in conjunction with reactor power distribution

³ Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402.

measurements, and (2) performance of a fixed fission rate neutron source (fixed-source) transport theory calculation to determine the neutron fluence rate distribution in the reactor core, through the internals and in the pressure vessel. Some neutronics modeling details for the benchmark, test reactor, or the power reactor calculation will differ; therefore, the procedures described herein are general and apply to each case. (See NUREG/CR-5049, NUREG/CR-1861, NUREG/CR-3318, and NUREG/CR-3319.)

3.1.2 It is expected that transport calculations will be performed whenever pressure vessel surveillance dosimetry data become available and that quantitative comparisons will be performed as prescribed by 3.2.2. All dosimetry data accumulated that are applicable to a particular facility should be included in the comparisons.

3.2 *Validation*—Prior to performing transport calculations for a particular facility, the computational methods must be validated by comparing results with measurements made on a benchmark experiment. Criteria for establishing a benchmark experiment for the purpose of validating neutronics methodology should include those set forth in Guides E944 and E2006 as well as those prescribed in 3.2.1. A discussion of the limiting accuracy of benchmark validation discrete ordinate radiation transport procedures for the LWR surveillance program is given in Reference (1). Reference (2) provides details on the benchmark validation for a Monte Carlo radiation transport code.

3.2.1 *Requirements for Benchmarks*—In order for a particular experiment to qualify as a calculational benchmark, the following criteria are recommended:

3.2.1.1 Sufficient information must be available to accurately determine the neutron source distribution in the reactor core,

3.2.1.2 Measurements must be reported in at least two ex-core locations, well separated by steel or coolant,

3.2.1.3 Uncertainty estimates should be reported for dosimetry measurements and calculated fluences including calculated exposure parameters and calculated dosimetry activities,

3.2.1.4 Quantitative criteria, consistent with those specified in the methods validation 3.2.2, must be published and demonstrated to be achievable,

3.2.1.5 Differences between measurements and calculations should be consistent with the uncertainty estimates in 3.2.1.3,

3.2.1.6 Results for exposure parameter values of neutron fluence greater than 1 MeV and 0.1 MeV [$\phi(E > 1 \text{ MeV}$ and 0.1 MeV)] and of displacements per atom (dpa) in iron should be reported consistent with Practices and E853.

3.2.1.7 Reaction rates (preferably established relative to neutron fluence standards) must be reported for $^{237}\text{Np}(n,f)$ or $^{238}\text{U}(n,f)$, and $^{58}\text{Ni}(n,p)$ or $^{54}\text{Fe}(n,p)$; additional reactions that aid in spectral characterization, such as provided by Cu, Ti, and Co-Al, should also be included in the benchmark measurements. The $^{237}\text{Np}(n,f)$ reaction is particularly important because it is sensitive to the same neutron energy region as the iron dpa. Practices and E853 and Guides E844 and E944 discuss this criterion.

3.2.2 *Methodology Validation*—It is essential that the neutronics methodology employed for predicting neutron fluence

in a reactor pressure vessel be validated by accurately predicting appropriate benchmark dosimetry results. In addition, the following documentation should be submitted: (1) convergence study results, and (2) estimates of variances and covariances for fluence rates and reaction rates arising from uncertainties in both the source and geometric modeling. For Monte Carlo calculations, the convergence study results should also include (3) an analysis of the figure-of-merit (FOM) as a function of particles history, and if applicable, (4) the description of the technique utilized to generate the weight window parameters.

3.2.2.1 For example, model specifications for discrete-ordinates method on which convergence studies should be performed include: (1) neutron cross-sections or energy group structure, (2) spatial mesh, and (3) angular quadrature. One-dimensional calculations may be performed to check the adequacy of group structure and spatial mesh. Two-dimensional calculations should be employed to check the adequacy of the angular quadrature. A P_3 cross section expansion is recommended along with a S_8 minimum quadrature.

3.2.2.2 Uncertainties that are propagated from known uncertainties in nuclear data need to be addressed in the analysis. The uncertainty analysis for discrete ordinates codes may be performed with sensitivity analysis as discussed in References (3, 4). In Monte Carlo analysis the uncertainties can be treated by a perturbation analysis as discussed in Reference (5). Appropriate computer programs and covariance data are available and sensitivity data may be obtained as an intermediate step in determining uncertainty estimates.⁴

3.2.2.3 Effects of known uncertainties in geometry and source distribution should be evaluated based on the following test cases: (1) reference calculation with a time-averaged source distribution and with best estimates of the core, and pressure vessel locations, (2) reference case geometry with maximum and minimum expected deviations in the source distribution, and (3) reference case source distribution with maximum expected spatial perturbations of the core, pressure vessel, and other pertinent locations.

3.2.2.4 Measured and calculated integral parameters should be compared for all test cases. It is expected that larger uncertainties are associated with geometry and neutron source specifications than with parameters included in the convergence study. Problems associated with space, energy, and angle discretizations can be identified and corrected. Uncertainties associated with geometry specifications are inherent in the structure tolerances. Calculations based on the expected extremes provide a measure of the sensitivity of integral parameters to the selected variables. Variations in the proposed convergence and uncertainty evaluations are appropriate when the above procedures are inconsistent with the methodology to be validated. As-built data could be used to reduce the uncertainty in geometrical dimensions.

3.2.2.5 In order to illustrate quantitative criteria based on measurements and calculations that should be satisfied, let ψ denote a set of logarithms of calculation (C_i) to measurement (E_i) ratios. Specifically,

⁴ Much of the nuclear covariance and sensitivity data have been incorporated into a benchmark database employed with the LEPRICON Code system. See Ref (6).

$$\psi = \{q_i; q_i = w_i \ln (C_i/E_i), i = 1 \dots N\} \quad (1)$$

where q_i and N are defined implicitly and the w_i are weighting factors. Because some reactions provide a greater response over a spectral region of concern than other reactions, weighting factors may be utilized when their selection method is well documented and adequately defended, such as through a least squares adjustment method as detailed in Guide E944. In the absence of the use of a least squares adjustment methodology, the mean of the set q is given by

$$\bar{q} = \frac{1}{N} \sum_{i=1}^N q_i \quad (2)$$

and the best estimate of the variance, S^2 , is

$$S^2 = \frac{1}{N-1} \sum_{i=1}^N (\bar{q} - q_i)^2 \quad (3)$$

3.2.2.6 The neutronics methodology is validated, if (in addition to qualitative model evaluation) all of the following criteria are satisfied:

- (1) The bias, $|\bar{q}|$, is less than ε_1 ,
- (2) The standard deviation, S , is less than ε_2 ,
- (3) All absolute values of the natural logarithmic of the C/E ratios ($|q|$, $i = 1 \dots N$) are less than ε_3 , and
- (4) ε_1 , ε_2 , and ε_3 are defined by the benchmark measurement documentation and demonstrated to be attainable for all items with which calculations are compared.

3.2.2.7 Note that a nonzero log-mean of the C_i/E_i ratios indicates that a bias exists. Possible sources of a bias are: (1) source normalization, (2) neutronics data, (3) transverse leakage corrections (if applicable), (4) geometric modeling, and (5) mathematical approximations. Reaction rates, equivalent fission fluence rates, or exposure parameter values [for example, $\phi(E > 1 \text{ MeV})$ and dpa] may be used for validating the computational methodology if appropriate criteria (that is, as established by 3.2.2.5 and 3.2.2.6) are documented for the benchmark of interest. Accuracy requirements for reactor vessel surveillance specific benchmark validation procedures are discussed in Guide E2006. The validation testing for the generic discrete ordinates and Monte Carlo transport methods is discussed in References (1, 2).

3.2.2.8 One acceptable procedure for performing these comparisons is: (1) obtain group fluence rates at dosimeter locations from neutronics calculations, (2) collapse the Guide E1018 recommended dosimetry cross section data to a multi-group set consistent with the neutron energy group fluence rates or obtain a fine group spectrum (consistent with the dosimetry cross section data) from the calculated group fluence rates, (3) fold the energy group fluence rates with the appropriate cross sections, and (4) compare the calculated and experimental data according to the specified quantitative criteria.

3.3 *Determination of the Fixed Fission Source*—The power distribution in a typical power reactor undergoes significant change during the life of the reactor. A time-averaged power distribution is recommended for use in determination of the neutron source distribution utilized for damage predictions. For multigroup methods, the fixed source may be determined from the equation

$$S_{rg} = x_g \bar{v} P_r \quad (4)$$

where:

- r = a spatial node,
- g = an energy group,
- $\bar{v}$ = average number of neutrons per fission,
- x_g = fraction of the fission spectrum in group g , and
- P_r = fission rate in node r .

3.3.1 Note that in addition to the fission rate, $\bar{v}$ and x_g will vary with fuel burnup, and a proper time average of these quantities should be used. The ratio between fission rate and power (that is, fission/s per watt) will also vary with burnup.

3.3.2 An adjoint procedure may be used as suggested in NUREG/CR-5049 instead of calculation with a time-averaged source calculation. The influence of changing source distribution is discussed in Reference (7).

3.4 *Calculation of the Neutron Fluence Rate Based on a Fixed Source in the Reactor Core*—The discussion in this section relates to methods validation calculations and to routine surveillance calculations. In either case, neutron transport calculations must estimate the neutron fluence rate in the core, through the internals, in the reactor pressure vessel, and outside the vessel, if for example, ex-vessel dosimetry is used. Procedures for methods validation differ very little from procedures for predicting neutron fluence rate in the pressure vessel or test facility; consequently, the following procedure is recommended:

3.4.1 Obtain detailed geometric and composition descriptions of the material configurations involved in the transport calculation. Uncertainty in the data should also be estimated.

3.4.2 Obtain applicable cross-section sets from appropriate data bases such as:

3.4.2.1 The evaluated nuclear data file (ENDF/B or its equivalent), or

3.4.2.2 A fine group library obtained by processing the above file (for example, see Reference (8)).

3.4.3 Perform a one-dimensional, fixed-source, fine-group calculation in order to collapse the fine-group cross sections to a broad-group set for multidimensional calculations. At least two broad-group sets are recommended for performing the one-dimensional group structure convergence evaluation. The broad-group structure should emphasize the high-energy range and should take cross section minima of important materials (for example, iron) into consideration.

3.4.4 Perform the convergence studies outlined in 3.2.2.

3.4.5 Perform two- or three-dimensional fixed-source transport calculations based on the model established in 3.4.1-3.4.4.

3.4.6 Compare appropriate dosimetry results with neutronics results from 3.4.5 according to the procedure given in 3.2.2. It is recommended that all valid lifetime-accumulated power reactor dosimetry data be included in this comparison each time new data become available except when dosimeter-specific comparisons are made and that a power reactor benchmark be utilized for power reactor calculations.

3.4.7 Repeat appropriate steps if validation criteria are not satisfied. Note that a power reactor dosimetry datum may be discarded if the associated C/E ratios differ substantially from the average of the applicable C/E ratios and a measurement error can be suspected. A measurement error can be suspected

if the deviation from the average exceeds the equivalent of three standard deviations. In addition, the source for power reactor calculations may be scaled to minimize the bias and variance defined by Eq 2 and Eq 3 provided that data are not discarded as a consequence of scaling the source.

3.4.8 Results from neutronics calculations may be used in a variety of ways:

3.4.8.1 Determine a single normalization constant that minimizes bias in the calculated values relative to the measurements in order to scale the group fluences. This is a simple and frequently used alternative to adjustment procedures. However, the magnitude of this constant should be critically examined in terms of estimated source uncertainties.

3.4.8.2 Use a spectrum adjustment procedure as recommended in Guide E944 using calculated group fluences and dosimetry data with uncertainty estimates to obtain an adjustment to the calculated group fluences and exposure parameters. Predicted pressure vessel fluences could then incorporate the spectral and normalization data obtained from the adjusted fluences.

3.4.8.3 Use the calculated fluence spectrum with Practice for damage exposure predictions.

3.4.8.4 It is expected that in some cases the procedure recommended above will be inconsistent with some methodologies to be validated. In these cases procedural variations are appropriate but should be well documented.

4. Documentation

4.1 The documentation of the neutronics calculations for the neutron fluence rates in the pressure vessel should be sufficient to perform a quality assurance audit. This includes: (1) an accurate description of the geometry and composition of the system, (2) a complete list, with description, of all input parameters for the computer programs utilized, (3) references for sources of the nuclear data, (4) comparisons of experimental data with calculated results, (5) the core power distribution,

(6) a normalization factor to obtain the neutron source distribution for any specified power, and (7) neutron spectra at the surveillance position, the inside surface of the pressure vessel, and through the pressure vessel wall. Any of these items may be documented by referencing other documents.

5. Precision and Bias

5.1 Uncertainties associated with specifications for neutronics calculations fall into several broad categories: (1) source distribution, (2) nuclear data, (3) geometry, (4) composition, (5) physical property data, and (6) system states (for example, temperature and pressure). Significant sources of uncertainty should be recognizable from the convergence and model specification studies outlined in 3.2.2. Additional direct or adjoint methods may be employed to generate supporting sensitivity data as required. Comments on accuracy requirements for benchmarks are given in Guide E2006.

5.2 A variance or standard deviation must be assigned to exposure and damage parameter values determined from uncertainty estimates for the neutronics calculation. Use of an adjustment procedure from Guide E944 is recommended for the determination and reduction of uncertainties for exposure parameters.

5.3 The uncertainty in calculated in-vessel neutron fast fluence [$\phi(E > 1 \text{ MeV})$] is typically in the range from 10-20 %. A discussion of the representative uncertainty contributions is provided in Reference (9). Reference (10) provides an overview of the international perspective on the state-of-the-art in radiation transport and the associated uncertainties in radiation transport calculations for pressure vessel fluence.

6. Keywords

6.1 discrete ordinates; dosimetry; exposure parameter; Monte Carlo; neutron fluence; pressure vessel; radiation transport

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