MATHEMATICS AND COMPUTATION

UNCERTAINTIES IN TRANSPORT THEORY MODELING FOR POWER REACTOR INTERNALS AND STRUCTURES

Cosponsored by the Mathematics and Computation, the Power, and the Radiation Protection and Shielding Divisions

Session Organizer: Ali Haghighat (Penn State Univ)

1. Uncertainties in Transport Theory Pressure Vessel Neutron Fluence Calculations, *A. Haghighat, B. Petrovic, J. C. Wagner, H. L. Hanshaw (Penn State), M. Mahgerefteh (GPU Nuclear, NJ), invited*

The desire for increasing safety margins (increased power production and plant availability), the fact that many existing plants are approaching the final years of their design lifetime, and the consideration of life extension have resulted in the need for performing more accurate estimation of parameters that affect plant performance and safety. This means that more accurate calculational and experimental methodologies for estimating the neutron and/or gamma fluence distributions are needed to ensure the structural integrity of the pressure vessel in pressurized water reactors (PWRs) and vessel internals in boiling water reactors. Such an estimation requires the use of particle transport theory methods and analysis; because of the existing uncertainties in the input parameters and numerical methods, it is necessary to estimate the uncertainties in the calculated results.

In this paper, we discuss our studies in identifying and estimating the uncertainties associated with transport theory calculations of the fast neutron fluence at the PWR pressure vessel. The common approach in the United States for pressure vessel fluence estimation is to perform fixed-source calculations using deterministic discrete ordinates methods. Specifically, three-dimensional multigroup flux/fluence distributions are calculated throughout one octant of a reactor and subsequently benchmarked based on measured reaction rates at in-vessel capsules and/or cavity dosimeters. The three-dimensional flux is obtained by synthesis of two two-dimensional (r-Θ and r-z) and one one-dimensional (r) flux distributions in cylindrical geometry as[1]

$$\phi(r,\Theta,z) = \phi(r,\Theta)\,\frac{\phi(r,z)}{\phi(r)} .$$

The reactor model is composed of rectangular regions (fuel assemblies) and cylindrical regions (including the core barrel and beyond). The cylindrical geometry is used because it adequately represents the pressure vessel, and the rectangular regions are projected onto it.

TABLE I

Ratios of Calculated to Experimental Activities

Reaction	Davis-Besse		TMI-1	
	In-Vessel Capsule at 26.5 deg, Cycles 1-6	Cavity Dosimetry at 11.5 deg, Cycle 6	Cavity Dosimetry at 30 deg, Cycle 7	Cavity Dosimetry at 30 deg, Cycle 8
$^{237}Np(n,f)^{137}Cs$	-	1.01[a]	-	0.88[a]
$^{238}U(n,f)^{137}Cs$	-	0.87[a]	-	0.87[a]
$^{58}Ni(n,p)^{58}Co$	0.91[b] (0.90-0.93)[c]	1.12 (1.09-1.15)	1.03 (1.01-1.05)	1.14 (1.08-1.20)
$^{54}Fe(n,p)^{54}Mn$	0.92 (0.91-0.94)	1.17 (1.13-1.20)	1.13 (1.12-1.15)	1.13 (1.08-1.19)
$^{46}Ti(n,p)^{46}Sc$	-	0.94 (0.89-0.99)	-	-
$^{63}Cu(n,\alpha)^{60}Co$	-	0.97 (0.95-0.99)	0.95 (0.94-0.97)	0.92 (0.91-0.93)

[a] Calculated activities for $^{237}Np(n,f)^{137}Cs$ and $^{238}U(n,f)^{137}Cs$ reactions do not include the photofission effect (it would increase C/E ratios by several percent).

[b] Median value for all available C/E ratios.

[c] Range of C/E ratios when several individual dosimeters exist.

For these calculations, a two-dimensional multigroup discrete ordinates code DORT (Ref. 2) is used. The r-Θ, r-z, and r fixed-source distributions are prepared using three-dimensional (x-y-z) pinwise beginning-of-cycle/end-of-cycle burnup distributions and an equivalent spectrum based on the isotopic composition of fissile nuclei (^{235}U, ^{239}Pu, and ^{241}Pu). The 47-group, P_3 SAILOR cross-section library[3] (modified to include the ENDF/B-VI iron cross sections) or BUGLE-93 library[4] are used.

To benchmark this methodology, we have modeled the Three Mile Island unit 1 (TMI-1) (GPU Nuclear Corporation) and Davis-Besse (Toledo Edison Company) reactors. In TMI-1, there is only one cavity dosimeter, while in Davis-Besse, there are several in-vessel capsules and cavity dosimeters. Table I presents the ratios of calculated to experimental (C/E) reaction rates for the TMI-1 cavity dosimeters for cycles 7 and 8 and the Davis-Besse in-vessel capsules and cavity dosimeters. These results (with no adjustments) demonstrate that the calculational results are in very good agreement with the experimental results (within 20%).

We have performed extensive studies to identify and categorize the causes of the uncertainties associated with these calculations. The causes can be grouped into five major categories: cross sections, fission source, reactor modeling, discrete ordinates (S_n) method, and synthesis procedure. Each category has several components:

1. cross sections
   a. basic pointwise cross-section data:
      (1) library evaluation/version (e.g., ENDF/B-VI)
      (2) pointwise cross-section uncertainties
      (3) iron cross section
   b. multigroup cross-section libraries preparation:
      (1) collapsing to fine-group structure (self-shielding)
      (2) collapsing from fine to broad group structure
      (3) response cross sections
      (4) multigroup cross sections
2. fission source
   a. power spatial distribution
   b. conversion to fission neutrons
   c. spectrum of fission neutrons
3. reactor model
   a. moderator density (former and downcomer region)
   b. stainless steel (baffle, core barrel, thermal shield, pressure vessel clad) density
   c. core barrel and thermal shield radial position
   d. pressure vessel eccentricity, density, and thickness
   e. concrete wall composition (steel, water contents, liner)
   f. cavity top/bottom reflector
   g. cavity dosimetry position
4. S_N method
   a. spatial discretization
   b. angular discretization
   c. order of anisotropy
   d. differencing
   e. scattering source negative fixup
   f. convergence criterion
   g. acceleration method
5. synthesis procedure
   a. synthesis formulation
   b. cylinderization.

We have estimated the individual uncertainties for the listed items and the overall uncertainty based on linear perturbation theory (using adjoint transport theory), sensitivity studies for limit cases, and performing more detailed/accurate calculations.[5,6] For the limit cases, we have considered the worst cases. For example, despite the fact we are using the ENDF/B-VI-based cross sections, to estimate the uncertainties we have used the ENDF/B-V and ENDF/B-IV cross sections as the possible deviations from the accurate data. This deviation is especially large for isotopes such as iron, which is the major constituent of the structure outside the reactor core (i.e., baffle plates, core barrel, thermal shield, and pressure vessel).

To combine these uncertainties, we have adopted the root-mean-squares approach. We have also estimated the overall uncertainty by using the LEPRICON (Least-Squares EPRI CONsolidation) code.[7] LEPRICON uses the calculational and experimental reaction rates along with its 44 benchmarks and a generalized least-squares methodology to estimate the uncertainties. Note that LEPRICON can also adjust the parameters and accordingly improve the precision of results.

Table II lists the uncertainties for different categories and the overall uncertainty obtained using our approach and the LEPRICON code. It is interesting that both approaches produce very similar results.

Because of the significant increase in the performance of computers, the Monte Carlo method is becoming possible as an alternative method for pressure vessel fluence calculations. We have developed an optimized Monte Carlo model[6] using the MCNP code[8]; for this, we utilized different variance reduction techniques along with the deterministic adjoint function distribution. The uncertainties with the Monte Carlo calculations are of a somewhat different nature; their causes can be summarized as (a) statistical, (b) tallying region, (c) cross sections, and (d) false convergence, i.e., not satisfying the central limit theorem. Finally, we note that the Monte Carlo method still requires large computation times for obtaining detailed flux distributions, which are necessary for a proper analysis of the results. Hence, for optimum transport theory simula-

TABLE II

Upper Limit of Uncertainty for the Cavity Dosimetry

Source of Uncertainty	Uncertainty PSU	Uncertainty LEPRICON (Before Adjustment)
Cross Section	23%	21%
Fission Source	10%	10%
Reactor Model	13%	12%
S_N Method	6%	n/a[a]
Synthesis Procedure	4%	n/a[a]
TOTAL UNCERTAINTY:	29%	30%

[a]These uncertainties are not available in the LEPRICON output, but their effects are included in the total uncertainty.

tions, it is necessary to use both deterministic and Monte Carlo methods.

In this paper, we have identified and categorized the major causes and quantified the associated uncertainties in calculated flux distributions obtained using the transport theory methods (deterministic and Monte Carlo). We have also presented a validation of the methodology based on experimental data from two PWRs, and a very good agreement has been observed. Nevertheless, it would be very beneficial to further reduce the uncertainties in transport theory calculations. As a part of our efforts in that direction, we have developed a new S_n differencing formulation,[9] a new multigroup cross-section generation methodology,[10] and advanced acceleration techniques for Monte Carlo simulations.[11]

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