Sensitivity Analysis of Reactivity Responses Using One-Dimensional Discrete Ordinates and Three-Dimensional Monte Carlo Methods

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Abstract

The TSUNAMI computational sequences currently in the SCALE 5 code system provide an automated approach to performing sensitivity and uncertainty analysis for eigenvalue responses, using either one-dimensional discrete ordinates or three-dimensional Monte Carlo methods. This capability has recently been expanded to address eigenvalue-difference responses such as reactivity changes. This paper describes the methodology and presents results obtained for an example advanced CANDU reactor design.

KEYWORDS: reactivity, sensitivity, perturbation theory, SCALE

1. Introduction

The SCALE 5 code system includes two major computational sequences and several auxiliary programs for sensitivity and uncertainty (S/U) analysis of k-eigenvalue responses. [1] The TSUNAMI-1D sequence [2] uses one-dimensional (1-D) discrete ordinates, while TSUNAMI-3D [3] uses the multigroup Monte Carlo code KENO V.a [4] to calculate k_{eff} sensitivities in arbitrary three-dimensional (3-D) geometry. Both of these automated <u>sequences</u> (a) perform self-shielding calculations for the unresolved and resolved resonance ranges; (b) execute transport codes to compute multigroup forward and adjoint flux distributions; (c) evaluate energy-dependent sensitivity coefficients relating k_{eff} to nuclear data of all nuclide-reaction pairs, and (d) fold the sensitivity profiles with cross section covariance data to obtain the uncertainty in the multiplication factor. TSUNAMI also includes techniques to account for implicit perturbations in the response caused by changes in cross section self-shielding, so that thermal and intermediate-spectra systems are treated more accurately. [5] Although originally developed primarily for k_{eff} responses in criticality safety work, the TSUNAMI S/U computation sequences were recently extended to address reactivity responses for reactor physics applications. In this paper, we describe the methodology implemented in SCALE to compute reactivity sensitivity coefficients, and we present several example applications.

2. Sensitivity/Uncertainty Expressions for Reactivity Responses

The static reactivity change due to a reactor transformation from an initial state with a k-eigenvalue of k_1, to a final state with a k-eigenvalue of k_2, is defined as

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$$\rho_{1\rightarrow 2} = \frac{1}{k_1} - \frac{1}{k_2} \quad . \tag{1}$$

It is assumed that the reactor states are distinct, uniquely defined by a finite change in number density, temperature, control rod position, or other state variable. The relative sensitivity coefficient for the reactivity response in Eq. (1) is defined as

$$S_{\rho,\alpha} \equiv \frac{\alpha}{\rho_{1\rightarrow 2}} \frac{\partial \rho_{1\rightarrow 2}}{\partial \alpha} = \frac{\frac{1}{k_2} S_{k2,\alpha} - \frac{1}{k_1} S_{k1,\alpha}}{\rho_{1\rightarrow 2}} \quad , \tag{2}$$

where α is an arbitrary data parameter (e.g., multigroup cross section) used in the transport calculations, and the relative sensitivity coefficient for the k-eigenvalue response is defined as

$$S_{k,\alpha} = \frac{\alpha}{k} \frac{\partial k}{\partial \alpha} \quad . \tag{3}$$

The TSUNAMI sequences in SCALE compute the above k-sensitivity coefficients for arbitrary material and geometric configurations. Therefore, $S_{k1,\alpha}$ and $S_{k2,\alpha}$ can be obtained from TSUNAMI Monte Carlo or discrete ordinates calculations at the initial and final reactor states, respectively; and then Eq. (2) can be utilized to compute the reactivity sensitivity coefficient, corresponding to the expression,

$$S_{\rho,\alpha} = \left\{ \frac{\left\langle \Phi_1^* \left(\frac{\alpha \partial \mathbf{L}_1}{\partial \alpha} - \lambda_1 \frac{\alpha \partial \mathbf{P}_1}{\partial \alpha} \right) \Phi_1 \right\rangle}{\rho_{1\rightarrow 2} \left\langle \Phi_1^* \mathbf{P}_1 \Phi_1 \right\rangle} - \frac{\left\langle \Phi_2^* \left(\frac{\alpha \partial \mathbf{L}_2}{\partial \alpha} - \lambda_2 \frac{\alpha \partial \mathbf{P}_2}{\partial \alpha} \right) \Phi_2 \right\rangle}{\rho_{1\rightarrow 2} \left\langle \Phi_2^* \mathbf{P}_2 \Phi_2 \right\rangle} \right\} \quad . \tag{4}$$

where λ is defined as the reciprocal of the k-eigenvalue.

This extends the general TSUNAMI methodology to treat responses such as coolant voiding reactivity (CVR), Doppler feedback, etc. The reactivity sensitivity coefficients can be utilized in subsequent analysis to obtain the reactivity uncertainty, [6] determine its similarity to other measurable responses, [7] and perform generalized least-squares adjustment calculations. [8]

For example, if $\mathbf{C}_{\alpha\alpha}$ represents the nuclear data covariance matrix, then the relative variance (square of the standard deviation) in the calculated reactivity due to cross section uncertainties is given by the expression,

$$\mathrm{Var}(\rho) = \left(\frac{\lambda_1}{\lambda_1 - \lambda_2} \right)^2 \mathbf{S}_{\lambda 1} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{\lambda 1}^{\mathrm{T}} + \left(\frac{\lambda_2}{\lambda_1 - \lambda_2} \right)^2 \mathbf{S}_{\lambda 2} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{\lambda 2}^{\mathrm{T}} - \left(\frac{2\lambda_1 \lambda_2}{(\lambda_1 - \lambda_2)^2} \right) \mathbf{S}_{\lambda 2} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{\lambda 1}^{\mathrm{T}} \quad . \tag{5}$$

Equation (5) shows that the variance in the reactivity is not simply the sum of the variances in the computed eigenvalues for states 1 and 2 because these uncertainties are correlated as a result of using the same nuclear data and models in the transport calculations. A positive correlation between the eigenvalue states reduces the uncertainty in the reactivity because common uncertainties tend to cancel from the eigenvalue-difference. It also can be seen that the relative variance of the reactivity can be substantially greater than the eigenvalue variances whenever the difference in the eigenvalues of the two states is small. Because this is usually the case for reactivity changes in a reactor, the relative uncertainties in reactivity responses are inherently large.

3. Application to ACR-700 Fuel Bundle Model

S/U analysis has been performed using TSUNAMI-3D for the CVR in a modified model of the advanced Canadian deuterium-uranium (CANDU) reactor, ACR-700. Figure 1 shows the fuel bundle model used for the KENO V.a Monte Carlo calculations. In this example, the initial reactor state includes water coolant within the pressure tube at the full-power conditions, and the final state has the water density reduced by 99.9%. The k-eigenvalues of the two states were calculated to a statistical precision of better than 0.01%. The CVR was found to be −211 pcm, with a precision of ±10 pcm.

Table 1 shows some energy-integrated sensitivities for the CVR to various nuclear data. The CVR has the highest sensitivity to the elastic cross section of the deuterium moderator. The sensitivity coefficient indicates that a uniform 1% increase in the elastic cross section of ^{2}H will cause the CVR to increase (become less negative) by more than 34%. Figure 2 shows the energy-dependent sensitivity profile for the deuterium total cross section. The largest (positive) sensitivities occur at the energies of the ^{238}U resonances, because when the light-water coolant is voided, the heavy-water moderator becomes essentially the only contributor to the resonance escape probability. Figure 3 shows the energy-dependent sensitivity profile for the hydrogen total cross section. The CVR has positive sensitivity to the ^{1}H thermal data because of loss of hydrogen absorption in the voided state, but it has large negative sensitivities within the energy intervals of the ^{238}U resonances where the loss of moderation decreases the resonance escape probability.

Table 1: Integrated cross section sensitivity coefficients
(Monte Carlo standard deviations are shown in parentheses).

Nuclide	Elastic	Capture	Fission
^{235}U	−0.0315 (±8.09E-06)	−1.386 (±8.39E-03)	−3.590 (±2.54E-02)
^{238}U	−0.628 (±5.22E-04)	−8.387 (±1.76E-02)	1.649 (±1.88E-03)
^{1}H	−17.287 (±2.39E-03)	14.915 (±2.04E-03)	0.0
^{2}H	34.159 (±1.08E-02)	0.0437 (±1.05E-04)	0.0
Dy-164	−0.0151 (±3.85E-06)	−2.647 (±1.33E-03)	0.0

Figure 1: Fuel bundle model used in Monte Carlo calculations for sensitivity coefficients.

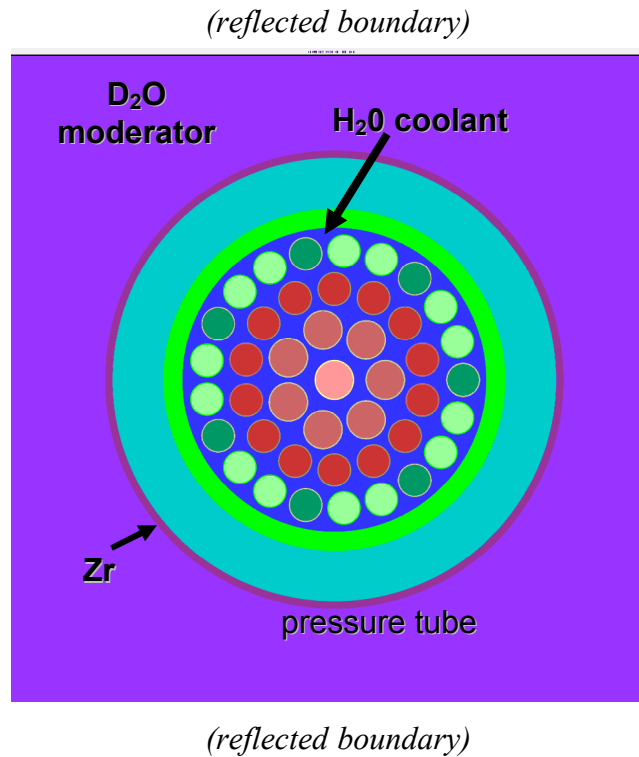*(reflected boundary)*

(reflected boundary)

Figure 2: CVR energy-dependent sensitivity profile to deuterium total cross section.
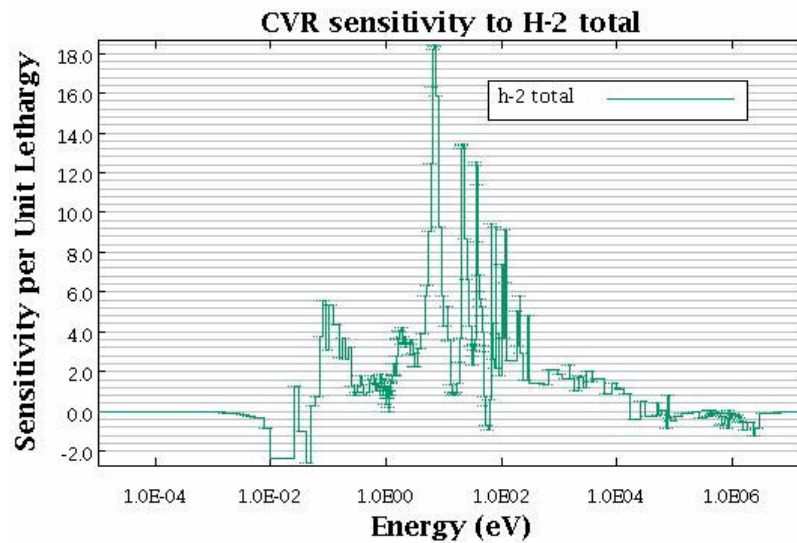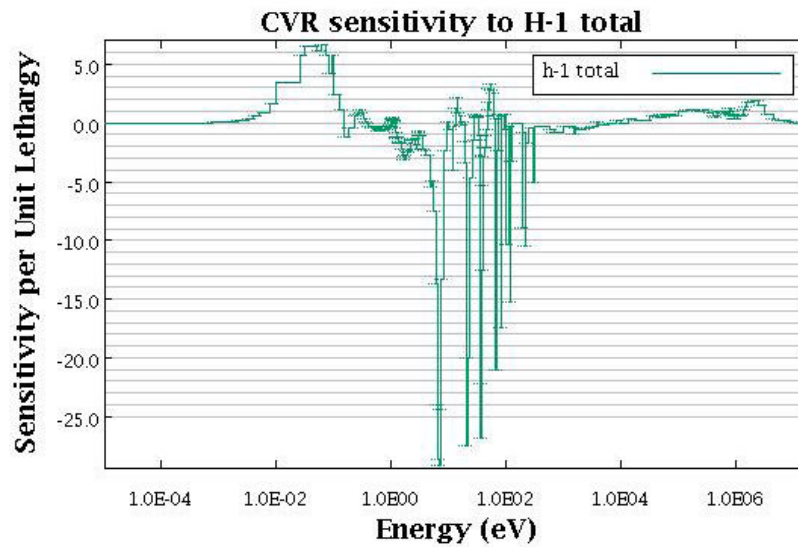

Figure 3: CVR energy-dependent sensitivity profile to hydrogen total cross section.

4. Summary

The automated S/U computation sequences in SCALE have been extended to address eigenvalue-difference responses. This provides the capability to compute data sensitivities for reactivity changes by using Monte Carlo in 3-D geometry and to determine the uncertainty in reactivity effects for reactor physics applications.

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