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Computational Methods for Sensitivity and Uncertainty Analysis in Criticality Safety

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COMPUTATIONAL METHODS FOR SENSITIVITY AND UNCERTAINTY ANALYSIS IN CRITICALITY SAFETY

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Abstract

Interest in the sensitivity methods that were developed and widely used in the 1970s (the FORSS methodology at ORNL among others) has increased recently as a result of potential use in the area of criticality safety data validation procedures to define computational bias, uncertainties and area(s) of applicability. Functional forms of the resulting sensitivity coefficients can be used as formal parameters in the determination of applicability of benchmark experiments to their corresponding industrial application areas. In order for these techniques to be generally useful to the criticality safety practitioner, the procedures governing their use had to be updated and simplified. This paper will describe the resulting sensitivity analysis tools that have been generated for potential use by the criticality safety community.

Introduction

The FORSS [1] system was developed at ORNL in the late 1970s primarily for use in the development of fast reactor systems. A version of the system is available from the Radiation Shielding Information and Computational Center (RSICC) as CCC-334. However, due to known deficiencies and the lack of availability on newer computational platforms, it was decided the most appropriate procedure was to start with the RSICC version of FORSS and reactivate the individual modules with the goal of putting portions of the original system into the SCALE [2] system. The SCALE philosophy is to include standard well-known computer codes into an application-specific computational sequence with a single integrated input file. Using this philosophy as a guide, a one-dimensional (1-D) sensitivity sequence, SEN1 [3], was produced for use in this work and for subsequent general use. This sequence performs standard resonance processing tasks, then computes sensitivity coefficients, estimates the uncertainty in the system k_{eff} value, and plots the sensitivity profiles.

The capability to generate 2-D sensitivities is also available; however, it is intended for use primarily as a tool to test the multidimensional nature of the sensitivities. This capability is not as fully integrated into the SCALE system as the 1-D sensitivity module. The 2-D sensitivity package, SEN2, is based on 2-D discrete-ordinates code DORT [4], which is not contained in the SCALE system. The documentation of the SEN2 sensitivity module is included in the same package as the SEN1 documentation [3].

The generation of sensitivity coefficients using 3-D Monte Carlo methods was also investigated under this project. A prototypical SCALE module, SAMS, was developed for performing limited sensitivity analyses using fluxes and cross sections obtained from the CSAS25 SCALE sequence, which uses KENO V.a.

Sensitivity Theory

The techniques used in this work to generate sensitivity information for the various critical benchmarks are based on the widely used perturbation theory approach [5–8]. The full derivation of the general procedure will not be given here; however, the specific theory for the generation of k_{eff} sensitivities is given below. For the full derivation of the general sensitivity equations the reader is referred to Ref. 1.

Considering the Boltzmann transport equation written in the form:

$$[A - \lambda B]\phi = 0 \tag{1}$$

and a perturbed system

$$[A' - \lambda' B']\phi' = 0 , \tag{2}$$

the equation adjoint to Eq. (1) is

$$[A^* - \lambda B^*]\phi^* = 0 . \tag{3}$$

Multiplying Eq. (2) by ϕ^*, and integrating over all phase space yields

$$\langle \phi^*(A' - \lambda' B')\phi' \rangle = 0 . \tag{4}$$

Defining:

$$A' = A + dA$$

$$B' = B + dB \tag{5}$$

$$\lambda' = \lambda + d\lambda$$

and using the property of adjointness for the operators A, A* and B, B*, we find

$$\langle \phi^*(dA - \lambda dB - B d\lambda - d\lambda dB)\phi' \rangle = 0 . \tag{6}$$

Ignoring second-order terms (e.g., $d\lambda dB$), substituting ϕ' with ϕ, and solving for the reactivity perturbation,

$$d\lambda/\lambda = \langle \phi^*(dA - \lambda dB)\phi \rangle / \langle \phi^*(\lambda B)\phi \rangle . \tag{7}$$

Hence, the sensitivity of λ, which is $1/k_{eff}$, with respect to the cross section, Σ, becomes

$$\frac{d\lambda/\lambda}{d\Sigma/\Sigma} = \frac{\Sigma \langle \phi^*(dA/d\Sigma - \lambda dB/d\Sigma)\phi \rangle}{\lambda \langle \phi^*(B)\phi \rangle} . \tag{8}$$

Note that since $\lambda = 1/k_{eff}$, then $d\lambda/\lambda = -dk_{eff}/k_{eff}$, such that the above equation is essentially the defining equation for the k_{eff} sensitivity. Note that first-order sensitivities to problem parameters besides Σ can be obtained, but this method has not been pursued in the current work.

Sensitivity Sequence Development

The k_{eff} sensitivity, as described above, was implemented in the FORSS [1,9] (Fantastic Oak Ridge Sensitivity System) package in the late 1970s. This package was placed into RSICC partially through the development process. While operational, it does not contain the complete package (e.g. thermal upscatter is not operational) that was locally available at ORNL at the time of the phase out of fast reactor funding in the mid 1980s. As a result of these deficiencies and the desire for an easy-to-use package, it was decided to reactivate the individual modules with the goal of putting portions of the original system into the SCALE [2] system.

One-Dimensional Sensitivity Tool

Using the SCALE philosophy as a guide, a one-dimensional (1-D) sensitivity sequence, SEN1 [3], was produced for use in this project and for subsequent general use. This sequence performs standard resonance processing tasks (BONAMI and NITAWL modules), then determines (using 1-D transport theory) the forward and adjoint angular fluxes needed for sensitivity coefficient generation. The radiation transport solver utilized was the XSDRNPM code, which is used extensively within the SCALE system. The sequence then calls modules VIP1D, LAKE, and PLOT, which compute the sensitivity coefficients, estimates the uncertainty in the system k_{eff} value, and plots the sensitivity profiles, respectively. The user input to SEN1 is very similar to the user input of the shielding module, SAS1, except that, since k_{eff} sensitivities do not require a source input, a fixed source is not required.

Typical user input for the two SCALE calculational types for the SEN1 module are shown in Figs. 1–2. The user input contains the standard composition input that is common to all SCALE modules, followed by a simple geometry description of the problem. The differences in the inputs for Figs. 1–2 are the use of the SCALE calculational types corresponding to INFHOMMEDIUM and LATTICECELL cross-section resonance-processing schemes. For the first option, no resonance shielding is performed; however, the latter technique treats resonance-shielding effects in lattice-pin geometry cases.

Two-Dimensional Sensitivity Tool

The capacity to generate 2-D sensitivities is also available via the SEN2 [3] module. This capability is not as fully integrated into the SCALE system as the 1-D sensitivity module. The 2-D sensitivity package is based on 2-D discrete-ordinates code DORT [4], which is not contained in the SCALE system. The objective of this package is to have the same functionality in both 1-D and 2-D, with the primary difference being the XSDRNPM versus DORT transport solvers. The 2-D sequence has not been made into an automated SCALE sequence because of the following considerations:

1. DORT calculations require much more computer time than those of the corresponding XSDRNPM calculations,

2. The DORT geometry and mesh input is more difficult to prepare than the 1-D inputs,

3. DORT calculations sometimes fail to converge adequately and need to be restarted or the input modified to obtain good convergence.

The first step in performing a 2-D sensitivity/uncertainty analysis is the preparation of problem-dependent cross sections. In SEN1 two cross-section files are used, an AMPX working library (used by XSDRNPM and LAKE) and a sensitivity cross-section library (used by LAKE). The LAKE code is used for both 1-D and 2-D sensitivity/uncertainty analyses. Thus, the two cross-sections files used in SEN1 are

also required in a 2-D analysis. In addition to these two cross-section files, two additional cross-section files are needed: a GIP cross-section file for the forward DORT calculation and a GIP file for the adjoint DORT calculation. A SCALE-type control sequence named SEN2 has been developed to produce all four of the cross-section files needed for a 2-D sensitivity analysis.

The second step in performing a 2-D sensitivity/uncertainty analysis is to execute both a forward and an adjoint DORT criticality calculation. Two interface files are saved from the forward calculation, and one interface file is saved from the adjoint calculation. The third step in obtaining 2-D sensitivity information is the execution of the VIP2D code. VIP2D reads the interface files written by DORT (and some other files and input data) and writes a file to be read by the LAKE code. The final step in a 2-D sensitivity analysis is the execution of the LAKE code. Unlike the SEN1 code, the individual inputs for VIP2D and LAKE must be generated by the user. However, the user input for these codes is minimal.

Three-Dimensional Sensitivity Tool

A prototypical SCALE module was developed to assess the feasibility of generating sensitivity coefficients from criticality calculations performed with the CSAS25 SCALE module. At the completion of this task, the SAMS module will be capable of calculating the sensitivity of k_{eff} to $\bar{\nu}$ and χ for any system that can be modeled using KENO V.a. SAMS is limited to these sensitivities because KENO V.a does not calculate angular fluxes or flux moments, which are necessary for the calculation of all other sensitivity parameters.

To use this 3-D analysis tool, the user must produce a KENO V.a restart file containing flux data for both the forward and adjoint solutions of the same system. The cross-section library used by KENO V.a must also be available. The SAMS module uses the KENO V.a scalar fluxes and geometry input to produce group-wise sensitivity coefficients for each KENO V.a geometry region. These are presented on an energy-integrated basis for each region and also for the entire system. Group-wise sensitivity data are written to a separate file that can be used for plotting sensitivity profiles.

Sensitivity coefficients generated with SAMS have been compared with those generated with SEN1 and SEN2. The results are nearly identical for both $\bar{\nu}$ and χ sensitivities. The development of SAMS continues with the focus primarily on adding angular flux and flux moment calculational methods to KENO V.a. Once these solutions can be obtained reliably, it will be possible to fully implement the FORSS sensitivity methodology into 3-D Monte Carlo calculations.

Sensitivity Coefficient Results

Sensitivity analyses can be excellent tools for understanding the underlying characteristics of systems. As an example of the information that can be gleaned from sensitivity plots, a total of twenty systems were analyzed using the 1-D sensitivity tool. These systems include six systems [11] with $U(2)F_4$ fuel and fourteen systems of $U(11)O_2$ with H/X values from 0 to 1000. The total (energy-integrated) sensitivity coefficients of k_{eff} for each of these systems to the ^{235}U fission, ^{238}U capture, and H total cross sections are plotted versus H/X in Fig. 3. This curve gives a visual representation of the similarities between the various systems. The sensitivity trend plots for the 11 wt % UO_2 systems look very similar to those of the 2 wt % UF_4 systems above an H/X of 200. The UF_4 curves are given for actual systems that had H/X values in the range 200 to 1000. The $U(11)O_2$ systems are "artificial" systems, that is to say that no such measurements exist, and they were generated for calculational comparison purposes. Each of these systems is a critical sphere with H/X values corresponding to 0, 3, 5, 10, 20, 40, 80, 200, 300, 400, 500, 600, 800, and 1000. The curves below an H/X of 200 exhibit large changes in slope along with maxima and minima. Clearly the curves indicate that the systems are changing rapidly at low values of H/X.

In order to understand the details behind the trends shown in the previous two plots, it is necessary to look at the individual sensitivity plots. The sensitivity information for ^{235}U fission seen in Fig. 4 for the 11 wt % systems clearly shows the differences between the systems with H/X values of 0, 3, and 5. The ^{235}U fission cross section of importance is very different for the H/X = 0 system. However, the systems with H/X values of 3 and 5 appear already quite similar. It can be seen from similar plots (not shown) for systems with H/X values of 10, 20 and 40 that *none* of these systems is similar to the other. Systems with H/X values above 200 show nearly identical sensitivities with respect to the ^{235}U fission cross sections. This region corresponds to the approximately linear region in the sensitivity trend plots shown in Fig. 3. Thus, these results confirm that for linear portions of the trend plots, the systems are indeed very similar with respect to that material. The underlying physical phenomenon appears to be the similarity in the system spectra. Thus far, we have only looked at the detailed sensitivity plots for ^{235}U fission cross sections. Similar studies were carried out for the ^{238}U capture and hydrogen-scattering cross sections by combining the various systems into 'local' groups of H/X values of 0, 3 and 5; H/X values of 10, 20, and 40; H/X values of 80, 200, and 300; and H/X values of 400, 600, and 1000. In each case, the individual scattering and capture profiles appear to have relatively constant spectral shapes, giving rise to the conclusion of very similar systems with respect to the hydrogen cross sections. Indeed, for the individual scattering and capture portions, the spectral shapes of these sensitivity profiles are relatively constant over *most* of the H/X range from about 10 to 1000.

Analyses such as the preceding studies are essential for understanding the mechanisms in the systems and are also valuable in determining the similarities between systems. However, for general validation studies, a more concise method is needed to convey the same information in a more compact manner [12].

Uncertainty Analysis Theory

The determination of uncertainties in the calculated values of the system multiplication factor is accomplished by two steps: the estimation/processing of uncertainties in the underlying cross-section data and the propagation of those uncertainties to the system k_{eff} value. The techniques for processing cross-section uncertainty data are well known [13,14] and will not be discussed here.

Once uncertainty information for the cross sections for all materials and reaction processes that are important to the systems one wishes to analyze is available, it is then possible to estimate the uncertainty in the system multiplication factor due to these data uncertainties. If we denote the matrices of uncertainty information for all of the cross sections as $C_{\alpha\alpha}$ and the sensitivity matrices relating changes in each constituent material and process to the system k_{eff} as S_k, the uncertainty matrix for the system k_{eff} values, C_{kk} is given as:

$$C_{kk} = S_k \, C_{\alpha\alpha} \, S_k^T. \tag{9}$$

The S_k matrix is I × N, where I is the number of critical systems being considered, N is the number of nuclear data parameters in the problem. Typically, N is the number of material/reaction processes times the number of energy groups. The $C_{\alpha\alpha}$ matrix is an N × N matrix, with the resulting C_{kk} matrix I × I. The C_{kk} matrix consists of variance values for each of the critical systems under consideration (the diagonal elements), as well as the so-called "covariance" between systems (the off-diagonal elements). These off-diagonal elements represent the shared or common variance, hence the term covariance, between the various systems. For presentation these off-diagonal elements are typically divided by the square root of the corresponding diagonal elements (i.e., the respective standard deviations) to generate a correlation coefficient matrix. The physical interpretation of the correlation matrix is as follows: a value of zero represents no correlation between the systems; a value of unity represents full correlation between the systems, and a value of −1 represents a full anticorrelation. Shown in Table 1 is a correlation matrix for the fourteen $U(11)O_2$

artificial systems discussed earlier. Since the diagonal elements are unity, each diagonal element is replaced by the corresponding fractional standard deviation.

The standard deviation values shown in Table 1 range from 0.87 to 1.91%. The highest uncertainties correspond to the lowest H/X values because a harder spectrum enhances the sensitivity to the higher-energy cross sections, which are usually less well known than the thermal values. Note that the off-diagonal elements are given as correlation coefficients, denoted as c_k, which indicate the fraction of the variance common to both systems. By setting a c_k criterion of 0.8 or greater as indicating similar systems, conclusions are reached that are nearly identical to those based on comparison of the sensitivity profiles. For example, the H/X of 0 system is only similar to the H/X of 3 system and then only marginally so (c_k is 0.8328). We see that for H/X values between 5 and 40, the similar systems include only the two or three neighboring systems with higher or lower H/X values. For systems with H/X values of 80 to 1000, the systems are typically similar to the nearest five neighboring systems with higher H/X values and to the two nearest neighboring systems with lower H/X values.

Table 1: Cross-Section Cross Correlation Coefficients for 11% Experiments

Critical system	11%-0	11%-3	11%-5	11%-10	11%-20	11%-40	11%-80	11%-200	11%-300	11%-400	11%-500	11%-600	11%-800	11%-1000
11% H/X=0	**.0191**													
11% H/X=3	.8328	**.0185**												
11% H/X=5	.7379	.9818	**.0188**											
11% H/X=10	.6011	.9205	.9725	**.0188**										
11% H/X=20	.4887	.8409	.9161	.9784	**.0176**									
11% H/X=40	.4067	.7562	.8403	.9253	.9763	**.0151**								
11% H/X=80	.3428	.6585	.7392	.8327	.9094	.9698	**.0128**							
11% H/X=200	.2800	.5240	.5888	.6760	.7696	.8705	.9526	**.0106**						
11% H/X=300	.2633	.4751	.5315	.6115	.7058	.8157	.9148	.9832	**.0099**					
11% H/X=400	.2557	.4452	.4953	.5687	.6604	.7727	.8798	.9668	.9846	**.0095**				
11% H/X=500	.2517	.4329	.4688	.5359	.6235	.7349	.8453	.9448	.9717	.9845	**.0091**			
11% H/X=600	.2490	.4076	.4482	.5097	.5927	.7014	.8123	.9200	.9543	.9742	.9847	**.0089**		
11% H/X=800	.2432	.3755	.4076	.4567	.5278	.6265	.7331	.8514	.8991	.9330	.9576	.9734	**.0087**	
11% H/X=1000	.2353	.3452	.3697	.4071	.4652	.5509	.6484	.7702	.8277	.8731	.9097	.9367	.9752	**.0087**

These c_k values are felt to be most appropriate for correlation with error trends in a criticality safety validation analysis because they are essentially the sensitivities to the individual cross sections weighted by their uncertainties. Thus, the c_k values represent the systems similarity with respect to materials with highest sensitivity/uncertainty combination.

Summary

This paper has described the various 1-D, 2-D and 3-D sensitivity and uncertainty analysis tools that have been developed at Oak Ridge National Laboratory for general use by the criticality safety community. The resulting tools are expected to be available with the next general release of the SCALE system. Examples of the uses of these tools for determining system similarity for criticality safety data validation tasks have also been described. Further results from the application of these tools are given in an accompanying paper, which is given as Ref. 12.

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```
=sen1
U(2)F4 H/X=294  raffety and milhalczo u(2)f4-2 unreflected (case 14)
44group         infhommedium
u-235  1 0 1.3303e-4 end
u-238  1 0 6.4370e-3 end
h      1 0 3.9097e-2 end
c      1 0 1.8797e-2 end
f      1 0 2.6280e-2 end
end comp
spherical  end
1 38.50 160
end zone
isn=8
stop
end
```

Figure 1. Example SEN1 input for infhommedium cross-section preparation.

```
=sen1x
u(10)o2 p=.7 1-d  leu-comp-therm-032  case 1
44groupndf5                  latticecell
u-234          1  0.0 1.7636e-5 293 end
u-235          1  0.0 2.1577e-3 293 end
u-236          1  0.0 1.53e-5 293 end
u-238          1  0.0 1.951e-2 293 end
o              1  0.0 4.4661e-2 293 end
fe             2  0.0 5.8894e-2 293 end
cr             2  0.0 1.6469e-2 293 end
ni             2  0.0 8.1061e-3 293 end
si             2  0.0 1.3551e-3 293 end
mn             2  0.0 1.299e-3 293 end
c              2  0.0 2.3766e-4 293 end
ti             2  0.0 4.4713e-4 293 end
h2o            3  1.0 293 end
h2o            4  1.0 293 end
end comp
triangpitch .7 .416 1  3  .51 2  .43 0  end
cylindrical   end
500 16.44 32
4   46.44 30
end zone
isn=10
stop
end
```

Figure 2. Example SEN1 input for latticecell cross-section preparation.

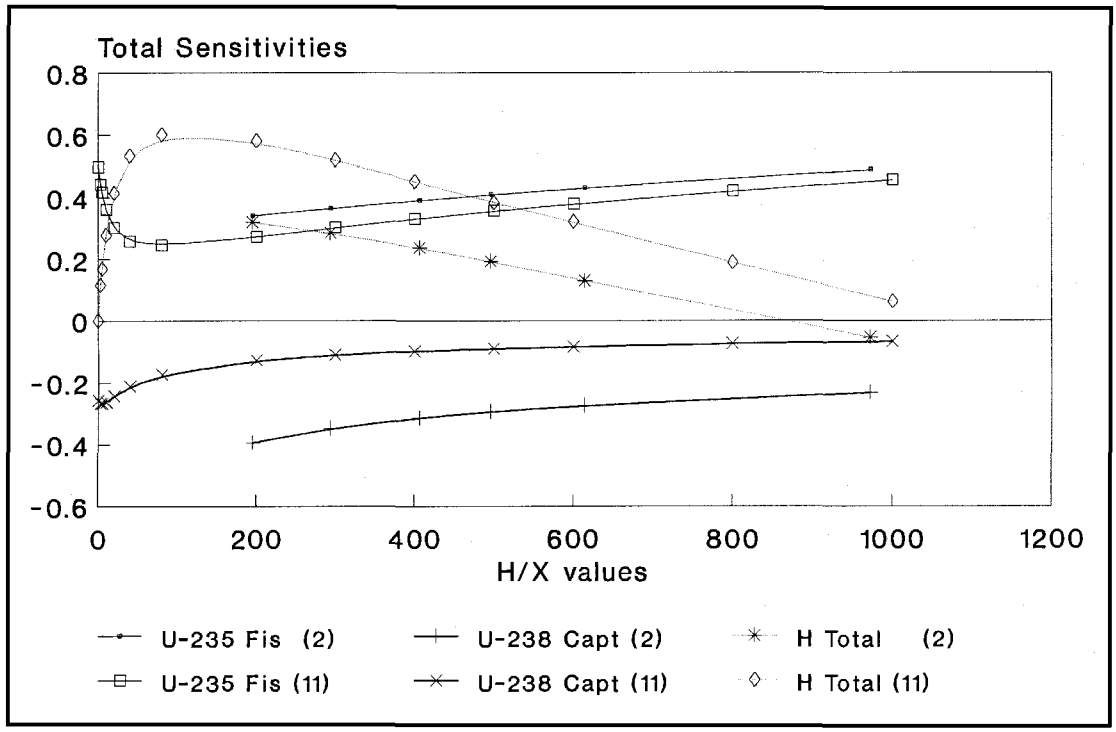

Figure 3. Total sensitivity trends with H/X for $U(2)F_4$ and $U(11)O_2$ systems.

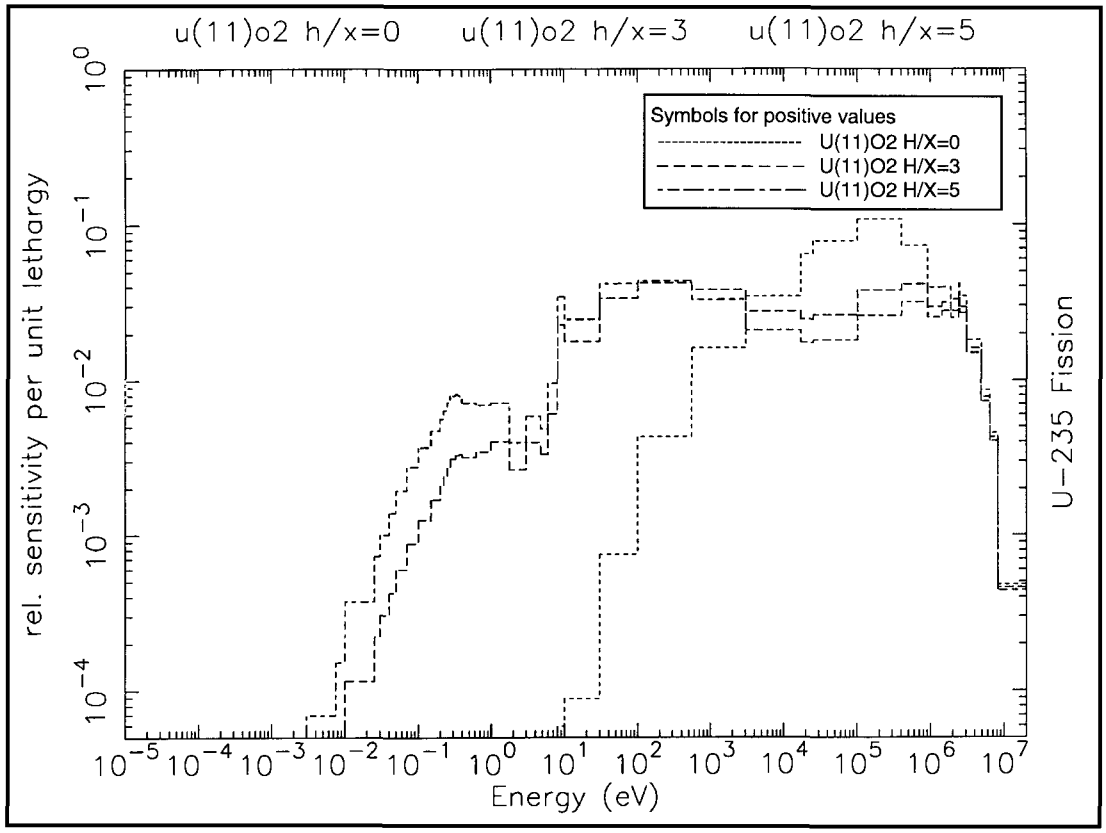

Figure 4. Comparison of ^{235}U fission sensitivities for $U(11)O_2$ systems with H/X values of 0, 3, and 5.