STOCHASTIC AND DATA UNCERTAINTY QUANTIFICATION OF MCNP PREDICTED NUCLIDE CONCENTRATIONS IN FUEL BURNUP SIMULATIONS

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ABSTRACT

Monte Carlo N-Particle transport code (MCNP) is used widely to simulate nuclear fuel burnup and depletion because it is efficient in solving the radiation transport equation for complex geometries. MCNP simulates fuel burnup and estimates the concentrations of actinides and fission products, which are useful in nuclear safeguards monitoring. The MCNP fuel burnup simulation does not estimate the uncertainties in the predicted nuclide concentration caused due to the uncertainties in nuclear data and the stochastic radiation transport methodology used. The nuclide concentration is calculated through CINDER 90 nuclide generation and depletion module, which uses the neutron reaction rates and flux values calculated by MCNP. Stochastic uncertainties in the neutron reaction rates and flux values are calculated by MCNP, which introduces stochastic uncertainty in the nuclide concentration, but this uncertainty is not propagated through each burnup time step to estimate the uncertainty in the nuclide concentrations predicted. This uncertainty is in addition to the systematic uncertainty caused due to the nuclear data. The neutron reaction rates can be broken down into neutron flux, number density, and microscopic neutron interaction cross section terms. The number density and neutron flux are provided by MCNP, and the neutron flux term calculated will contain stochastic uncertainty; however, the microscopic cross sections used in MCNP will contain systematic uncertainties. Propagating the effects of both sources of uncertainties using a Backward Euler numerical scheme allows for the reporting of the total relative error in the predicted nuclide concentrations. The MCNP depletion calculation uses a one group neutron flux and therefore a one group microscopic neutron cross section is necessary to find the neutron reaction rates. The microscopic neutron cross sections are dependent on the energy spectrum of the flux in the fuel burnup simulation. The process of acquiring these microscopic cross sections and weighting them by the flux is automated in our study for estimating both stochastic and systematic uncertainties. The final product of the study will be a software that calculates and reports stochastic, systematic, and total nuclide concentration uncertainties by utilizing the MCNP fuel burnup simulation output file.

INTRODUCTION

There are two types of uncertainties that are discussed in this paper related to the Monte Carlo N-particle (MCNP) fuel burnup simulations [1]. One is the stochastic uncertainty and the other is systematic uncertainty. Stochastic uncertainty results from the stochastic nature of radiation transport simulation carried out in the MCNP simulations. Systematic uncertainty results from discrepancies in nuclear data sets used by the MCNP code. The MCNP code is used to simulate fuel burnup and predict concentrations of actinides and fission products. During the fuel burnup simulations, nuclide concentration uncertainties emanating from the stochastic and systematic uncertainties are not estimated and predicted at any fuel burnup time step. These nuclide concentrations are calculated through CINDER 90 nuclide generation and depletion module in MCNP. Stochastic uncertainty in the neutron reaction rates and flux values are calculated by MCNP. MCNP uses a predictor-corrector scheme to determine the nuclide concentrations. The predictor step solves the neutronics using material composition at the beginning of the depletion time step. The corrector step solves the neutronics again using the depleted nuclide composition from the predictor step. The nuclide generation and depletion in CINDER90 module use Eq. (1)

$$\frac{dN_x}{dt} = \sum_i \gamma_{x,i}\sigma_{f,i}\phi N_i - \sigma_a \phi N_x - \lambda_x N_x + \sum_j \lambda_j Y_j N_j + \sum_k \sigma_k \phi N_k \qquad \text{---------} \ (1)$$

$\frac{dN_x}{dt}$ = Derivative of the number density of nuclide x with respect to time

$\gamma_{x,i}$ = Fission yield of target nuclide x from fission isotope i

$\sigma_{f,i}$ = The fission microscopic cross section

ϕ = Flux

N_i = The number density of fission isotope i

σ_a = The absorption microscopic cross section

λ_x = The decay constant of target nuclide x

λ_j = The decay constant of isotope j that produces istope x

Y_j = The branching ratio of j that produces x

N_j = The number density of isotope j

σ_k = The microscopic cross section for all non n reactions that produce isotope x

N_k = The number density of isotope k

The main objectives of this research are to determine the stochastic relative error for the MCNP-predicted nuclide concentrations. Also, to account for nuclear data uncertainty in the MCNP-predicted nuclide concentrations, which will give the systematic relative error. The overall goal is to combine both to calculate the total error in MCNP nuclide concentrations.

METHODOLOGY

The Backward Euler method Eq. (2) is used to propagate and estimate the stochastic and systematic uncertainties [2]. The 'y' term in this case will be the nuclide concentration and the sub-time step size in the python script used to implement the Backward Euler method is 0.01 days. The Backward Euler method tends to undershoot because of the indexing. So, for example, y_{k+1} is the nuclide concentration at time step 2 and y_k is the concentration at time step 1 and then Δt*f is the production and depletion of that concentration over time step 2. The Backward Euler method is a method of solving ordinary differential equations. The method is done 1000 times by using Gaussian sampling of the mean neutron reaction rates and its predicted standard deviation calculated by the MCNP code at each fuel burnup timestep. This repetition of 1000 times enable us to estimate the nuclide concentration mean value and its associated standard deviation. This method has been used in stochastic uncertainty calculations [3], which will be used in systematic uncertainty calculations. The MCNP models used to test the Backward Euler method and the automation of the process to acquire the one-group microscopic neutron interaction cross sections are a Pressurized water reactor (PWR) fuel assembly and a Fast breeder reactor (FBR) fuel subassembly. The PWR fuel enrichment chosen is 3.2% ^{235}Uranium with water as the coolant. The FBR assembly uses a Mixed oxide (MOX) fuel with sodium as coolant. The two test cases were chosen based on the differences in the neutron energy spectrum so that the problem dependent one-group neutron interaction microscopic cross section generations can be tested for two very different cases.

$$\frac{dy}{dt} = f(t, y, x_1, x_2, x_3, \dots, x_n) \qquad \text{---------} \ (2)$$

$$\mathrm{y}(0) = y_o$$

$$y_{k+1} = y_k + \Delta t f(t_{k+1}, y_{k+1}, x_{1,k+1}, x_{2,k+1}, x_{3,k+1}, \dots, x_{n,k+1})$$

Δt = sub time step

k=sub step number

t= time

y = what is being solved

$x_{n,k+1}$ = the variables for *y* evaluated at sub step *k*

RESULTS AND DISCUSSION

Preliminary steps have been completed by considering the nuclear data uncertainty by generating a one-group microscopic neutron interaction rate, which was tested for the case of ^{137}Cs production. Neutron reaction rates are used to determine components of the nuclide depletion equations. The one-group microscopic neutron interaction cross sections play a role in the neutron reaction rates. The one-group microscopic neutron interaction cross sections for nuclides of interest are estimated by weighting them by the F4 tally (cell neutron flux in the material being depleted) neutron flux spectrum using Eq. (3).

$$< \sigma_{avg} >= \frac{\int_{1E-11}^{20MeV} \phi_i(E)\sigma_i(E)dE_i}{\int_{1E-11}^{20MeV} \phi_i(E)dE_i} \qquad \text{---------} \ (3)$$

i = 252 groups

The one-group microscopic neutron interaction cross sections must be adjusted according to temperature dependence prior to the weighting by the neutron flux spectrum. Data is gathered from the International Atomic Energy Agency (IAEA) point temperature data files and available cross section and standard deviation data files from Java-based Nuclear Information Software (JANIS) [4]. The process of acquiring the one-group cross sections and weighting them by the neutron flux spectrum is automated in the python script developed. Figures 1 and 2 are 2-dimensional renderings (top and side views) created using Visual Editor software for the FBR hexagonal fuel subassembly and PWR fuel assembly test cases. Tables 1 and 2 are the results comparing two test cases and the two methods of calculating the one-group microscopic neutron fission cross sections of ^{235}U. The test cases are FBR subassembly and PWR fuel assembly.

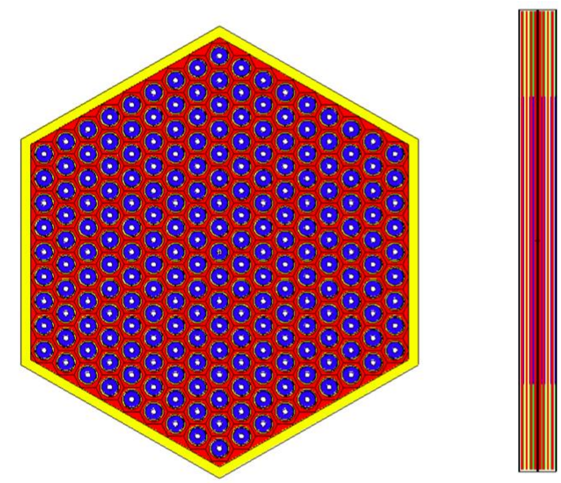

Figure 1. Top and side view of the FBR fuel subassembly modeled in MCNP.

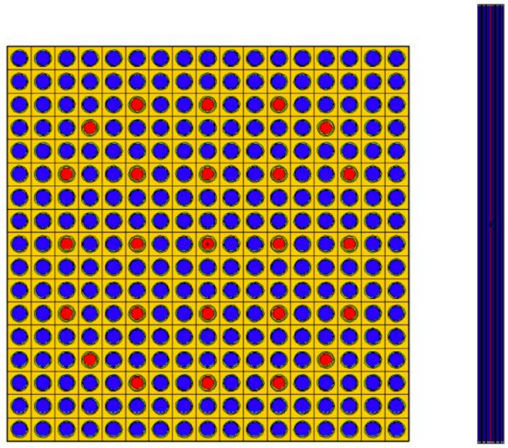

Figure 2. Top and side view of the PWR fuel assembly modeled in MCNP.

Table 1. One-group microscopic neutron fission cross section of ^{235}U generated by two methods for the FBR test case and the corresponding systematic data uncertainty.

Fast Breeder Reactor Assembly Excel Results				Fast Breeder Reactor Assembly Python Results			
^{235}U (n,f)				^{235}U (n,f)			
Time Step	1-Group Cross Section (barns)	1-Group Cross Section Error	Systematic Relative Error	Time Step	1-Group Cross Section (barns)	1-Group Cross Section Error	Systematic Relative Error
1	1.88	7.72E-03	0.41%	1	1.88	7.71E-03	0.41%
2	1.88	7.71E-03	0.41%	2	1.88	7.69E-03	0.41%
3	1.88	7.68E-03	0.41%	3	1.88	7.67E-03	0.41%

Table 2. One-group microscopic neutron fission cross section of ^{235}U generated by two methods for the PWR test case and the corresponding systematic data uncertainty.

Pressurized Water Reactor Assembly Excel Results				Pressurized Water Reactor Assembly Python Results			
^{235}U (n,f)				^{235}U (n,f)			
Time Step	1-Group Cross Section (barns)	1-Group Cross Section Error	Systematic Relative Error	Time Step	1-Group Cross Section (barns)	1-Group Cross Section Error	Systematic Relative Error
1	41.2	5.44E-02	0.13%	1	41.2	5.44E-02	0.13%
2	40.7	5.37E-02	0.13%	2	40.7	5.37E-02	0.13%
3	40.5	5.35E-02	0.13%	3	40.5	5.35E-02	0.13%

Tables 3 and 4 are the results comparing two test cases and the two methods of calculating the one-group microscopic neutron capture cross sections of ^{137}Cs.

Table 3. One-group microscopic neutron capture cross section of ^{137}Cs generated by two methods for the FBR test case and the corresponding systematic data uncertainty.

Fast Breeder Reactor Assembly Excel Results				Fast Breeder Reactor Assembly Python Results			
^{137}Cs (n,y)				^{137}Cs (n,y)			
Time Step	1-Group Cross Section (barns)	1-Group Cross Section Error	Systematic Relative Error	Time Step	1-Group Cross Section (barns)	1-Group Cross Section Error	Systematic Relative Error
1	1.52E-02	1.09E-03	7.20%	1	1.52E-02	1.09E-03	7.20%
2	1.52E-02	1.09E-03	7.20%	2	1.52E-02	1.09E-03	7.20%
3	1.52E-02	1.09E-03	7.20%	3	1.52E-02	1.09E-03	7.20%

Table 4. One-group microscopic neutron capture cross section of ^{137}Cs generated by two methods for the PWR test case and the corresponding systematic data uncertainty.

Pressurized Water Reactor Assembly Excel Results				Pressurized Water Reactor Assembly Python Results			
^{137}Cs (n,y)				^{137}Cs (n,y)			
Time Step	1-Group Cross Section (barns)	1-Group Cross Section Error	Systematic Relative Error	Time Step	1-Group Cross Section (barns)	1-Group Cross Section Error	Systematic Relative Error
1	2.84E-02	1.28E-03	4.50%	1	2.84E-02	1.28E-03	4.50%
2	2.82E-02	1.27E-03	4.50%	2	2.82E-02	1.27E-03	4.50%
3	2.81E-02	1.26E-03	4.50%	3	2.81E-02	1.26E-03	4.50%

The ^{235}U one-group neutron interaction cross sections demonstrate the difference between the two neutron energy spectra for the two MCNP mode test cases and the of ^{137}Cs one-group neutron interaction cross sections displays a comparatively large systematic relative error. A proof-of-concept python script was developed to calculate the systematic uncertainty in the nuclide concentration for ^{137}Cs buildup considering its buildup chain. The results for the two test cases (FBR and PWR) are displayed in Tables 5 and 6.

Table 5. ^{137}Cs concentration generated for the FBR test case and the corresponding systematic data concentration relative uncertainty.

FBR Systematic Error for ^{137}Cs		
MCNP Time Step (days)	Concentration Average (atoms·cm^{-3})	Concentration Relative Uncertainty
0.3	2.83E+16	0.23%
0.3	8.57E+16	0.24%
0.4	1.52E+17	0.24%

Table 6. ^{137}Cs concentration generated for the PWR test case and the corresponding systematic data concentration relative uncertainty.

PWR Systematic Error for ^{137}Cs		
MCNP Time Step (days)	Concentration Average (atoms·cm^{-3})	Concentration Relative Uncertainty
0.3	9.90E+15	0.13%
0.3	3.00E+16	0.13%
0.4	5.31E+16	0.13%

CONCLUSIONS

A python script to estimate systematic and stochastic uncertainties using Backward Euler method is developed to go along with the MCNP predicted nuclide concentrations. The script contains the method for generating one-group neutron cross section those are required for computing neutron reaction rates for substitution in the nuclide buildup equation. The script was tested for two sample cases of PWR and FBR, specifically for the production of ^{137}Cs.

FUTURE WORK

The python script will be further developed to calculate the one-group microscopic neutron cross sections and will be integrated with the Backward Euler method to estimate systematic and stochastic uncertainties for the other nuclides of interest predicted by MCNP.

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