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Investigation of antineutrino spectral anomaly with reactor simulation uncertainty

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ABSTRACT

Recently, three successful antineutrino experiments (Daya Bay, Double Chooz, and RENO) measured the neutrino mixing angle θ_{13}; however, significant discrepancies were found, both in the absolute flux and spectral shape. Much effort has been expended investigating the possible reasons for the discrepancies. In this study, Monte Carlo-based sampling was used to evaluate the fission fraction uncertainties. We found that fission cross-section uncertainties are an important source of uncertainty for ^{235}U, ^{239}Pu, and ^{241}Pu, but for ^{238}U, elastic and inelastic cross-sections are more important. Among uncertainty related to manufacturing parameters, fuel density is the main uncertainty; however, the total manufacturing uncertainty was very small. The uncertainties induced by burnup were evaluated through the atomic density uncertainty of the four isotopes. The total fission fraction uncertainties from reactor simulation were 0.83%, 2.24%, 1.79%, and 2.58% for ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu, respectively, at the middle of the fuel cycle. The total fission fraction uncertainty was smaller than the previously derived value of 5%. These results are helpful for studying the reactor antineutrino anomaly and precisely measuring the antineutrino spectrum in the Daya Bay antineutrino experiment.

1. Introduction

Antineutrinos produced by nuclear reactors are used to study neutrino oscillations and search for signatures of nonstandard neutrino interactions in the kilometer-baseline reactor experiments Daya Bay [1], Double Chooz [2], and RENO [3]. Antineutrinos can also be used to monitor reactor conditions to safeguard operations [4]. Although the neutrino mixing angle θ_{13} was successfully determined by these experiments, comparison of the measured spectra of kilometer- and short-baseline experiments to the most up-to-date predictions showed significant discrepancies both in the absolute flux and spectral shape. A 2.9σ deviation was found in the measured inverse beta decay positron energy spectrum compared to predictions. In particular, an excess of events at energies of 4–6 MeV was found in the measured spectrum [5–7], with a local significance of 4.4σ. These results have brought home the notion that neutrino fluxes are not as well understood as had been thought. At present, it is not clear what physical processes give rise to the neutrino spectra bump. Much effort has been focused on the reactor antineutrino anomaly, which arose from improved calculations of the antineutrino spectra derived from a combination of information from nuclear databases with reference β spectra [8–11].

In reactor antineutrino experiments, the following formula is usually applied to calculate the antineutrino spectrum for the reactor:

$$S(E_\nu) = \frac{W_{th}}{\sum_j f_j e_j} \sum_i f_i S_i(E_\nu), \quad (1)$$

where W_{th} (MeV/s) is the reactor thermal power, f_j is the fission fraction associated with each isotope (^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu), e_j is the thermal energy release per fission event for each isotope, and $S_i(E_\nu)$ is a function of the $\bar{\nu}_e$ energy E_ν signifying the $\bar{\nu}_e$ yield per fission for each isotope. Therefore, the bump in the reactor neutrino spectra may be caused mainly by one isotope or by some important fission event [12–14].

The antineutrino flux is an important source of uncertainty associated with measurements in reactor neutrino experiments. To evaluate uncertainties in reactor simulations, the calculated concentrations of each isotope using different reactor simulation codes were compared with a benchmark [15], and a proximate method was proposed to determine the fission fraction uncertainty using concentration uncertainty. Using the Takahama-3 benchmark and the largest burnup sample calculated with MURE and DRAGON, the concentration differences of each isotope between the calculated value and experimental data were about 5% [16]. The fission fractions for the Daya Bay reactor were also simulated using DRAGON and compared with results obtained with the SCIENCE code [17]. It was found the average deviation for ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu were 0.71%, 4.2%, 2.1%, and 3.5% [18], respectively. However, the fission fraction uncertainty as a function of burnup was not reported. To investigate this question and determine the correlation coefficient of the fission fraction of different isotopes, a new Monte Carlo-based method was proposed using the one-group fission

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cross section and concentration of each isotope [19]. That paper also discussed a coefficient to correlate the results with the burnup function. However, these previous studies did not solve the problem of identifying the main source of uncertainty in the fission fractions. Thus, the purpose of this study was to investigate fission fraction uncertainties induced by neutron cross section and fuel manufacturing uncertainties in a reactor simulation.

This paper is structured as follows. The Monte Carlo-based sampling method used for evaluation of uncertainties of fission fractions is introduced in Section 2. To generate a library of samples for the transport calculation, the Sensitivity and Uncertainty Analysis Code for Light Water Reactor (SUACL) was developed, and the Three Mile Island Unit 1 (TMI-1) benchmark and a mixed oxide fuel (MOX) test were used to verify the code, as described in Section 3. Section 4 discusses how all the reaction types for the four isotopes and other important isotopes, atomic density uncertainties induced by burnup, and manufacturing parameters were taken into account to evaluate uncertainty of fission fractions. The last section provides conclusions.

2. Monte Carlo-based sampling method

In reactor simulations, we always focus on the neutronics characteristics because the fission power and chain reaction are determined by the neutron flux. Therefore, reactor simulation is generally called a neutronics calculation. The simulation results are affected by various uncertainties, including material composition, geometry, operation conditions, measured plant data, neutron cross section, and model approximations. In this study, the impact of cross section and fuel manufacturing parameter uncertainty on the fission fraction results was evaluated.

Propagation of cross section uncertainties to core characteristics has been traditionally evaluated by the sandwich variance formula [20,21]. There are three difficulties in using the sandwich formula for pressurized water reactor (PWR) uncertainty analysis: complicated calculation sequence, nonlinear effects of thermal hydraulics and burnup, and the large number of input and output parameters. Recently, the Monte Carlo-based sampling method has attracted attention, since it can avoid these major difficulties. The procedures for uncertainty estimation of the fission fraction for antineutrino experiments using Monte Carlo-based sampling method is shown Fig. 1. Generally, cross sections can be divided into basic and integral sections. The integral cross sections are composed of basic cross sections. The cross section uncertainties are stored in their covariance data. Different approaches to evaluating a nuclear data library may lead to different analysis results. The covariance data used in this study were produced using the NJOY code [22] based on the ENDF/B-VII.1 [23] and JENDL-4.0 libraries [24]. The covariance matrices for ^{235}U and ^{238}U for the (n,γ) cross section are shown in Fig. 2. Other important inputs are the engineering parameters for fuel/assembly manufacturing [25], which are crucial to the simulation model. The uncertainty of these parameters can propagate to the results and reduce their accuracy. The SUACL code was designed specifically to analyze the uncertainty of neutron cross section and manufacturing parameters.

In the Monte Carlo-based sampling method, samples are randomly taken from the parent population. In this study, multi-group microscopic cross sections were randomly sampled using the covariance matrix. Multi-group means that the neutron energy have been divided many segments, and each segment is called one group. Sets of sampled cross sections approximately represent the distribution of the microscopic cross sections due to the nature of measurement error. Cross sections are randomly perturbed [26] by

$$\sigma_{x,g}^{per} = P_{x,g} \times \sigma_{x,g} \tag{2}$$

where $P_{x,g}$ is the perturbation factor for a microscopic cross section, $\sigma_{x,g}^{per}$ is the perturbed microscopic cross section, $\sigma_{x,g}$ is the unperturbed microscopic cross section in the original cross section library, x is the type of cross section, and g is the energy group. The total sample number is set 100 for each reaction type of each isotope. Multi-group, microscopic cross sections in the original cross section library were perturbed by Eq. (2) to generate the perturbed cross section library. A procedure for generating vectors of dependent random variables consistent with a given covariance matrix involves performing a spectral decomposition of the matrix.

Table 1
Parameters of TMI-1 and MOX cell.

Parameters	MOX cell	TMI-1 cell
Fuel material	$(U,Pu)O_2$	UO_2
Gap material	N/A	He gas
Clad material	Zircaloy-4	Zircaloy-4
Moderator	H_2O	H_2O
Fuel pellet/mm	9.020	9.391
Gap thickness/mm	0.0	0.955
Clad thickness/mm	0.380	0.673
Unit cell pitch/mm	12.60	14.427

$$\mathbf{\Sigma} = \mathbf{V} \times \mathbf{D} \times \mathbf{V^T}. \tag{3}$$

The matrix of relative covariance, $\mathbf{\Sigma}$, is decomposed into three matrices, where $\mathbf{V}$ is a matrix whose columns are eigenvectors of $\mathbf{\Sigma}$ and $\mathbf{D}$ is a diagonal matrix of eigenvalues that correspond to the eigenvectors in $\mathbf{V}$. Matrix $\mathbf{\Sigma^{1/2}}$ is defined as

$$\mathbf{\Sigma^{1/2}} = \mathbf{V} \times \mathbf{D^{1/2}} \times \mathbf{V^T} \tag{4}$$

where $D^{1/2}$ is a diagonal matrix whose elements are the roots of the elements in $\mathbf{D}$. The perturbed factor can be calculated using Eq. (5) [27].

$$\mathbf{P(\Sigma)} = \mathbf{\Sigma^{1/2}G(0,1)} + \mathbf{I}, \tag{5}$$

where $\mathbf{G}$ is a vector of n normally distributed dependent random variables with a mean of zero and standard deviation of 1 and $\mathbf{I}$ is a identity matrix.

3. Validation of SUACL for PWR pin cell analysis

The SUACL code evaluates fission fraction uncertainty in the reactor simulation using Monte Carlo sampling [28]. The perturbed nuclear library is generated by SUACL, as shown in Fig. 1, and then the reactor simulation code DRAGON [29] applies the perturbed nuclear library to do the transport calculation. To verify the SUACL code, the TMI-1 PWR fuel cell benchmark [25] and MOX cell were used. Parameters of the TMI-1 and MOX datasets are shown in Table 1. The uncertainty of the infinity multiplication factors for the TMI-1 and MOX cells, which were evaluated using SUACL, are shown in Table 2. We found that the SUACL results were consistent with those obtained with other codes, such as TSUNAMI-1D, for the TMI-1 and MOX cells.

4. Reactor simulation uncertainty for antineutrino experiment

Four isotopes, namely ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu, are important to antineutrino experiments because more than 99.0% of the antineutrinos are emitted from these isotopes. To predict antineutrino flux for an antineutrino experiment, the fission fraction of each isotope is needed according to Eq. (1). The process of evaluating the fission fraction depends on how neutrons are handled in the reactor simulation. In general, the neutron behavior is described by a neutron transport equation and the cross sections of neutrons with matter are the coefficients of the transport equation. The fission fraction of isotopes f_i (i = ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu) can be defined as

$$f_i = \frac{N_i \sum_{g=1}^{G} \sigma_{i,g,f} \phi_g}{\sum_i N_i \sum_{g=1}^{G} \sigma_{i,g,f} \phi_g}, \tag{6}$$

where $\sigma_{i,g,f}$ is the microscopic cross section of isotope i in group g, g is the neutron energy number, G is the total neutron energy group