Physics-based Uncertainty Quantification for $\text{ZrH}_x$ Thermal Scattering Law

Weixiong Zheng

Nuclear Engineering,
Texas A&M University,
2013 ANS Winter Meeting
Synopsis

- Background
- Motivations
- Introduction
- Parameterized Models and Model Tests
- Calibration based on MCNP Simulations
- Conclusions and Future Work
- References
Background

- Basics for TRIGA Reactors
  - TRIGA reactors are thermal reactors using U-ZrH$_x$ fuel
  - Thermal neutrons, which are heavily affected by thermal scattering, are important

- Scattering Complexity
  - Binding forces affect thermal neutron scattering cross sections
  - Different ZrH$_x$ compositions (different x) result in different bindings, and then different vibration frequency distributions (also called phonon spectrum), thus different scattering cross sections
  - Different temperatures result in different bindings, thus different phonon spectra and cross sections

- Existing data
  - ENDF based on Slaggie’s study on ZrH$_2$; IKE simplified the H phonon spectrum for ZrH$_2$; the evaluations use phonon spectra at RT for all temperatures

- Possible Problem
  - x=1.523 (i.e. ZrH$_{1.523}$)
  - Accurate scattering cross scattering data specific for x=1.523 at multiple temperature are needed
Motivations

- Establish valid parameterized phonon spectrum models for H and Zr in ZrH$_x$
- Find sensitive quantities of interest in the TRIGA simulations which could be used to calibrate the parameters in the phonon spectrum models
- Tabulate the reasonably accurate thermal scattering law table for TRIGA at TAMU for future reactor simulation uses
Introduction

• Theory

Double differential scattering cross section

\[ \sigma(E' \rightarrow E, \Omega' \cdot \Omega) = \frac{\sigma_b}{4\pi kT} \sqrt{\frac{E}{E'}} S(\alpha, \beta) \]

where \( \alpha \equiv \frac{E + E' - 2\mu\sqrt{EE'}}{AkT} \) and \( \beta \equiv \frac{E - E'}{kT} \).

The \( S(\alpha, \beta) \) is the scattering law. It can be given by:

\[ S(\alpha, \beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\beta t} e^{-\gamma(t)} dt \]

where

\[ \gamma(t) = \alpha \int_{-\infty}^{\infty} P(\beta)[1 - e^{-i\beta t}] e^{-\beta/2} d\beta \]

and \( P(\beta) = \frac{\rho(\beta)}{2\beta \sinh(\beta/2)} \)

The \( \rho(\beta) \) is the phonon spectra in terms of \( \beta \).
Introduction

- Theory
  Double differential scattering cross section

\[
\sigma(E' \rightarrow E, \Omega' \cdot \Omega) = \frac{\sigma_b}{4\pi kT} \sqrt{\frac{E}{E'}} S(\alpha, \beta)
\]

where \( \alpha \equiv \frac{E+E'-2\mu\sqrt{EE'}}{AkT} \) and \( \beta \equiv \frac{E-E'}{kT} \).

The \( S(\alpha, \beta) \) is the scattering law. It can be given by:

\[
S(\alpha, \beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\beta t} e^{-\gamma(t)} dt
\]

where

\[
\gamma(t) = \alpha \int_{-\infty}^{\infty} P(\beta)[1 - e^{-i\beta t}] e^{-\beta/2} d\beta \quad \text{and} \quad P(\beta) = \frac{\rho(\beta)}{2\beta \sinh(\beta/2)}
\]

The \( \rho(\beta) \) is the phonon spectra in terms of \( \beta \).
Introduction

• Theory

Double differential scattering cross section

$$\sigma(E' \rightarrow E, \Omega' \cdot \Omega) = \frac{\sigma_b}{4\pi kT} \sqrt{\frac{E}{E'}} S(\alpha, \beta)$$

where $\alpha \equiv \frac{E+E'-2\mu\sqrt{EE'}}{AkT}$ and $\beta \equiv \frac{E-E'}{kT}$.

The $S(\alpha, \beta)$ is the scattering law. It can be given by:

$$S(\alpha, \beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\beta t} e^{-\gamma(t)} dt$$

where

$$\gamma(t) = \alpha \int_{-\infty}^{\infty} P(\beta)[1 - e^{-i\beta t}] e^{-\beta/2} d\beta \text{ and } P(\beta) = \frac{\rho(\beta)}{2\beta \sinh(\beta/2)}$$

The $\rho(\beta)$ is the phonon spectra in terms of $\beta$. 
Introduction

• Theory

Double differential scattering cross section

\[ \sigma(E' \to E, \Omega' \cdot \Omega) = \frac{\sigma_b}{4\pi kT} \frac{\sqrt{E}}{\sqrt{E'}} S(\alpha, \beta) \]

where \( \alpha \equiv \frac{E+E'-2\mu\sqrt{EE'}}{AkT} \) and \( \beta \equiv \frac{E-E'}{kT} \).

The \( S(\alpha, \beta) \) is the scattering law. It can be given by:

\[ S(\alpha, \beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\beta t} e^{-\gamma(t)} \, dt \]

where

\[ \gamma(t) = \alpha \int_{-\infty}^{\infty} P(\beta)[1 - e^{-i\beta t}]e^{-\beta/2} \, d\beta \]

and \( P(\beta) = \frac{\rho(\beta)}{2\beta \sinh(\beta/2)} \).

The \( \rho(\beta) \) is the phonon spectra in terms of \( \beta \).
Parameterized Model and Model Tests

- Some existing spectra
Parameterized Model and Model Tests

- Some existing spectra
  - Phonon spectra for H in ZrH_x
  - Phonon spectra for Zr in ZrH_x
  - Debye distribution

Phonon spectra for H in ZrH_x

- Acoustic mode
- Optical mode

Phonon spectra for Zr in ZrH_x

- Acoustic mode
- Optical mode
Parameterized Model and Model Tests

- Some existing spectra

Debye distribution

Phonon spectra for H in ZrH$_x$
- Pink: Gaussian distribution
- Black dashed line: three Gaussian specific for ZrH$_{1.58}$

Phonon spectra for Zr in ZrH$_x$
- ENDF-VII
- Debye spectrum
Parameterized Model and Model Tests

- Some existing spectra

Phonon spectra for H in ZrH$_x$

- Debye Temperature
- Optical Peak Position
- Branching Ratio
- FWHM

Phonon spectra for Zr in ZrH$_x$

- Debye Temperature

Acoustic mode

Optical mode
Parameterized Model and Model Tests

- Parameterized Phonon Spectra (PPS)
  - For H:
    \[
    \rho(\omega)_{\text{H}} = \begin{cases} 
    \frac{3b}{2T_{\text{DH}}^3} \omega^2, & \omega < T_{\text{DH}} \\
    \frac{3b}{2T_{\text{DH}}^3} (\omega - 2T_{\text{DH}})^2, & T_{\text{DH}} \leq \omega \leq 2T_{\text{DH}} \\
    \frac{c(b)}{\sqrt{2\pi\sigma}} \exp \left[ -\frac{(\omega - p)^2}{2\sigma^2} \right], & 2T_{\text{DH}} \leq \omega \leq \omega_{\text{max,H}} 
    \end{cases}
    \]
  - For Zr:
    \[
    \rho(\omega)_{\text{Zr}} = \begin{cases} 
    \frac{r(1+c)}{T_{\text{DZr}}^{1+c}} \omega^c, & \omega \leq T_{\text{DZr}} \\
    \frac{(1+c)r}{T_{\text{DZr}}} \exp \left[ (1+c)^r \left( 1 - \frac{\omega}{T_{\text{DZr}}} \right) \right], & T_{\text{DZr}} \leq \omega \leq \omega_{\text{max,Zr}} 
    \end{cases}
    \]
  - Parameters:
    \[
    T_{\text{DH}}, b, p, \text{FWHM}, r, c \text{ and } T_{\text{DZr}}
    \]

<table>
<thead>
<tr>
<th>Parameters</th>
<th>FWHM/meV</th>
<th>(b)</th>
<th>(p)/meV</th>
<th>(T_{\text{DH}})/meV</th>
<th>(T_{\text{DZr}})/meV</th>
<th>(r)</th>
<th>(c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ranges</td>
<td>[25,31]</td>
<td>[1/361,1/91]</td>
<td>[127,147]</td>
<td>[16,24]</td>
<td>[16,24]</td>
<td>[0.4,0.8]</td>
<td>[2,2.8]</td>
</tr>
</tbody>
</table>
Parameterized Model and Model Tests

- Some existing spectra for H in ZrH_x
Parameterized Model and Model Tests

- Latin Hypercube sampling design (LHS)
  - Sampled 3000 sets of parameters over the seven dimensional input space
  - Generated 3000 realizations of phonon spectrum based on the LHS design
  - Each realization gives unique phonon spectra for H and Zr, respectively.
Parameterized Model and Model Tests

- For each realization, we get a unique phonon spectrum
Parameterized Model and Model Tests

- Model Tests: $\bar{\mu}_{\text{ZrH}_{1.84}}$
Parameterized Model and Model Tests

- Model Tests: $\sigma_{g'}^{\text{tot, ZrH}_{1.5229}}$
Calibration based on MCNP Simulations

- Calculation and Analysis Procedure

- Parameterized phonon spectra generation
- Thermal scattering data generations and simulations
- Sensitivity tests and calibration based score estimations
Calibration based on MCNP Simulations

- Calculation and Analysis Procedure

Generate phonon spectra

- Parameter ranges
  - Latin Hypercube Sampling
  - Parameter sets
    - Spectrum generator
      - PPS spectra

Thermal scattering data generations and simulations

Sensitivity tests and calibration based score estimations
Calibration based on MCNP Simulations

- Calculation and Analysis Procedure

Generate phonon spectra

Data generations and simulations

<table>
<thead>
<tr>
<th>Parameter ranges</th>
<th>Latin Hypercube Sampling</th>
<th>Parameter sets</th>
<th>Spectrum generator</th>
<th>PPS spectra</th>
</tr>
</thead>
</table>

NJOY

Thermal Scattering Cross Sections

MCNP

QOIs

Sensitivity tests and calibration based score estimations
Calibration based on MCNP Simulations

Calculation and Analysis Procedure

1. Parameter ranges
2. Latin Hypercube Sampling
3. Parameter sets
4. Spectrum generator
5. PPS spectra

Data generations and simulations

1. NJOY
2. Thermal Scattering Cross Sections
3. MCNP
4. QOIs

QOI sensitivities analyses

1. ANOVA
2. Significant factors for specific QOIs
3. Cross-validations to test indicated sensitivities
4. Calibrations based on score estimations
5. Appropriate parameter ranges

Calibrations based on score estimation
Calibration based on MCNP Simulations

- Geometry in MCNP
  - TRIGA lattice model at TAMU
  - 3000 MCNP simulations
- QOIs
  - $\rho$: reactivity
  - FRD: fission rate density

```
Fuel
Central zirconium rod
SS304 cladding
Water moderator
Axial graphite reflector
```
Calibration based on MCNP Simulations

- Scatterplot on reactivity ($\rho$)-FRD plane
  - Reference results are surrounded by PPS model results
  - Two reference results stay in different parts of the plot
Calibration based on MCNP Simulations

- ANOVA indicated reactivity is sensitive to the parameters
- Cross-validation for reactivity $\rho$
  - To test the indicated sensitivities
  - 2400 realizations were used to get the regression models based on the parameters
  - Use the regression models to predict outputs for the rest 600 realizations and compare the predictions with the simulations
Calibration based on MCNP Simulations

- Sensitivity for reactivity $\rho$
  - Sensitive to proposed parameters
  - Most sensitive to two main factors
  - Main factors:
    - Optical peak position in H
    - Branching ratio of acoustic mode to optical mode in H
  - By “main”, it means QOIs are most sensitive to it (them)
Calibration based on MCNP Simulations

- **Geometry in MCNP**
  - Simplified full-core TRIGA model at TAMU
  - Configuration: to make TRIGA near critical ($k_{\text{eff}} = 1.00000 \pm 0.00013$ with ENDF)

- **QOIs**
  - $\rho$: reactivity (not the phonon spectrum!)
  - $\Lambda$: neutron mean generation time
  - $\alpha_{T_{\text{fuel}}}$: fuel temperature feedback coefficient
  - $\beta_{\text{eff}}$: effective delayed neutron fraction
  - $R_{\text{abs}}$: ex-core detector absorption rate
Calibration based on MCNP Simulations

- Cross-validation test the significances of the factors indicated by ANOVA
  - 1331 MCNP simulation results in total
    - 1064 for forming regression models
    - 267 for comparing simulations and predictions based on regression models
- Complex model (right upper): based on all “significant” factors from ANOVA
- Main-factor model (right lower): based on optical peak position and branching ratio of acoustic mode to optical mode in H
- Reactivity is most sensitive to these two factors
Calibration based on MCNP Simulations

• Calculation and Analysis Procedure

Parameterized phonon spectra generation

Thermal scattering data generations and simulations

QOI sensitivity analyses

Calibrations based on score estimations

Appropriate parameter ranges
Calibration based on MCNP Simulations

- Calibration
- MC quantities of interest (QOIs): given in forms of normal distributions
- Score estimation: overlaps of QOI distributions
  - It measures how close each realization is to the reference QOI

\[ f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \]

Target distribution for QOI

Particular realization distribution for QOI
Calibration based on MCNP Simulations

- Score Estimation for Calibration
  - ENDF and IKE scattering data were used as calibration examples
  - $X_2$: standardized form of branching ratio of acoustic mode to optical mode in $\text{H in ZrH}_x$
  - $X_3$: standardized form of optical peak position in $\text{H in ZrH}_x$
  - They have different high score regions
  - What if we have multiple QOIs sensitive to proposed parameters?
Calibration based on MCNP Simulations

- Score Estimation for Calibration
  - ENDF and IKE scattering data were used as calibration examples
  - They have different high score regions
- What if we have multiple QOIs sensitive to proposed parameters?
  - Multiplications of multiple score distributions
  - Calibrated parameter ranges shrink
Calibration based on MCNP Simulations

- An example of the products
Conclusions and Future Work

- **Model tests:**
  - It would be reasonable to hypothesize PPS models for ZrH$_x$ phonon spectra

- **Methodology:**
  - NJOY-MCNP chain is compatible with this UQ study;
  - ANOVA and cross-validations are effective to determine the main-factor affecting QOIs and find the relationship between the parameters and QOIs;
  - Score estimation may be appropriate to take the calibration.

- **QOI sensitivities:**
  - Several QOIs (e.g. $\rho$, $\alpha_{T_{\text{fuel}}}$, $\Lambda$, etc.) are found to be sensitive to proposed parameters

- **Future work:**
  - Investigate in-core neutron detectors to further constrain the parameters in the model.
  - Calibrate parameters for TRIGA reactor at TAMU for different temperatures.
  - Tabulate $S(\alpha, \beta, T)$ for TRIGA reactor at TAMU
References


• Thank you!