Effective Physics-based Uncertainty Quantification for ZrH_x Thermal Neutron Scattering in TRIGA Reactors

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TRIGA reactor and ZrH_x thermal scattering in TRIGA reactor facts

- TRIGA reactor: A type of thermal reactor utilizing U-ZrH_x fuel material for its good moderation and large negative temperature feedback coefficient due to the presence of ZrH_x
- Scattering complexity: H concentration, x, in ZrH_x affects the scattering cross section
  - It affects the bond types of atoms in ZrH_x solid lattice
  - Different bonds result in distinct phonon spectra of Zr and H in ZrH_x, which result in different cross sections[5]
  - Total scattering cross section measurement captured the effects from changing ZrH_x composition[1]
- Existing data: Slaggie (1960s) suggested centered force model based on lattice dynamics research assuming composition of ZrH_2, with which ENDF data was calculated[8]
- Potential data problem: TRIGA at Texas A&M University has a concentration of 1.523

Connection between phonon spectrum and thermal scattering

The thermal scattering cross section could be written as[3, 4]:

$$\sigma(E' \to E, \mu) = \frac{\sigma_{\mathrm{b}}}{4\pi kT}\sqrt{\frac{E}{E'}}S(\alpha, \beta), \tag{1}$$

The functional $S(\alpha, \beta)$ is the scattering law calculated via:

$$S(\alpha, \beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\hat{t}\ e^{i\beta\hat{t}} \exp\left\{-\alpha \int_{-\infty}^{\infty} d\beta' \ \frac{f(\beta')\left[1 - e^{-i\beta'\hat{t}}\right]}{2\beta' \sinh\left(\beta'/2\right)} e^{-\beta'/2}\right\} \tag{2}$$

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

- $f(\beta)$ is the dimensionless phonon spectrum as a function of β
- The connection between phonon spectrum and thermal scattering is via Eq. (2) and Eq. (1)[11, 10]

Aims

- Establish valid phonon spectra with user-controlled parameters
- Find sensitive quantities of interest (QOIs) in TRIGA simulations
- Develop algorithms for calibration
- With results from experiment (or surrogate experiment) of TRIGA at TAMU, calibrate plausible parameters and generate corresponding thermal scattering data of ZrH_x

Phenomenological spectra and parameterized model

Previous researchers tried using simple mathematical models to replace the ENDF spectra (or some modes in the spectra)[8, 5, 6].

- Roughly mimic the shape and position of modes in spectra
- It is flexible to manipulate the spectra because of its simple-math nature
- Such simplified models performs well or even better in comparison with experimental results after mode optimization (e.g. Mattes's model)

Phenomenological spectra and parameterized model

We proposed a seven-parameter parameterized phonon spectrum (PPS) model (as functions of energy transfer, ω, in units of eV)[11, 10]

For H:

$$f(\omega)_{\mathrm{H}} = \begin{cases} \frac{3b}{2T_{\mathrm{DH}}^3}\omega^2 & \omega < T_{\mathrm{DH}} \\ \frac{3b}{2T_{\mathrm{DH}}^3}(\omega - 2T_{\mathrm{DH}})^2 & T_{\mathrm{DH}} \le \omega \le 2T_{\mathrm{DH}} \\ \frac{g(b)}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(\omega-p)^2}{2\sigma^2}\right] & 2T_{\mathrm{DH}} \le \omega \le \omega_{\mathrm{max,H}}. \end{cases} \tag{3}$$

For Zr:

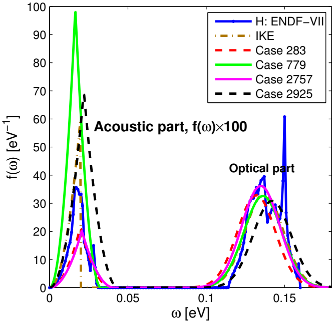
$$f(\omega)_{\mathrm{Zr}} = \begin{cases} \frac{r(1+c)}{T_{\mathrm{DZr}}^{1+c}}\omega^c & \omega < T_{\mathrm{DZr}} \\ \frac{(1+c)r}{T_{\mathrm{DZr}}} \exp\left[\frac{(1+c)^r}{1-r}\left(1 - \frac{\omega}{T_{\mathrm{DZr}}}\right)\right] & T_{\mathrm{DZr}} \le \omega \le \omega_{\mathrm{max,Zr}}. \end{cases} \tag{4}$$

Note:

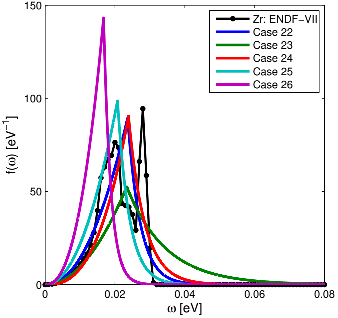
$$f(\omega)d\omega = f(\beta)d\beta \qquad \text{and} \qquad \beta = \frac{\omega}{kT} \tag{5}$$

Phenomenological spectra and parameterized model

- Used Latin Hypercube sampling (LHS) design to sample given numbers of parameter combinations
- Each combination specifies a realization of spectrum, which specifies a unique scattering cross section set



(a) H spectrum examples from 3000-set LHS designs



(b) Zr spectrum examples from 3000-set LHS designs

Sensitive QOIs and main parameters

LHS generated several sets of parameters, which are propagated through data generating and transport simulations to QOIs. Questions arise:

- Which QOI(s) is(are) sensitive to parameters?
- Which parameter affect QOI variations most?

Facts:

- Not all seven parameters are important, nor are the pairwise interactions
- Necessity in picking significant parameters out to simplify the problem

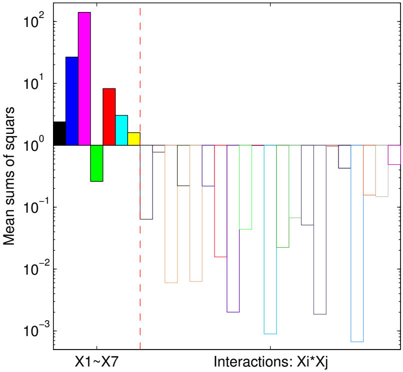
Dimension reduction example

- The ANOVA technique is used to discriminate the sensitive QOIs and significant parameters to those sensitive QOIs (see ex. for ρ)[7, 2, 9]
- The means of squared sums indicate the significances
- Current sensitive QOIs: reactivity ρ, mean neutron generation time Λ and fuel temperature coefficient α_{T}
- Significant parameters: branching ratio of acoustic mode in H model b, optical peak position in H model p

Dimension reduction example

Example of ANOVA mean of squared sums for ρ

- ρ is most sensitive to $X_2(b)$ and $X_3(p)$
- Dimension reduced from $(7 + 21) = 28$ to 2
- Insignificant ones are excluded from other statistical test results, e.g. F-test and p-value, included in ANOVA results



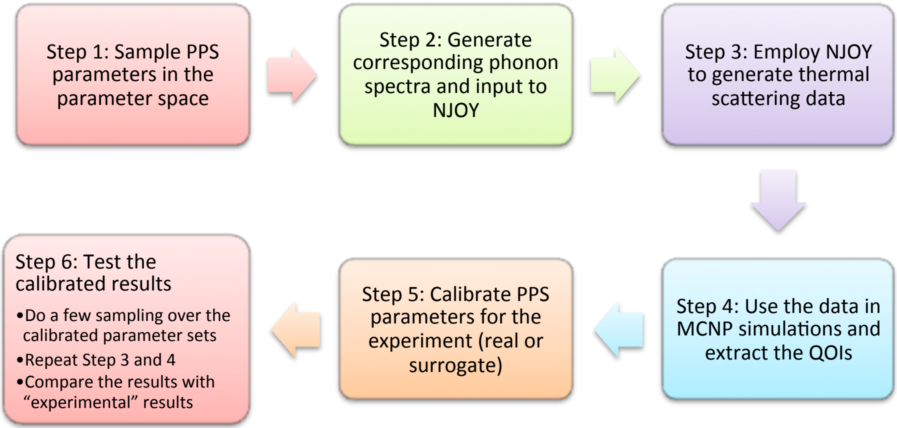
Section 2

What is calibration?

Calibration:

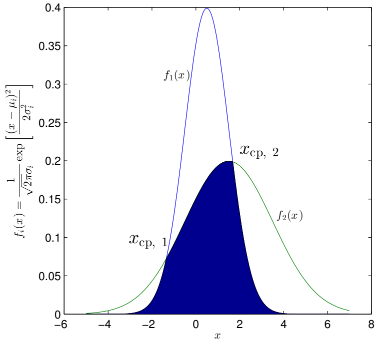
- With QOI values from experiments (or surrogates) and a bunch of simulation results, one could measure which sets of simulations are close to experiments
- Project those "close" sets into parameter space may calibrate plausible parameter ranges
- Simulations propagated from those calibrated subsets of parameters would present closer results to experiments

Flow chart


Step 1: Sample PPS parameters in the parameter space
Step 2: Generate corresponding phonon spectra and input to NJOY
Step 3: Employ NJOY to generate thermal scattering data
Step 4: Use the data in MCNP simulations and extract the QOIs
Step 5: Calibrate PPS parameters for the experiment (real or surrogate)
Step 6: Test the calibrated results
•Do a few sampling over the calibrated parameter sets
•Repeat Step 3 and 4
•Compare the results with "experimental" results

How to measure how close?

- MCNP simulations present results informed by normal distributions
- Assuming experimental results subject to normal distribution (surrogate with MCNP simulations is naturally subject to a normal.)
- Measures can be overlaps of simulation distributions and experiments
- We refer the measure to as score



Surrogate experiment

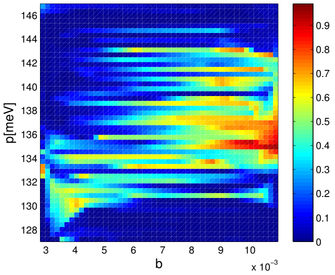
Facts:

- No experimental results currently
- Calibration frameworks are being developed and need testing to assure the feasibility and efficacy of such methodologies

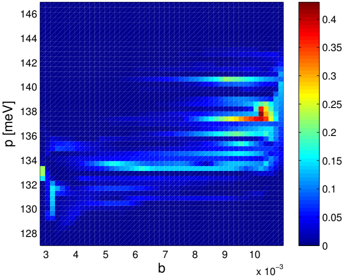
Solutions:

- Run simulations with existing data library, e.g. ENDF-VII or IKE
- Use the QOIs generated in such simulations as surrogates of experiments
- Perform calibrations of parameters in PPS model and test simulation results from data generated with the calibrated parameters
- One would claim the calibration framework works if the calibrated parameters generate close results to the surrogate results
- Such framework then would be used in calibration with real experiments

- Estimate the scores of all simulation with all QOIs individually
- Projection help capture significant subsets
- Calibration with multiple QOIs narrow down the size of such subsets



(c) Direct calibation with ρ



(d) Direct calibration with all three sensitive QOIs

Potential problem and solutions

Potential problems:

- Score distribution is sparse.
- Hard to tell if "low score" is really low score (could also be induced by lack of simulations)
- Not smooth

Solutions:

- Increase the number of simulations (not affordable)
- Emulate the mapping from parameters to QOIs
  - One can easily calculate a emulated QOI value at place where simulation is missing
  - Cheap
  - Smooth results

Emulation based calibrations

Properties wanted from emulators:

- Results informed by probability distribution functions (PDFs)
- Smooth results

Candidates:

- Gaussian process regression (GPR)
- Bayesian multivariate adaptive regression splines (BMARS)

Emulators

GPR:

- Generate a normal distribution of function values at user-defined input grids

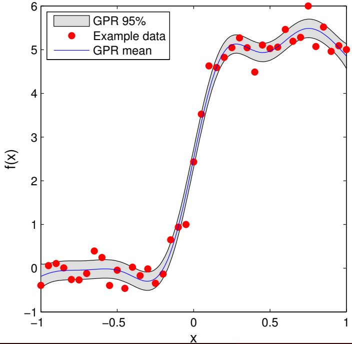
BMARS:

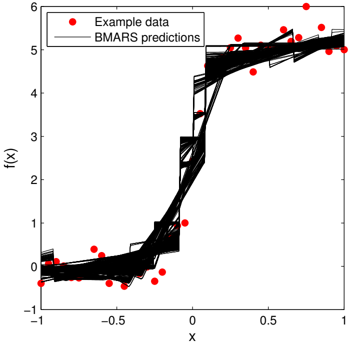
- Uses splines as basis functions and appropriate sum of such basis functions as prediction at user-defined grids
- Employed Markov Chain Monte Carlo (MCMC) in making inference
- Generates a bunch of predictions of functions at user-defined inputs. Each prediction is a draw of a posterior distribution

1D Emulation examples

Example model: logistic function with Gaussian distributed error.

- GPR (left) generates smooth mean results and corresponding standard deviations
- BMARS (right) generates a bunch of predictions of functions scratched from posterior distributions
- Both generate results informed by PDFs





BMARS scoring implementation

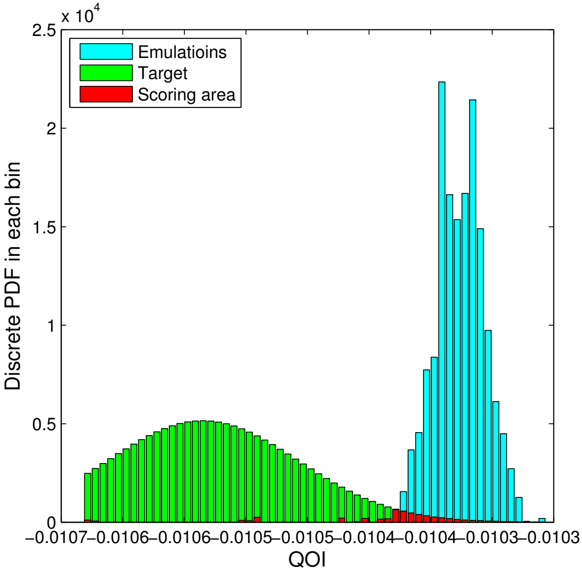
GPR generate normal distributions so original scoring strategy from direct calibration works for GPR. BMARS generates distributions in a "non-analytic" form:

- No explicit expression
- Original scoring not available

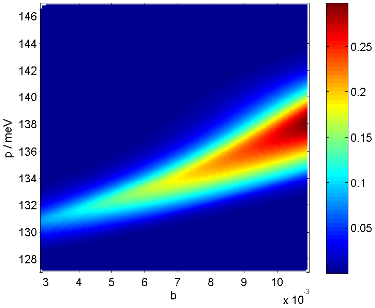
Solutions:

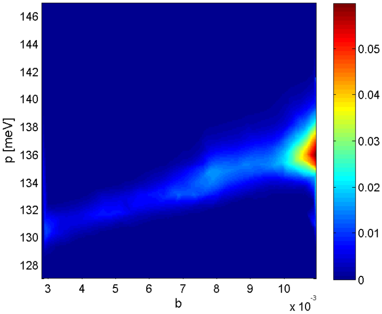
- Collect all the predictions and regenerate the posterior distribution discretely in several bins
- Discretize experimental distributions in the same bins
- Calculate the overlap bin by bin and sum the sub-scores up

BMARS scoring example



Following the calibration flow chart, we calibrated the two main parameters using GPR (left) and BMARS (right) with all three sensitive QOIs.





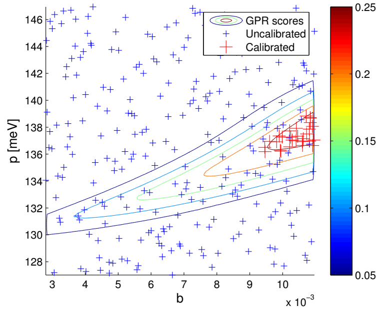
Section 3

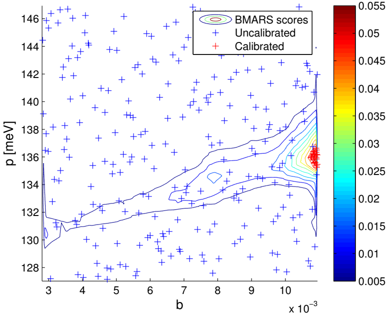
Sampling over calibrated parameters

Tests are needed to assure if those collections will result in close results to experiments. One could uniformly sample parameters over the high score regions. For the two main parameters, regions with scores higher than 0.8 times the highest scores are sampled and the other five are sampled together using LHS designs.

Sampling over calibrated parameters

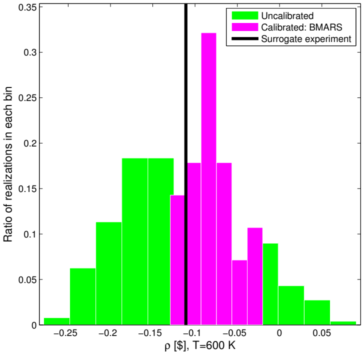
GPR sampling is on left and BMARS is on right.

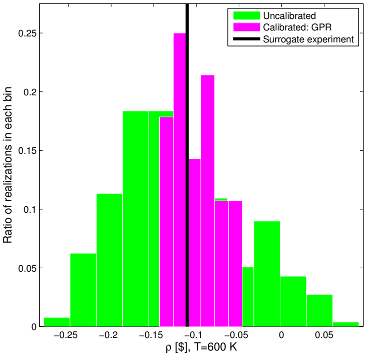




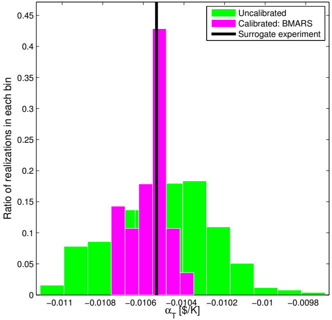
Testing results

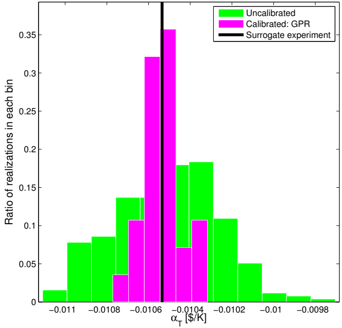
- Uncertainties of QOIs shrink
- Both emulators perform well



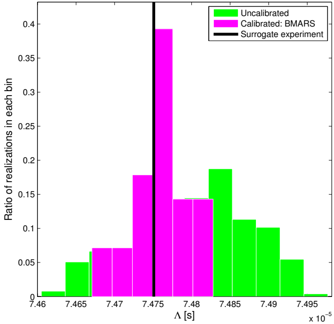


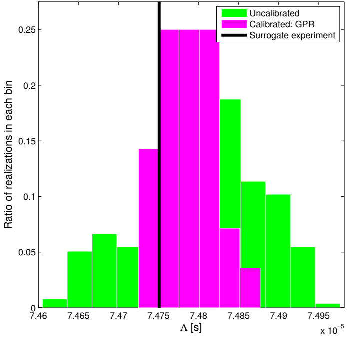
Testing results





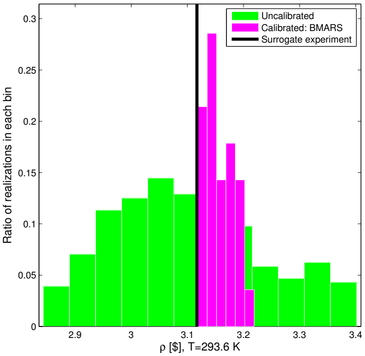
Testing results

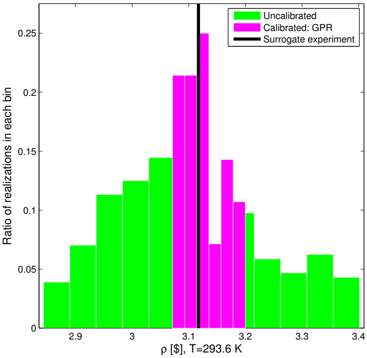




Testing results

Extension: no calibration done with reactivity at room temperature, but the simulation results with calibrated data works well





Section 4

Conclusions and future work

Conclusions:

- Developed emulator based calibration frameworks to calibrate parameters in previously proposed PPS spectra for ZrH_x
- Investigated the performances of two emulators in the calibration framework
- Calibrated most important two parameters, b and p, and with the calibrated results, MCNP simulation QOIs get close to the surrogate experiments

Future Work:

- Conduct real experiment on TRIGA at TAMU, and perform the calibration
- Explore techniques like GPR, LASSO regression etc. on parameter significance recognition
- Develop more simplified parameterized phonon spectra

Thanks!

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