Uncertainty quantification of optical model parameters using Unscented Transform Kalman filter technique

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Introduction

1. Uncertainty quantification of nuclear reaction model parameters is very important for calculating the uncertainties associated with the model predictions.
2. Model Parameters can be highly correlated.
3. Different techniques have been developed over time for the parameter estimation and uncertainty quantification, e.g. Extended Kalman Filter [1], χ^2 minimization [2], Monte Carlo techniques [3] etc.
4. All these techniques either reacquire to calculate the Jacobian of model equation with respect to parameters or take very large computational time and power.
5. In order to overcome these issues, we have used the Unscented Transform Kalman filter (UTKF) technique for the estimation of the optical model parameters and their uncertainties.

Optical model potential

1. We have used the Wood-Saxon phenomenological optical model potential.
2. The phenomenological optical model potential for the interaction of neutron and nucleus is generally given as:

$$\mathcal{U}(r,E) = -\mathcal{V}_V(r,E) - i\mathcal{W}_V(r,E) - i\mathcal{W}_D(r,E) +$$
$$\mathcal{V}_{SO}(r,E).1.\sigma + i\mathcal{W}_{SO}(r,E).1.\sigma \tag{1}$$

3. Different terms in this potential can be separated in to energy dependent and independent parts.
4. Energy independent part can be further simplified and we get various parameters v_1, v_2, v_3, w_1, w_2, d_1, d_2, d_3, $v_{so1}, v_{so2}, w_{so1}$, w_{so2} etc. which can be estimated by fitting the model predictions to the experimental results.
5. A detailed information can be found in ref.[7]

Unscented Transform Kalman Filter for parameter estimation

1. Consider a N dimensional vectors of the experimental measurements (d) and a prior estimate of the parameter vector (θ_0) of dimension L and their covariance matrix P_0.
2. Let $G(\theta_k)$ is the model. Here the index k represents the calculations for the k^{th} experimental data set $(k \in 1, 2, 3...\infty)$.
3. We can write the time update equations for estimating the parameters for k^{th} experimental data set as $\theta_k^- = \theta_{k-1}$, $P_{\theta_k}^- = P_{k-1} + R_{k-1}^r$.
4. For θ_k^- and $P_{\theta_k}^-$ we can generate a $L \times (2L+1)$ dimensional matrix (W) containing $(2L+1)$ sets of the sigma points using the unscented transform as given below.

$$W_{k|k-1} = \left[\theta_k^- \quad \theta_k^- + \sqrt{(L+\lambda)P_{\theta_k}^-} \quad \theta_k^- - \sqrt{(L+\lambda)P_{\theta_k}^-}\right] \tag{2}$$

Unscented Transform Kalman Filter for parameter estimation

1. The corresponding weights to these sigma points are given in the following equations

$$w_0^{(m)} = \lambda/L + \lambda \tag{3}$$

$$w_0^{(c)} = \lambda/(L+\lambda) + (1 - \alpha^2 + \beta) \tag{4}$$

$$w_i^{(m)} = w_i^{(c)} = 1/2(L+\lambda); \quad i = 1, 2, ...2L \tag{5}$$

2. Using $(2L+1)$ sets of the parameters, we can generate a $N \times (2L+1)$ dimensional matrix (D) containing $(2L+1)$ sets of model predictions using the model function $G(\theta_k)$.
3. From this ensemble we will calculate the quantities required to calculate the updated parameters and their covariance matrix given by following equations:

$$\theta_k = \theta_k^- + K_k(d_k - \hat{d}_k) \tag{6}$$

$$P_{\theta_k} = P_{\theta_k}^- - K_k P_{\hat{d}_k \hat{d}_k} K_k^T \tag{7}$$

Unscented Transform Kalman Filter for parameter estimation

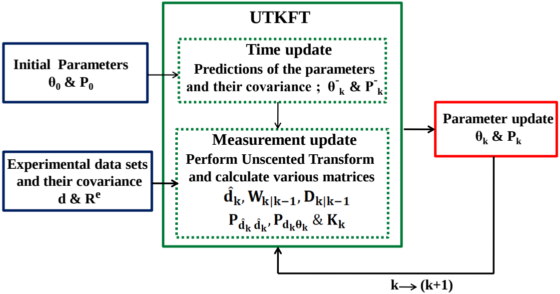
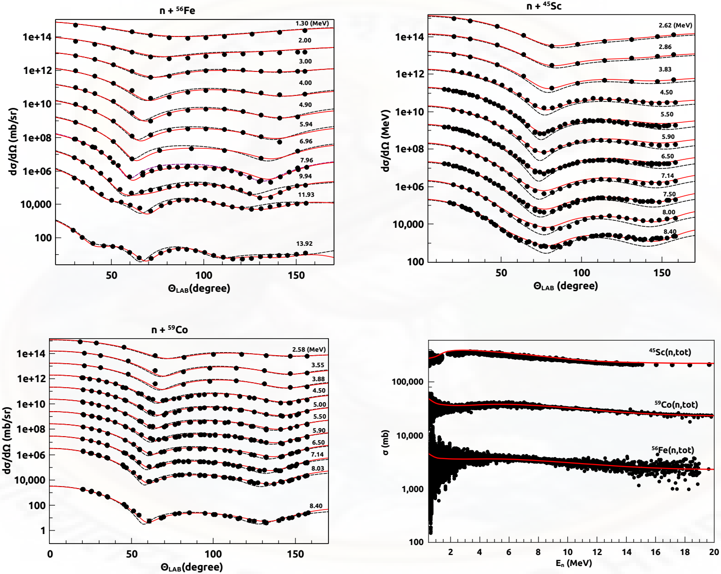


Figure: Flow chart for UTKF technique calculation for the present work.

Methodology

1. The DWBA calculations of the differential cross sections for the elastically scattered neutrons n+^{56}Fe, n+^{45}Sc and n+^{59}Co, were compared with the experimental data from EXFOR data library using the UTKF algorithm.
2. DWBA calculations were carried out using the TALYS nuclear reaction code.
3. We have determined 18 optical model parameters in this work.
4. We have used the global optical model parameters of Koning and Delaroche [5] as our initial estimate of the parameters, and an initial estimate of the uncertainties of these parameters was used from ref. [6].

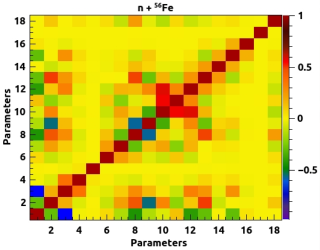
Results

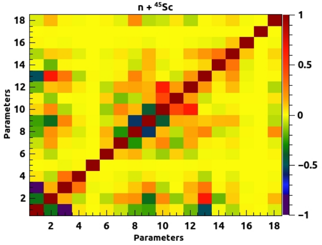

n + ^{56}Fe
dσ/dΩ (mb/sr)
ΘLAB(degree)
1.30 (MeV)
2.00
3.00
4.00
4.90
5.94
6.96
7.96
9.94
11.93
13.92
n + ^{45}Sc
dσ/dΩ (MeV)
ΘLAB (degree)
2.62 (MeV)
2.86
3.83
4.50
5.50
5.90
6.50
7.14
7.50
8.00
8.40
n + ^{59}Co
dσ/dΩ (mb/sr)
ΘLAB(degree)
2.58 (MeV)
3.55
3.88
4.50
5.00
5.50
5.90
6.50
7.14
8.03
8.40
^{45}Sc(n,tot)
^{59}Co(n,tot)
^{56}Fe(n,tot)
σ (mb)
En (MeV)

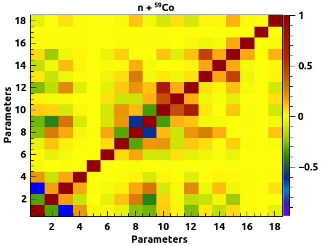
Results

1. The average χ^2 value of the model prediction for n+^{56}Fe reaction was 11.683 with initial set of parameters, while 4.796 with the new set of parameters.
2. The value of average χ^2 was 15.990 with initial parameters and 5.018 with the new parameters for n+^{45}Sc reaction.
3. Similarly for n+^{59}Co reaction the average χ^2 was 9.350 with the initial set of parameters, while 3.238 with the updated set of parameters.
4. The total reaction cross sections obtained through the new set of the optical model parameters are consistent with the experimental data.

Results


n + 56Fe
Parameters
Parameters
1
0.5
0
−0.5


n + 45Sc
Parameters
Parameters
1
0.5
0
−0.5
−1


n + 59Co
Parameters
Parameters
1
0.5
0
−0.5

Results

1. It is observed that parameters r_v and v_1 are strongly anti-correlated.
2. It is also observed that most of the parameters are anti-correlated (e.g. r_v and a_v, d_1 and a_d, a_d and a_v, r_d and a_d, r_d and w_2 etc.).
3. These observations are consistent with the observations of Duan *et al.,* [3], however they had used a completely different method for calculating the correlation matrix.
4. Some of the parameters also indicate strong positive correlations e.g. d_1 and d_2, d_1 and d_3, a_v and v_1, r_d and r_{so}, a_v and r_d etc. are positively correlated

Conclusion

1. In this study, we have determined the optical model parameters and their correlation matrices using the Unscented Transform Kalman Filter technique successfully.
2. The results clearly verify the use of the UTKF for the parameter estimation and uncertainty quantification of the optical model parameters.
3. This study clearly indicates that the optical model parameters are correlated to each other; hence these correlations should be considered while using them to predict the nuclear reaction cross sections.
4. The quality of the estimated optical model parameters and their uncertainties depends on the quality of the initial set of parameters, their uncertainties and the experimental data used for the estimation.

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Thank You!