

Production of Model Parameter Covariance Matrix for the LEAPR model of NJOY with the CONRAD code, preliminary results

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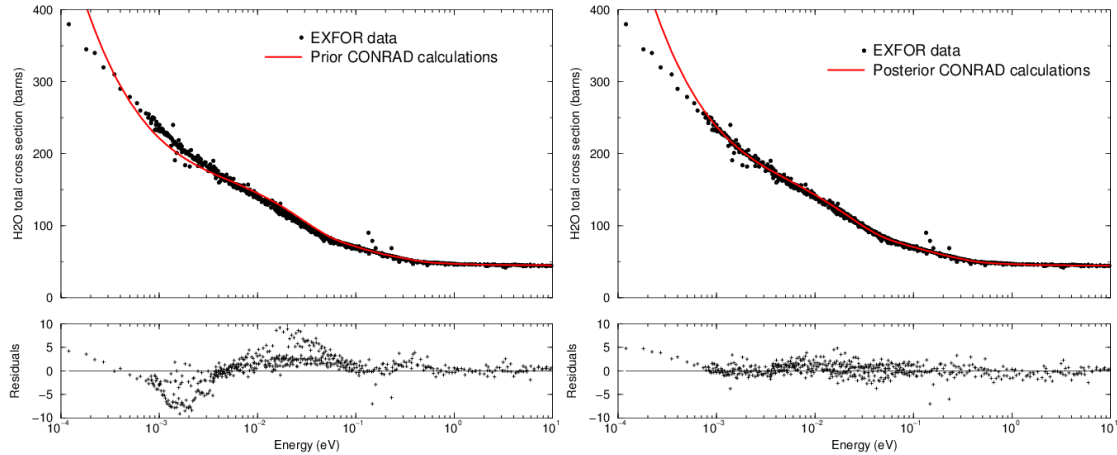


Figure 1 : Prior (left hand plot) and posterior (right hand plot) H2O total cross section calculated with the CONRAD code by using the IKE parameters established by Mattes.

The CONRAD code (developed at the CEA Cadarache [1]) was used to produce the covariance matrix between the model parameters involved in the LEAPR model of NJOY for H in H₂O. The model parameters established by Mattes (IKE) were used as prior parameters. Posterior uncertainties and covariances were obtained from a two-step CONRAD calculation. The first step consists in fitting experimental data. The second step consists in propagating the uncertainties of the experimental corrections with a marginalization procedure. Analytic or Bayesian Monte-Carlo methods (or a mix of both) can be used [2-5].

Preliminary results were obtained for H in H₂O by converting total cross sections retrieved from the EXFOR data base in transmission data. Prior and posterior results are shown in Figure 1. The posterior uncertainties and correlations between the model parameters are given in Table 1. They take into account uncertainties on the flight path length, time offset, normalisation, background, temperature and sample composition. Figure 2 represents the H in H₂O total cross section, relative uncertainty and correlation matrix calculated with the CONRAD code by using parameters listed in Table 1. The final covariance matrix is dominated by the uncertainties of the experimental corrections.

Parameters	values	correlation matrix
delta (eV)	= 0.00201 +/- 0.00013 (6.5%)	100
twt	= 0.02454 +/- 0.00304 (12.4%)	76 100
tbeta	= 0.47110 +/- 0.01626 (6.5%)	-18 14 100
en1 (eV)	= 0.22210 +/- 0.01627 (7.3%)	3 -49 -64 100
en2 (eV)	= 0.40770 +/- 0.03348 (8.2%)	63 28 -63 43 100
w1	= 0.17020 +/- 0.05116 (30.0%)	-49 -84 -60 81 9 100
w2	= 0.34250 +/- 0.05378 (15.7%)	61 92 40 -73 7 -97 100

Table 1 : Values, uncertainties and correlation matrix between the IKE parameters obtained from the marginalization procedure implemented in the CONRAD code.

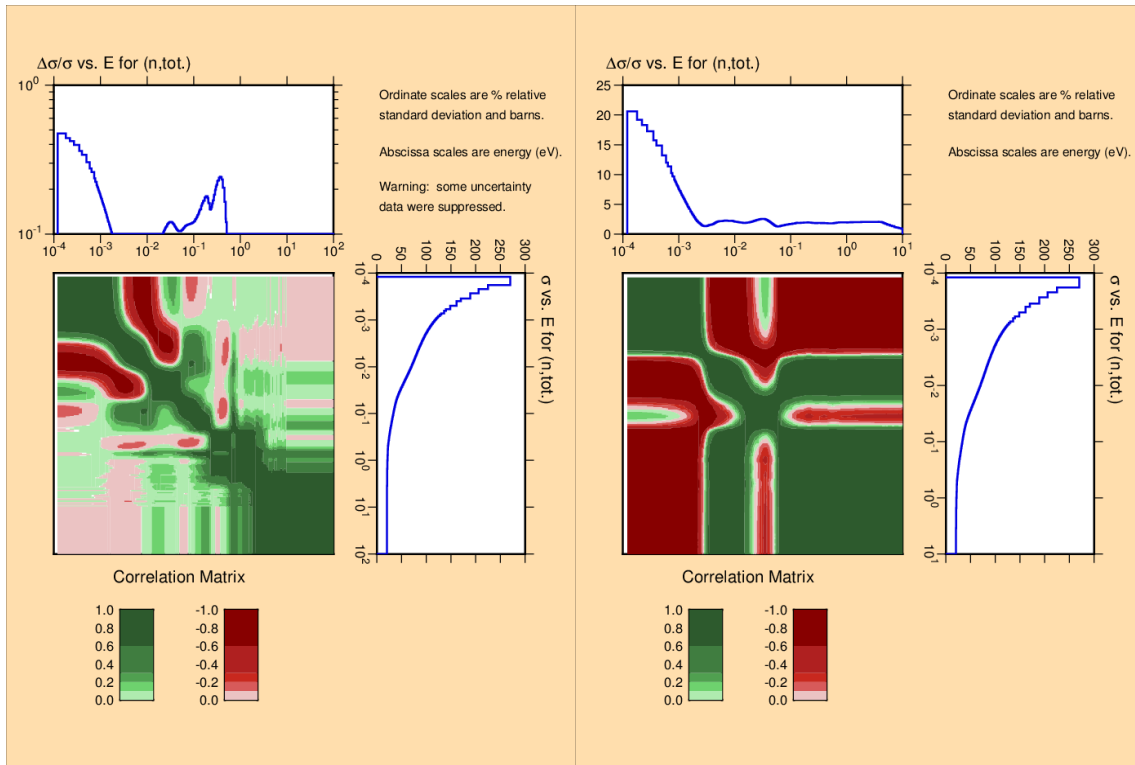


Figure 2 : H in H₂O total cross section, relative uncertainty and correlation matrix calculated with the CONRAD code. The left hand plot represents the contribution of the the « fitting » uncertainty. The right hand plot takes into account the uncertainties of the experimental corrections.

A better set of parameters cannot be obtained by using the IKE model (no diffusion component). A new analysis has to be performed by using a refine model (such as the CAB model) and double-differential data. The optimized CONRAD calculations will consist to start from the model parameters involved in Molecular Dynamic calculations.

References

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- [5] C. De Saint Jean et al., Evaluation of Cross Section Uncertainties Using Physical Constraints: Focus on Integral Experiments, Nucl. Data Sheets 123, 178 (2015)