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OECD-NEA Workshop on Future Criticality Safety Research Needs

Use of covariance data for reactor applications.

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- Sensitivity and Uncertainty Analysis
- Examples of Application
- New Covariance Data
- Perspectives
- Conclusions

Sensitivity and uncertainty analysis have played an important role in nuclear reactor (core, fuel cycle, shielding) analysis for more than forty years.

Major applications were made for:

- **uncertainty estimates,**
- **design optimization,**
- **determination of target accuracy requirements,**
- **adjustment of input parameters,**
- **evaluations of the "representativity" of an experiment with respect to a reference design configuration.**

For any integral parameter:

$$I_S = \langle \sigma_S \Phi \rangle$$

sensitivity coefficients to nuclear data variations can be calculated using GPT (Generalized Perturbation Theory):

$$\frac{\sigma}{\langle \sigma_S \Phi \rangle} \frac{d\langle \sigma_S \Phi \rangle}{d\sigma} = \sigma \left\{ \frac{\left\langle \left(\frac{\partial \sigma_S}{\partial \sigma} \right) \Phi \right\rangle}{\langle \sigma_S \Phi \rangle} - \left\langle \tilde{\Psi}^*, \left(\frac{\partial A}{\partial \sigma} - \frac{\partial F}{\partial \sigma} \right) \Phi \right\rangle \right\}$$

The Generalized Importance Function Ψ^* satisfies the inhomogeneous equation:

$$\left(A^* - \frac{F^*}{K_{eff}} \right) \tilde{\Psi}^* = \frac{1}{I_S} \frac{\partial I_S}{\partial \Phi} = \frac{\sigma_f(r,E)}{\langle \sigma_f \Phi \rangle}$$

Φ (and Φ^*) are the solutions of the real (and adjoint) Boltzmann equations:

$$A\Phi = \frac{F\Phi}{K_{eff}} \qquad A^*\Phi^* = \frac{F^*\Phi^*}{K_{eff}}$$

The ERANOS code system has been used to calculate sensitivity coefficients (by isotope, nuclear reaction,energy group, space region etc) for:

- **Criticality (multiplication factor)**
- **Any type of reaction rate or any type of adjoint flux functional**
- **Doppler Reactivity Coefficient**
- **Coolant Void Reactivity Coefficient**
- **Any other reactivity coefficient**
- **Effective Delayed Neutron Fraction**
- **External neutron source importance**
- **Reactivity Loss during Irradiation**
- **Transmutation Potential**
- **Peak Power Value**
- **Control Rod Reactivity Worth**
- **Decay Heat**
- **Radiation Source at Fuel Discharge or in a Repository**
- **Radiotoxicity in a Repository**
- **Shielding related parameters**
- **…and more**

Sensitivity coefficients: the case of Reaction Rates

Case of e.g. damage rate or He-production in structures, or to the power peak factor in the core (linear functionals of the flux):

$$R = \langle \underline{\Phi}, \underline{\Sigma}_R \rangle$$

The sensitivity coefficients are given by:

$$S_j^R = \langle \underline{\Psi}_R^*, \sigma_j \underline{\Phi} \rangle$$

$\underline{\Psi}_R^*$ **is the solution of:**

$$M^* \underline{\Psi}_R^* = \underline{\Sigma}_R$$

and M^* is the adjoint of the operator M.

In the case of the power peak:

$$R = \frac{\langle \Sigma_p \underline{\Phi} \rangle_{MAX}}{\langle \Sigma_p \underline{\Phi} \rangle_{Reactor}}$$

Σ_p = power cross-section, defined as $E_f \cdot \Sigma_f$, E_f being the average energy released per fission.

The sensitivity coefficients are defined as:

$$S_j = \langle \underline{\Psi}^*, \sigma_j \underline{\Phi} \rangle$$

$\underline{\Psi}^*$ **is the importance function solution of:**

$$M^* \underline{\Psi}^* = \frac{\Sigma_{p,MAX}}{\langle \Sigma_p \underline{\Phi} \rangle_{MAX}} - \frac{\Sigma_{p,Reactor}}{\langle \Sigma_p \underline{\Phi} \rangle_{Reactor}}$$

where $\Sigma_{p,MAX}$ is the Σ_p value at the spatial point where $\langle \Sigma_p \underline{\Phi} \rangle \equiv \langle \Sigma_p \underline{\Phi} \rangle_{MAX}$, and

$\Sigma_{p,Reactor}$ is the Σ_p value at each spatial point of the reactor

Sensitivity Coefficients for Reactivity Coefficients, EGPT: Equivalent Generalized Perturbation Theory

A reactivity coefficient (like the Doppler effect) can be expressed as a variation of the reactivity of the unperturbed system (characterized by a value K of the multiplication factor, a Boltzmann operator M, a flux $\underline{\Phi}$ and an adjoint flux $\underline{\Phi}$*) :

$$\Delta\rho = \left(1 - \frac{1}{K_p}\right) - \left(1 - \frac{1}{K}\right) = \frac{1}{K} - \frac{1}{K_p}$$

where K_p corresponds to a variation of the Boltzmann operator such that :

$$M \rightarrow M_p \left(= M + \delta M_p\right) \quad \underline{\Phi} \rightarrow \underline{\Phi}_p \left(= \underline{\Phi} + \delta\underline{\Phi}_p\right)$$
$$\underline{\Phi}^* \rightarrow \underline{\Phi}_p^* \left(= \underline{\Phi}^* + \delta\underline{\Phi}_p^*\right) \quad K \rightarrow K_p \left(= K + \delta K_p\right)$$

The sensitivity coefficients (at first order) for $\Delta\rho$ to variations of the σ_j are given as :

$$S_j = \frac{\partial(\Delta\rho)}{\partial\sigma_j} \cdot \frac{\sigma_j}{\Delta\rho} = \left\{ \frac{1}{I_f^p} \left\langle \underline{\Phi}_p^*, \sigma_j \underline{\Phi}_p \right\rangle - \frac{1}{I_f} \left\langle \underline{\Phi}^*, \sigma_j \underline{\Phi} \right\rangle \right\}$$

where $I_f = \left\langle \underline{\Phi}^*, F\underline{\Phi} \right\rangle$ **and** $\mathbf{I_f^p = \left\langle \underline{\Phi}_p^*, F\underline{\Phi}_p \right\rangle}$

F being the neutron fission production part of the M (= F - A) operator.

Sensitivity Coefficients : The Case of Nuclide Transmutation (i.e. nuclide densities at end of irradiation)

The generic nuclide K transmutation during irradiation can be represented as the nuclide density variation between time t_0 and t_F. If we denote n_F^K the "final" density, the appropriate sensitivity coefficients are given by :

$$S_j^K = \frac{\partial n_F^K}{\partial \sigma_j} \cdot \frac{\sigma_j}{n_F^K} = \frac{1}{n_F^K} \int_{t_0}^{t_F} \underline{n}^* \sigma_j \, \underline{n} \, dt$$

where the time dependent equations to obtain $\underline{n}^*$ and $\underline{n}$ are the solution of the classical Bateman equation and its adjoint equation, with appropriate boundary conditions.

Perturbation of the source term

An example is related to the γ-heating of a material j : $H_\gamma^j = < \underline{K}_\gamma^j \underline{\phi}_\gamma >$

The photon flux $\underline{\phi}_\gamma$ is the solution of the inhomogeneous equation $M_\gamma \underline{\phi}_\gamma = \underline{G}_{(n\to\gamma)}$

where Mγ is the Boltzmann operator for the transport of γ, and $\underline{G}_{(n\to\gamma)}$ is the photon source due to neutron reactions which, at a photon energy Eγ, S is given by :

$$G(E_\gamma) = \sum_K \int \sigma_k(E_n) P_k(E_n \to E_\gamma) \phi_n(E_n) dE_n$$

To compute the sensitivity of H_γ^j to uncertainties in the γ-source $\underline{G}_{(n\to\gamma)}$ it is necessary to

define an "adjoint" equation : $M_\gamma^* \underline{\phi}_{\gamma,j}^* = \underline{K}_\gamma^j$

$\underline{K}_\gamma^j$ being the photon KERMA for material j

The sensitivity coefficients are of the type : $S = \dfrac{\partial H_\gamma^j}{H_\gamma^j} \Big/ \dfrac{\partial \underline{G}_{(n\to\gamma)}}{\underline{G}_{(n\to\gamma)}} = \left\langle \underline{\phi}_{\gamma j}^* . \underline{G}_{(n\to\gamma)} \right\rangle$

Statistical input parameter adjustments

- **For input parameter adjustments, the sensitivity coefficients are used within a fitting methodology (e.g. least square fit, Lagrange multipliers with most likelihood function, etc.) in order to reduce the discrepancies between measured and calculation results.**
- **The resulting adjusted input parameters can be subsequently used, sometimes in conjunction with bias factors, to obtain calculation results to which a reduced uncertainty will be associated.**
- **If we define: $y_j=(\sigma_j^{adj}-\sigma_j)/\sigma_j$ and $y_{Qi}^{exp}=(Q_i^{exp}-Q_i)/Q_i$, the y_j are given by:**

$$\bar{y}=\left(S^T D_Q^{-1} S+D^{-1}\right)^{-1} S^T D_Q^{-1}\,\bar{y}_Q^{\,ex}$$

where D_Q is the covariance matrix of the experiments, D the covariance matrix of the cross sections and S is the sensitivity matrix.

It will also result an adjusted covariance matrix for the nuclear data:

$$\left(D^{adj}\right)^{-1}=D^{-1}+S^T D_Q^{-1}\,S$$

Representativity

- **A further use of sensitivity coefficients is, in conjunction with a covariance matrix, a representativity analysis of proposed or existing experiments .**
- **The calculation of correlations among the design and experiments allow to determine how representative is the latter of the former, and consequently, to optimize the experiments and to reduce their numbers.**

- **Formally one can reduce the estimated uncertainty on a design parameter by a quantity that represents the knowledge gained by performing the experiment:**

$$\Delta \mathbf{R}_1^2 = \Delta \mathbf{R}_0^2 (1 - \mathbf{r}_{\mathbf{RE}}^2)$$

$$\mathbf{r}_{\mathbf{RE}} = \frac{\left(\mathbf{S}_{\mathbf{R}}^{+} \mathbf{D} \mathbf{S}_{\mathbf{E}}\right)}{\left[\left(\mathbf{S}_{\mathbf{R}}^{+} \mathbf{D} \mathbf{S}_{\mathbf{R}}\right)\left(\mathbf{S}_{\mathbf{E}}^{+} \mathbf{D} \mathbf{S}_{\mathbf{E}}\right)\right]^{1/2}}$$

Target Accuracy Assessments

- **Target accuracy assessments are the inverse problem of the uncertainty evaluation.**
- **In order to establish priorities and target accuracies on data uncertainty reduction, a formal approach can be adopted by defining target accuracy on design parameter and finding out required accuracy on data.**
- **The unknown uncertainty data requirements can be obtained by solving a minimization problem where the sensitivity coefficients are used together with the existing constraints:**

$$\sum_{i} \lambda_i / d_i^2 = \min \qquad i = 1 \ldots I$$

$$\sum_{i} S_{ni}^2 d_i^2 < Q_n^T \qquad n = 1 \ldots N$$

where d_i are the uncertainties to be found, S_{ni} are the sensitivity coefficients for the integral parameter Q_n, Q^T are the target accuracies on the N integral parameters, and λ_i are cost parameters.

Uncertainty analysis: an example

Recent extensive sensitivity/uncertainty studies, performed partly in the frame of AFCI and extensively supported within an international OECD-NEA initiative, have quantified for the first time the impact of current nuclear data uncertainties on design parameters of the major Gen-IV systems, and in particular for fast reactors with different fuels (oxide or metal), fuel composition (e.g. different Pu/TRU ratios), different conversion ratios and different coolants.

These studies have pointed out that present uncertainties on the nuclear data should be significantly reduced, in order to get full benefit from the advanced modeling and simulation initiatives.

Only a parallel effort in advanced simulation and in nuclear data improvement will enable to provide designers with more general and well validated calculation tools that would be able to meet design target accuracies.

High Burn up VHTR: Uncertainties (%)

	k_{eff} BOC	k_{eff} EOC	Peak Power BOC	Peak Power EOC	Doppler BOC	Doppler EOC	Burnup [pcm]
BOLNA	0.53	0.46	1.0	1.1	1.7	2.0	530

High Burn up PWR: Uncertainties (%)

	k_{eff} BOC	k_{eff} EOC	Doppler BOC	Doppler EOC	Burnup [pcm]
BOLNA	0.51	0.74	1.4	1.9	851

Δρ burnup uncertainty breakdown into components [pcm]

System / Δρ component	VHTR	PWR
Actinides	±530	±851
Fission Products	±215	±244
Total	±572	±885

Examples of results obtained by Subgroup 26

Target Accuracy (1 sigma) for UO_2- and PuO_2-fuelled HTR's

(Source: AREVA-NP, reproduced with permission for WPEC/SG26)

Criticality	300 pcm (operation) 500 pcm (safety)
Local power (in fuel compact)	6% 2% in pin-wise fission rate of fresh fuel and 4% in main fissile isotope concentration of irradiated fuel
Burn-up (cycle length)	1000 pcm
Doppler coefficient	20%
Moderator temperature coefficient	1 pcm/°C
Nuclide inventories at EOL Main fissile isotopes Fertile isotopes MAs and FPs	 4% 5% 20%

PWR Target Accuracy (1 sigma)

k_{eff}	Temperature React. Coeff.	Burn-up $\Delta\rho$	Transmutation
±0.5%	±10%	500 pcm	±5%

VHTR: Uncertainty Reduction Requirements Needed to Meet Integral Parameter Target Accuracies

Isotope	Cross-Section	Energy Range	Uncertainty (%)	
			Initial	Required (λ=1)
U238	σ_{capt}	454 - 22.6 eV	1.7	1.2
C	σ_{inel}	19.6 - 6.07 MeV	30.0	7.1
C	σ_{capt}	19.6 - 6.07 MeV	20.0	7.1
		4 - 0.54 eV	20.0	5.0
Pu239	σ_{capt}	0.54eV - 0.1eV	1.4	0.9
Pu241	σ_{fiss}	454 - 22.6 eV	19.4	6.4
		4 - 0.54 eV	26.8	9.4
		0.54eV - 0.1eV	2.9	1.5
Pu241	σ_{capt}	0.54eV - 0.1eV	6.8	2.4

PWR: Uncertainty Reduction Requirements Needed to Meet Integral Parameter Target Accuracies

Isotope	Cross-Section	Energy Range	Uncertainty (%)	
			Initial	Required (λ=1)
O	σ_{capt}	19.6 - 6.07 MeV	100.0	12.1
		6.07 - 2.23 MeV	100.0	9.9
Pu241	σ_{fiss}	454 - 22.6 eV	19.4	4.7
		4 - 0.54 eV	26.8	7.7
		0.54eV - 0.1eV	2.9	1.7
		0.1eV - thermal	3.3	1.9
Pu239	σ_{capt}	0.54eV - 0.1eV	1.4	1.0
U238	σ_{capt}	24.8 - 9.12 keV	9.4	4.6
		454 - 22.6 eV	1.7	1.4
U238	σ_{inel}	6.07 - 2.23 MeV	14.6	5.1
Pu241	σ_{capt}	0.54eV - 0.1eV	6.8	3.0
Pu240	σ_{capt}	0.1eV - thermal	4.8	3.1
O	σ_{inel}	6.07 - 2.23 MeV	54.9	12.6
		19.6 - 6.07 MeV	84.6	15.6

New covariance data have been produced very recently at BLN:

AFCI 1.2

SFR : keff Uncertainty (%) using AFCI 1.2 and BOLNA Covariance Data

ISOTOPE	CAPTURE	NU	INELASTIC	FISSION	TOTAL
Pu-238	0.06	0.16	0.02	1.31	1.32
	0.06	0.36	0.01	0.53	0.65
Pu-241	0.13	0.03	0.01	0.99	1.00
	0.07	0.04	0.00	0.99	1.00
Pu-240	0.47	0.44	0.03	0.39	0.76
	0.31	0.43	0.01	0.36	0.64
Am-242M	0.09	0.05	0.02	0.65	0.66
	0.05	0.06	0.01	0.73	0.73
Pu-242	0.20	0.08	0.03	0.38	0.44
	0.18	0.08	0.04	0.36	0.41
Cm-245	0.01	0.05	0.00	0.42	0.42
	0.01	0.05	0.00	0.40	0.40
Fe-56	0.20	0.00	0.04	0.00	0.29
	0.12	0.00	0.45	0.00	0.47
Cm-244	0.18	0.11	0.01	0.14	0.25
	0.05	0.08	0.01	0.38	0.39
U-238	0.05	0.03	0.23	0.01	0.24
	0.07	0.03	0.22	0.01	0.23
Pu-239	0.13	0.08	0.06	0.13	0.21
	0.13	0.07	0.06	0.13	0.21
TOTAL	0.64	0.51	0.27	1.91	2.11
	0.46	0.58	0.57	1.55	1.81

- **The process for producing the improved (i.e. with reduced uncertainties) nuclear data involves several ingredients and steps:**

  - Selection of a set of relevant experiments,
  - Sensitivity analysis of selected configurations including reference design configurations,
  - Production and use of science based covariance data for uncertainty evaluation and target accuracy assessment,
  - Analysis of experiments using the best methodologies available,
  - Use of calculation/experiment discrepancies in a statistical adjustment

Statistical adjustments have successfully used to improve multigroup data for fast reactor design.

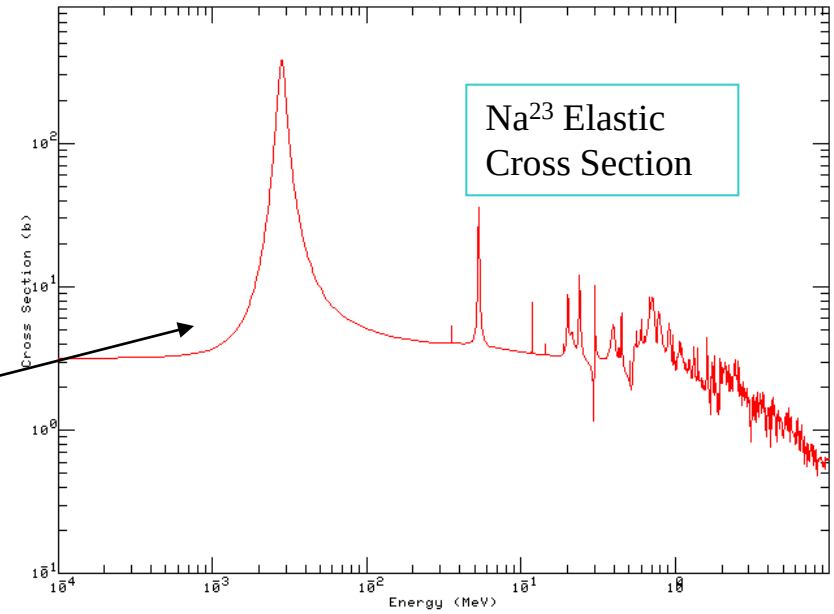
However, to extend the validity of an adjusted set, one can adjust the model basic nuclear parameters used in an evaluation: the **« consistent »** method.

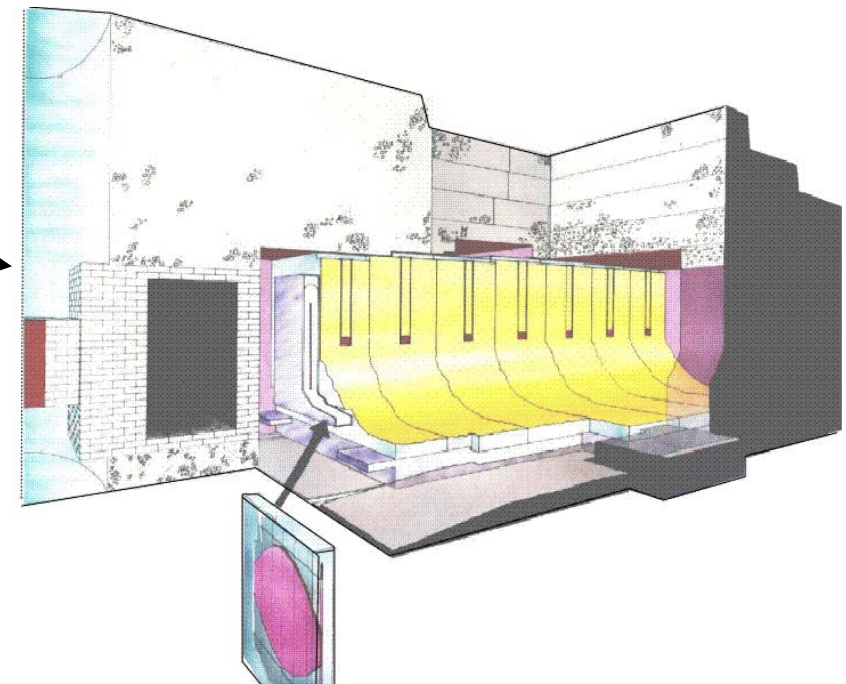
Consistent Data Assimilation: a first step is underway

From Meters to Femtometers

A first attempt of consistent data assimilation is under way using neutron propagation experiments.

The parameters characterizing **10 major resonances** of the sodium elastic cross section and **16 basic nuclear parameters** (optical model) will be tuned using the C/E of reaction rates measured in the EURACOS experiment (propagation in 3 meters of sodium).





Conclusions

- **Sensitivity and uncertainty analysis is available for a very wide range of parameters and applications**

- **The adjoint method (as implemented e.g. in the ERANOS code system) provides an effective tool**

- **Covariance data play a crucial role and the data produced at BNL (with the support of LANL and ORNL) are a real « breakthrough » that will have significant impact in:**

  - **Advanced Simulation Experimental Validation,**
  - **Design Optimisation and**
  - **New, Science-based Experiment planning.**

Sensitivity Coefficients : The Case of the Reactivity Loss during Irradiation, $\Delta\rho^{cycle}$

At first order :

$$\Delta\rho^{cycle} = \sum_K \Delta n^K \rho_K \qquad \Delta n^K = n_F^K - n_0^K$$

and ρ_K is the reactivity per unit mass associated to the isotope K.

The related sensitivity coefficients associated to the variation of a σ_j, are given by :

$$S_j^{cycle} = \frac{\sigma_j}{\Delta\rho^{cycle}} \frac{\partial \Delta\rho^{cycle}}{\partial \sigma_j} = \frac{\sigma_j}{\Delta\rho^{cycle}} \left(\sum_K \frac{\partial n^K}{\partial \sigma_j} . \rho_K + \sum_K \Delta n_K \frac{\partial \rho_K}{\partial \sigma_j} \right)$$

or:

$$S_j^{cycle} = \sum_K \frac{\rho_K}{\Delta\rho^{cycle}} \int_{t_0}^{t_F} \underline{n}^* \sigma_j \underline{n} \; dt + \left\{ \frac{1}{I_f^p} \left\langle \underline{\Phi}_p^*, \sigma_j \underline{\Phi}_p \right\rangle - \frac{1}{I_f} \left\langle \underline{\Phi}^*, \sigma_j \underline{\Phi} \right\rangle \right\}$$