International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

COMPUTING SENSITIVITY AND HANDLING DATA UNCERTAINTIES IN ACTIVATION PROBLEMS

J. Cartier*
CEA-DIF Bruyères-le-Châtel
91297 Arpajon Cedex
julien.cartier@cea.fr

ABSTRACT

This paper presents sensitivities computation techniques and how to handle data uncertainties in activation problems. We describe a direct and an adjoint method for calculating the sensitivities of an observable (solution in some sense of an activation problem). Some numerical results are also exposed to validate these techniques. Moreover, we simulate an experiment of yttrium irradiation. This experiment was done at CEA by using the PROSPERO reactor. We use the new cross sections variance-covariance matrices related to yttrium evaluation from BRC6 and ENDF-B7 to estimate the error committed on some observable.

Key Words: Activation, sensitivities, uncertainties, neutron flux, PROSPERO reactor

1. INTRODUCTION

The aim of this paper is to present some techniques used to compute sensitivity and to handle data uncertainties in activation problems. Controlling uncertainties and sensitivity of an observable (or solution) for a given parametric problem is a major issue. It allows for anticipating, optimizing and orienting the scientific and engineering requirements related to the elaboration of experiments. It also allows for quantifying the error associated with the solution of a given physical problem and for taking into account the uncertainties related to the parameters of this problem. Some evaluations of cross sections [2, 3] are currently available with variance-covariance matrices to show uncertainties on these evaluations (ENDF-B7, EAF 2007). First, we describe the general equations of our activation model problem. Then, we present two sensitivities calculation techniques integrated into the code TRACT, developed in CEA. In one hand, we deal with a direct method derived from A.Khursheed's work [5] and in the other hand we derive an adjoint method. The originality of our work is to apply this adjoint method for activation calculation. Indeed, most of the activation's codes use a direct method. Finally, we illustrate the efficiency of our techniques with some numerical results. We particularly insist on the simulation of Yttrium irradiation experiment. This experiment was performed at CEA with the PROSPERO reactor [1].

2 MODEL PROBLEM

In this section, we write general equations for a given activation problem. At CEA, the TRACT code solves this problem. Some sensitivity computing and uncertainties handling techniques were integrated into TRACT code. We consider the general situation in which a medium is subject to a neutron flux. The flux is supposed to be known and is denoted $\varphi(E, \vec{r}, t)$ where E is the energy, $\vec{r}$ the position and t the time. We

*CEA

focus on a sufficiently small volume in order to have an homogeneous flux and population (i.e. $\varphi(E,\vec{r},t)=\varphi(E,t)$). Each isotopic proportion follows Bateman's classical equation :

$$\frac{dN}{dt}=MN,$$

where $N(t)\in\mathbb{R}^m$ represents the unknown atomic composition. We denote $N_i(t)$ the i-th component of $N(t)$, equals to the atom number of species i and M is the evolution matrix for this system with

$$M_{ij}(t)=\lambda_{j\to i}-\delta_{i,j}\sum_k\lambda_{i\to k}+\int_0^{+\infty}\varphi(E,t)\left(\sigma_{j\to i}(E)-\delta_{i,j}\sum_k\sigma_{i\to k}(E)\right)dE,$$

where $\sigma_{i\to j}(E)$ represents the neutron cross-section of reaction $n+X_i\to X_j+\dots$, and $\lambda_{j\to i}$ is the decay constant of nuclide j to nuclide i.

3 SENSITIVITY COMPUTATION TECHNIQUES

In this paragraph, we give a definition of the "sensitivity" notion and we describe several sensitivity techniques applied to the previous model problem. The quantity R will represent an observable.

3.1 The observable and sensitivity notions

The observable mainly relates to the concentration (or atoms number) N_i of the nucleids of a given species i, to the weighted sums of atoms number or isotopical ratios (ratios of weighted sums of atoms number). The observable always take the general form

$$R=\frac{<D,N>}{q+<Q,N>},\tag{1}$$

where $D\in\mathbb{R}^m$ and $Q\in\mathbb{R}^m$ are constant vectors in $\mathbb{R}^m$, $<,>$ represents the common scalar product between $\mathbb{R}^m$ and $q\in\{0,1\}$ where $q=0$ if $Q\neq 0$ and $q=1$ otherwise. This general form allows to mathematically describe observables in terms of concentration, sum of concentrations from different nuclides and ratio of nuclides concentrations. Thus we have

$$\frac{\partial R}{\partial x_j}=\frac{<D,\frac{\partial N}{\partial x_j}>}{q+<Q,N>}-\frac{<D,N><Q,\frac{\partial N}{\partial x_j}>}{(q+<Q,N>)^2}.\tag{2}$$

The sensitivity of one observable R or , of one concentration (or atom number of a given nuclei N_i) on parameter x_j is denoted $S(R;x_j)$ (or $S(N_i;x_j)$ respectively) is defined by the following expression:

$$S(R;x_j)=\frac{\partial R}{\partial x_j}\frac{x_j}{R}.$$

Several techniques are available to compute the sensitivities of a given observable using cross-sections and decay data. We give a detailed review of deterministic methods. Some stochastic methods also exist, for instance, the Monte-Carlo based methods. A detailed review may be found in [4].

3.2 A. Khursheed direct method

The most common approach to sensitivity computing is the direct method (see, for instance, Khursheed [5]). This method is used in FISPACT code [7]. Given a matricial problem (called a direct problem) :

$$\frac{dN}{dt} = MN, \tag{3}$$

with $N(t = 0) = N_0$. Let denote x_j a parameter implied in the problem (3). Assuming each term of this equation is differentiable with respect to x_j, we obtain an equation satisfied by $\frac{\partial N}{\partial x_j}$ by deriving (3) along the x_j-component :

$$\frac{d}{dt}\left(\frac{\partial N}{\partial x_j}\right) = M\left(\frac{\partial N}{\partial x_j}\right) + \left(\frac{\partial M}{\partial x_j}\right)N. \tag{4}$$

Assuming N was previously numerically computed, the problem becomes similar to (3) and can be solved using the same numerical methods (Runge-Kutta, for instance): that is the main interest for this kind of methods. The natural initial conditions used to close this problem (4) in the case of sensitivity computed with parameters x_j are:

$$\frac{\partial N}{\partial x_j} = 0.$$

We may notice that computing the solution sensitivities for n parameters of the problem requires to solve $n + 1$ matricial first order differential equations (so $n + 1$ Runge-Kutta, for instance), which can increase the computing cost. An alternative approach exists, lighter in term of computing cost (with a speed-up of $\frac{n+1}{2}$, for instance) : the adjoint method.

3.3 The adjoint method

In this section, we present a method using the adjoint problem of (3). This method is called adjoint state method or simply adjoint method [6]. The adjoint method has been presented by R. Sentis (CEA) for activation problems. We can also find in the paper of Williams [10] a very interesting similar adjoint method used to compute sensitivities in the context of coupled neutron/nuclide fields. Remembering we try to evaluate the quantity $\frac{\partial N}{\partial x_j}$ where x_j is a given parameter occuring in the problem (3). We consider the adjoint problem of (3) with the vectorial unknown Ψ:

$$\frac{d\Psi}{dt} = -M^*\Psi, \tag{5}$$

where M^* is the adjoint operator of the M operator. In the case of our activation problem, M^* is simply the transposed matrix of M matrix. Remembering an important property of adjoint operators : if X and Y are two vectors belonging to $\mathbb{R}^m$ then

$$< X\,,\, MY >=< M^*X\,,\, Y >$$

where $<,>$ represents the euclidian scalar product in $\mathbb{R}^m$. The adjoint method consists in solving in the same time problem (3) and its adjoint problem (5) in order to compute $\frac{\partial N}{\partial x_j}(t = T)$. From equation (2), we have a general expression of $\frac{\partial R}{\partial x_j}(t = T)$ that we can write as

$$\frac{\partial R}{\partial x_j}(t = T) =< \Psi_T, \frac{\partial N}{\partial x_j}(t = T) >,$$

where Ψ_T is deduced from (2) (in particular Ψ_T depends on $N(T)$). Thus, if we indeed choose an initial condition $\Psi(t = T) = \Psi_T$ to the adjoint backwards problem, then we can write

$$\frac{\partial R}{\partial x_j}(t = T) = \int_0^T \frac{d}{dt}\left(< \Psi(t), \frac{\partial N}{\partial x_j}(t) > \right) dt,$$

$$= \int_0^T \left(< \frac{d}{dt}\Psi(t), \frac{\partial N}{\partial x_j}(t) > + < \Psi(t), \frac{d}{dt}\frac{\partial N}{\partial x_j}(t) > \right) dt,$$

$$= \int_0^T < \Psi(t), \frac{\partial M}{\partial x_j} N(t) > \, dt. \tag{6}$$

Expression (6) can be computed with little computing cost as it only requires one direct computation in order to get $N(t)$ and only one adjoint computation for $\Psi(t)$, and it only remains to evaluate the $\frac{\partial M}{\partial x_j}$ derivatives for each interesting parameter using a simple numerical integration. We notice for adjoint computation we need to know $N(t)$, we need so to solve the direct problem first. Indeed, the initial condition of the adjoint problem Ψ_T depends on $N(T)$. Moreover, the adjoint computation can be done by using the same kind of numerical solver than that used for direct computation. It is also necessary to store the values obtained for the solutions at each time step in order to evaluate the integrals in time (6). Furthermore, the main advantage of the adjoint technique in comparison with direct one is its little computing cost. Indeed, if we denote by d the number of uncertains parameters, then we need to solve $d + 1$ evolution problems with direct method whereas we need to solve only 2 evolution problems with the adjoint method.

4 NUMERICAL RESULTS

In this section, we present some numerical test cases in order to evaluate and to illustrate the sensitivity computing module features and uncertainties handling for the TRACT code. First, we present an analytical test case and we compare it to the numerical solution obtained using the TRACT code and with the one obtained using the FISPACT activation code. Finally, we present the numerical resolution for a problem modeling some material irradiations with the PROSPERO experimental reactor. We compare the experimental results with the numerical results for the TRACT and FISPACT codes. We are using the cross sections covariances data ENDF-B7 and BRC6 (CEA) for Yttrium [2, 3] in order to give the numerical solution uncertainty.

4.1 Analytical test case

We consider the model problem involving three species denoted $\{Z_i\}_{i=1,\cdots,3}$ with respective concentrations $\{N_i\}_{i=1,\cdots,3}$. Let us assume that at time $t = 0$, Z_1 is the only one present with concentration $N_1 = N_0$. Two nuclear reactions are to be taken into account, they transform Z_1 in Z_2 with a cross section $\sigma_{1\to2}$ and Z_1 in Z_3 with a differential cross-section $\sigma_{1\to3}$. The time-integrated flux φ and the cross-sections are supposed to be such that :

$$\int_0^{+\infty} \varphi(E)\sigma_{1\to2}(E)dE = \sigma_2,$$

and

$$\int_0^{+\infty} \varphi(E)\sigma_{1\to3}(E)dE = \sigma_3,$$

where σ_2 and σ_3 do not depend on time and energy. We also assume that Z_3 species spontaneously decays to Z_2 with a decay constant equals to λ. Thus, the set of equations to solve is

$$\frac{dN}{dt} = \begin{pmatrix} -\sigma_2 - \sigma_3 & 0 & 0 \\ \sigma_2 & 0 & \lambda \\ \sigma_3 & 0 & -\lambda \end{pmatrix} N,$$

with $N(t=0) = (N_0, 0, 0)^t$ where N represents the concentration vector. We perform $\lambda = \sigma_2 = \sigma_3 = N_0 = 1$. The solution of this problem can be written as :

$$N(t) = \begin{pmatrix} e^{-2t} \\ 1 - e^{-t} \\ e^{-t}(1 - e^{-t}) \end{pmatrix}.$$

We can also analytically compute the sensitivities. Table I shows the sensitivities numerically computed inventory using TRACT at time $t = 1$ and the sensitivities computed using previous formulae. The table I

Sensitivity	**TRACT**	**Analytical**
$S(N_1;\sigma_2)$	-0.99980	-1
$S(N_1;\sigma_3)$	-0.99980	-1
$S(N_1;\lambda)$	0	0
$S(N_2;\sigma_2)$	0.36782	0.36787
$S(N_2;\sigma_3)$	$0.13204 \cdot 10^{-10}$	0
$S(N_2;\lambda)$	0.21409	0.21409
$S(N_3;\sigma_2)$	-0.21409	-0.21409
$S(N_3;\sigma_3)$	0.58186	0.58197
$S(N_3;\lambda)$	0.58197	0.58197

Table I. Comparisons between TRACT code and analytical formulas

presents the sensitivity computing results obtained with the TRACT code and the exact numerical values. These results are close, but it remains some minor differences related to the numerical integration method used to compute the term (6) coming from the adjoint problem. With this table, we can evaluate each reaction influence on the considered species set. We particularly see that the decay reaction has no influence on the evolution of the concentration of the Z_1 concentration (nullity of the sensitivity), and also of the $Z_1 \rightarrow Z_3$ reaction on the Z_2 concentration. In the case of a more complicated problem where numerous species, and for which no analytical solution exists, the sensitivity computation can be greatly useful in order to know the influence of each reaction on each considered species.

4.2 Irradiation with the PROSPERO reactor: comparison TRACT vs FISPACT

In this section, we illustrate an application of our method in a case where some irradiations experiments have been done with the PROSPERO reactor [1] at CEA.

4.2.1 The PROSPERO reactor

PROSPERO is a small reactor with a 31.4cm diameter and 35.2cm length (see picture 1). The reactor core

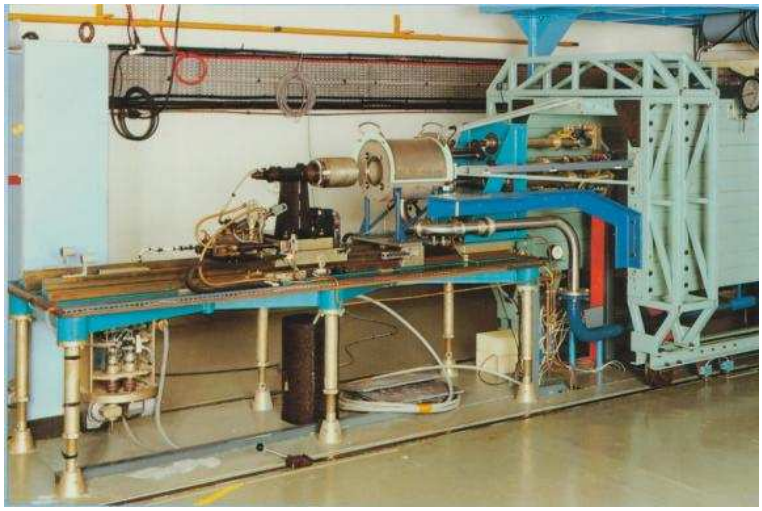

Figure 1. Photography of the PROSPERO reactor

is made of two enriched uranium cylinders and a natural uranium reflector. Three control bars and a compensation bar allows for piloting this system. It produces an intensive and continuous neutron and fission gamma-ray source. The sample we want to irradiate is put inside the central cavity between the two cylinders. Each target is associated to gold made target in order to control the neutron flux. It is 125 μm width shells of 20 mm diameter. These targets are irradiated with a 3000 W power by a neutron flow equals to $9 \cdot 10^{11} n.cm^{-2}.s^{-1}$ during 3h to 3h30. Temperatures at heart and at the sample can reach respectively 175 $°C$ and 85 $°C$. The PROSPERO reactor modelisation has been done using the neutron transport codes : Monte Carlo MCNP (A. Umbert) and deterministic, developed at CEA, STYX (C. Aussourd, see [8]) and PANDA (P. Humbert, see [9]). In these numerical simulations, the neutron data related to the reactor components come from ENDF B6 library. MCNP does some computation with continuous energy and then the resulting flow is put in group. The neutron energy domain is divided by 172 groups between 10^{-10} and 20 MeV. To handle covariance data, we have decided to work with the 53 groups format proposed in the BRC6-cross sections file containing the covariance data. We have put together the ENDF-B7 data in this format using the NJOY software.

4.2.2 Numerical results: Yttrium irradiation

We focus on a 3h Yttrium capsule irradiation in the PROSPERO reactor. Table II shows activity of Yttrium 89M and associated uncertainties. Uncertainties are computed using the covariance data on cross-sections as presented on figure 2. We use the sandwich-rule formula to compute the uncertainties:

$$V(R) = \sum_{i,j} \frac{\partial R}{\partial x_i} \frac{\partial R}{\partial x_j} Cov(x_i, x_j).$$

The results obtained by TRACT code for BRC6 and ENDF-B7 libraries for 53 energy groups are really close to results obtained with FISPACT and EAF-2007 codes. The uncertainty on result is only equal to 8.6% in the case of BRC6 data, and 15.42% for ENDF-B7. The uncertainty coming from FISPACT activation code is equal to 15%. We notice that all error bars cross each other. In Table III, we can see that Yttrium 89M isomer is mainly sensitive to the reaction $^{89}Y(n,n')^{89M}Y$ and to its spontaneous decay.

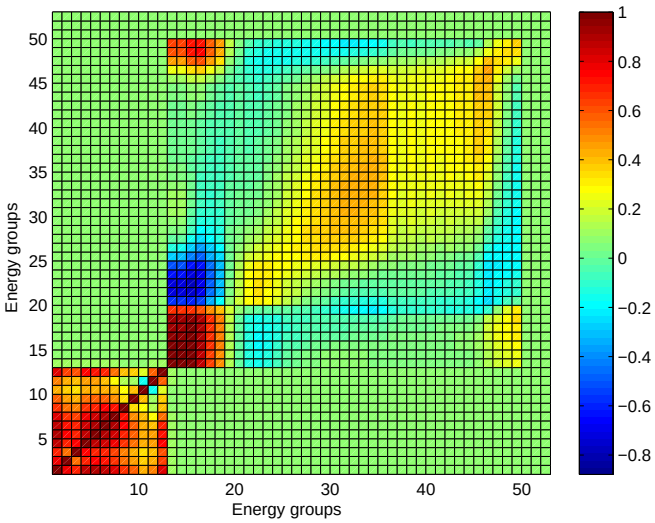

Figure 2. Correlation BRC6 matrix between (n, n') and $(n, 2n)$ reactions for Yttrium 89

Evaluated uncertainty on Yttrium 89M activity is then principally due to the uncertainty of the cross sections for the reaction $^{89}Y(n, n')^{89M}Y$.

TRACT Comput.				**FISPACT Comput.**	
BRC6		ENDF-B7		EAF-2007	
Activity	Uncert.	Activity	Uncert.	Activity	Uncert.
7.27	8.6%	7.75	15.42%	8.42	15%

Table II. Yttrium 89M activities for a 3h irradiation in PROSPERO

The global uncertainty on $^{89}Y(n, n')^{89M}Y$ cross-section is around 7.45% for BRC6 and 20.76% for ENDF-B7. These uncertainties are equivalent to these obtained on Yttrium 89M activity as expected. The small noticeable differences are linked to the correlations between different energy groups of cross-sections and also to the variation (as a function of the energy) of the observable sensitivity along cross-sections.

5. CONCLUSIONS

We have presented in this paper some techniques in order to compute sensitivities and handle uncertainties on activation problem data. We have implemented a sensitivity computing method in the TRACT code at CEA. This method is based on the adjoint problem resolution. This method requires few resources and little numerical cost compared to concurrent methods. The numerical results with TRACT code are satisfying (very good agreement with respect to FISPACT activation code). We can use this code to give an error bar on one observable from uncertainties on data. The first sensitivities computing results are very encouraging and the exploitation thanks to TRACT code of covariances data is particularly practical and useful.

	TRACT Sensitivities		FISPACT Sensitivities	
	^{89M}Y	^{90}Y	^{89M}Y	^{90}Y
$(n, 2n)$	$-4 \cdot 10^{-13}$	$-4 \cdot 10^{-13}$	$-8 \cdot 10^{-13}$	$-8 \cdot 10^{-13}$
(n, γ)	$-3 \cdot 10^{-11}$	$0,983$	$-7 \cdot 10^{-11}$	0.988
(n, n')	1	$-3 \cdot 10^{-12}$	1	$-6 \cdot 10^{-10}$
(n, p)	$5 \cdot 10^{-13}$	$-6 \cdot 10^{-13}$	$3 \cdot 10^{-13}$	$-3 \cdot 10^{-13}$
(n, α)	$-5 \cdot 10^{-15}$	$-6 \cdot 10^{-13}$	$-9 \cdot 10^{-14}$	$-9 \cdot 10^{-14}$
$(n, 3n)$	0	0	0	0

Table III. Sensitivities of some Yttrium observables

6. *

REFERENCES

REFERENCES

[1] Y. Calzavara, N. Authier, S. Wisniewski, X. Jacquet, *Experimental facilities for mixed field neutron/γ irradiation* , proceeding RADECS (2005).

[2] E. Bauge, P. Dossantos-Uzarralde, S. Hillaire, *Evaluations des Incertitudes associées aux sections efficaces de la réaction n + ^{89}Y, méthodologie, résultats, mise en forme* (CEA's report).

[3] M.B. Chadwick et al., *ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology*, Nuclear Data Sheets 107, pp 2931-3060 (2006).

[4] I. Thibault, *Restitution d'expériences de transmission neutronique. Sensibilité aux données de base.*, Thèse de l'Université Paris VI (1990).

[5] A. Khursheed, *Neutron-Induced Activation of Materials for the First Wall of Conceptual Fusion Reactors*, Ph.D. University of London (1989).

[6] M. Ionescu-Bujor, D.G. Cacuci, *A Comparative Review of Sensitivity and Uncertainty Analysis of Large-Scale Systems – I: Deterministic Methods*, Nuclear Science and Engineering, 147, pp.189-203 (2004).

[7] *FISPACT-2007: User manual*, published by Euratom/UKAEA Fusion Association (2007).

[8] C. Aussourd, *Styx: A Multidimensional AMR SN Scheme*, Nuclear Science and Engineering, 143, pp.281-290 (2003).

[9] P. Humbert, *Results for the C5G17 Extension Benchmark Using the Discrete Ordiantes Code PANDA*, Progress in Nuclear Energy, 48, pp.394-400 (2006).

[10] M. L. Williams, *Development of Depletion Perturbation Theory for Coupled Neutron/Nuclide Fields*, Nuclear Science and Engineering, 70, pp.20-36 (1979).