

## VARIATIONS ON THE RESONANT SELF-SHIELDING FACTOR IN PROCESSES WITH TEMPERATURE FEEDBACK

**Franciole Marinho, fmarinho@physics.gla.ac.uk**

Instituto de Física Teórica - Universidade Estadual Paulista, ZIP Code: 01140-070 – São Paulo, SP, Brasil.

**Laura Paulucci, lapaulucci@gmail.com**

Instituto de Astronomia, Geofísica e Ciências Atmosféricas – IAG/USP, ZIP Code: 05508 – 090 – São Paulo, SP, Brasil.

**Daniel Artur Pinheiro Palma, dpalmaster@gmail.com**

**Wallace Vallory Nunes, w.vallory@gmail.com**

Instituto Federal do Rio de Janeiro, Rua Lúcio Tavares, 1045, ZIP Code: 28630-050 – Nilópolis, RJ, Brasil

**Aquilino Senra Martinez, aquilino@imp.ufrj.br**

COPPE/UFRJ – Programa de Engenharia Nuclear, ZIP Code: 21941-914 – Rio de Janeiro, RJ, Brasil

***Abstract.** The activation technique allows precise measurements of relative or absolute neutron intensity. Fast and accurate calculations of the self-shielding factors in ephithermal range are necessary for the neutron flux monitoring in real time. An analysis of the behaviour of the self-shielding factor according to temperature variations defined by a process with thermal hydraulic feedback is presented in this work. The calculations were evaluated for a disk with fixed source. An analytical approximation for the evaluation of the temperature in the nuclear core was implemented. The results were compared with the numerical method of reference and values obtained by Monte Carlo simulations providing satisfactory accuracy.*

***Keywords:** Self-shielding factor, Point kinetics, Temperature feedback, Doppler broadening function, Monte Carlo*

### 1. INTRODUCTION

Self-shielding factors are important in the treatment of nuclear data in the energy ranges corresponding to the resonances. There are countless applications of these parameters in reactor physics (Shcherbakov and Harada, 2002), (Bitelli and Gonçalves, 2007), (Bitelli et. al., 2007), (Caldeira, 2007).

A technique that is widely used in research reactors to measure the neutron flux is the activation method. Also known as the cadmium rate technique ( $^{113}\text{Cd}$ ), the activation technique consists in the evaluation of the absolute thermal neutron flux in the reactor core from an analysis of the activation of irradiated gold sheets, with or without (bare) cadmium coating. A description of the technique can be found in literature (Bekurts & Wirtz, 1964).

A study of the behavior of the self-shielding factors as a function of the temperature variation in a reactor's core is performed in this paper. A satisfactory estimate of the global temperature of a reactor's core can be obtained by solving the point kinetics equations considering thermal-hydraulic feedback.

The point kinetics equations for reactors constitute a system of coupled ordinary differential equations. It is a simple model which is able to provide satisfactory answers from the physics point of view. Through this set of equations, which depend only on time, it is possible to investigate the behavior of the neutron in the reactor from a small perturbation caused in the reactor's core. Besides the density of neutrons, other time dependent quantities as the reactivity, the temperature of operation of the reactor and the concentration of precursors of delayed neutrons are essential to the design of the reactor's core and to perform its control and monitoring (Stacey, 2001).

This paper considers an approximate solution of the point kinetics equations with thermal-hydraulic feedback proposed by Palma et. al. (2009). Although, there are other approximate solutions in the literature (Nahla and Aboanber, 2002, Chen et. al., 2007, Li et. al., 2007; Nahla, 2009), the method proposed by Palma et. al. achieves small percentage deviations with respect to the reference values and offers the advantage of explicit time dependence in its functional form. Subsequently, a comparison of self-shielding factors obtained using a Monte Carlo GEANT4 simulation is performed.

### 2. THE SELF-SHIELDING FACTOR $G_{epi}(\xi, \tau)$

Let us consider the case where the object of activation is a circular disk with thickness  $t$ , negligible in relation to the diameter of the plate exposed to an isotropic neutrons flux with the spectrum in the neighborhood of resonance energy  $E_0$ . The macroscopic absorption cross section in the resonance is  $\Sigma_0 = \sigma_0 N_a$ , where  $N_a$  is the number of target nuclei per unit volume. Assuming that the neutron scattering is negligible when compared to the absorption the expression for the self-shielding factor for an isolated resonance located in the epithermal range is written by (Palma et. al, 2008):

$$G_{epi}(\xi, \tau) = \frac{1}{\pi\tau} \int_0^{+\infty} \left[ 1 - (1 - \tau\psi) \exp(-\tau\psi) - \tau^2 \psi^2 E_1(\tau\psi) \right] dx, \quad (1)$$

where  $\tau = t\Sigma_0$  is named effective thickness,  $E_1(\tau\psi)$  is the integral exponential function of order 1 (Gradshteyn and Ryzhik., 2008) written by

$$E_1(\mu) = \int_1^{\infty} \frac{dy}{y} \exp(-\mu y). \quad (2)$$

and it indicated the Doppler broadening function  $\psi(x, \xi) \equiv \psi$ , written in its integral form by:

$$\psi(x, \xi) = \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{dy}{1+y^2} \exp\left[-\frac{\xi^2}{4}(x-y)^2\right]. \quad (3)$$

Variables  $x$  and  $\xi$  are set by the nuclear parameters of the resonance (Stacey, 2001):

$$x = \frac{2}{\Gamma}(E - E_0) \quad (4)$$

$$\xi = \frac{\Gamma}{(4E_0 kT / A)^{1/2}}, \quad (5)$$

where  $E$  is the energy of the neutron,  $E_0$  the resonance energy,  $\Gamma$  the total resonance width,  $T$  the temperature of the medium, and  $k$  the Boltzmann constant.

Palma et. al. (2006) proposed the following approximation for the Doppler broadening function:

$$\psi(x, \xi) = \frac{\xi\sqrt{\pi}}{2} \exp\left[-\frac{1}{4}\xi^2(x^2 - 1)\right] \cos\left(\frac{\xi^2 x}{2}\right) \left\{ 1 + \operatorname{Re}[\eta(x, \xi)] + \tan\left(\frac{\xi^2 x}{2}\right) \operatorname{Im}[\eta(x, \xi)] \right\}, \quad (6)$$

where  $\eta(x, \xi) = \operatorname{erf}\left(\frac{i\xi x - \xi}{2}\right)$ .

Equation (6) provides a simple and accurate expression for the Doppler broadening function and will be used for the calculation of  $G_{epi}(\xi, \tau)$  according to Eq. (1). The disk temperature is approximated as the reactor's core temperature. This is a reasonable assumption given: the reduced dimensions of the disk used in the activation technique; direct contact of the disk with the moderator; and disk location close to the reactor's fuel. The  $\xi$  parameter in this approach is considered a time dependent quantity. The main goal of this paper is to determine the function that predicts how the global temperature of the reactor's core varies with time.

### 3. THE POINT KINETICS EQUATIONS WITH TEMPERATURE FEEDBACK

Considering adiabatic thermal-hydraulic feedback, the point kinetics equations with a group of precursors can be written as follows:

$$\frac{dn(t)}{dt} = \frac{\rho(t) - \beta}{l} n(t) + \lambda C(t) \quad (7)$$

$$\frac{dC(t)}{dt} = \frac{\beta}{l} n(t) - \lambda C(t) \quad (8)$$

$$\rho(t) = \rho_0 - \alpha [T(t) - T_0] \quad (9)$$

$$\frac{dT(t)}{dt} = K_c n(t), \quad (10)$$

where  $n(t)$  is the density of neutrons,  $\rho(t)$  is the reactivity,  $\beta$  is the fraction of retarded neutrons,  $l$  is the time of generation of ready neutrons,  $\lambda$  is the decay constant of precursors of retarded neutrons,  $C(t)$  is the average density of precursors of retarded neutrons,  $\alpha$  ( $\alpha > 0$ ) is the coefficient of reactivity, and  $K_c$  is the reactor's heat capacity. Although there are models that consider the variation of the coefficient of reactivity  $\alpha$  with temperature (Stacey, 2001), (Jian and Cotta, 2000), it is considered constant in this paper. This assumption is valid as the temperature variation in the core is usually not large enough to significantly change the coefficient of reactivity transients when considering thermal-hydraulic feedback.

By solving the set of Eq.s (7), (8), (9) and (10) one can write the following expression, valid near the supercriticality, for the temperature of the reactor core as a function of time (Palma et. al., 2009):

$$T(t) = T_0 + \left( \frac{\sigma + \rho_0}{\alpha} \right) \left( 1 - e^{-\frac{\lambda t}{2}} \right), \quad (11)$$

where  $\sigma = \sqrt{\rho_0^2 + \frac{2}{\lambda} \alpha K_c n_0 (\beta - \rho_0)}$ . The temperature function displays a simple shape and is used to predict the time dependence of the self-shielding factors. From the Eq. (11) one can estimate the asymptotic behavior of the temperature:

$$T_{ass}(t) = \lim_{t \rightarrow \infty} T(t) = T_0 + \left( \frac{\sigma + \rho_0}{\alpha} \right). \quad (12)$$

Substituting Eq. (10) in Eq. (4), we obtain an expression for the  $\xi(t)$  function:

$$\xi(t) = \Gamma \sqrt{\frac{\alpha A}{4E_0 k \left[ \alpha T_0 + (\sigma + \rho_0) \left( 1 - e^{-\lambda t/2} \right) \right]}}. \quad (13)$$

#### 4. MONTE CARLO SIMULATION

A Monte Carlo simulation was developed to confirm the evaluation of the temperature dependence of the self-shielding factors obtained through the method described in sections 2 and 3. This simulation was performed using the GEANT4 package which is a toolkit for the simulation of the passage of particles through matter based on Object-Oriented technology implemented in C++ (Agostinelli, S. et al, 2003). This section describes the implementation of this MC simulation. It explains which physics processes are included in the simulation, describes the geometry used and the neutron flux generation.

A subset of C++ classes is implemented in Geant4 to describe neutron interactions with matter at thermal energies which can be used to perform accurate simulations (G4NeutronHP). Its precision models and cross sections data sets are based on the ENDF/B-VII files format. Thermal neutron scattering from chemically bound atoms is taken into account since effects of atomic translational motion as well as vibration and rotation of the chemically bound atoms affect the neutron scattering cross section, the energy and angular distribution of secondary neutrons. Neutron capture processes are also detailed in the simulation.

In order to exactly reproduce the physical situation described in section 2 the following geometry was developed. A target with a thin disk shape was implemented. It was placed inside an empty cubic box of 1m x 1m x 1m dimensions. Table 1 shows the physical characteristics and dimensions of the target material.

Table 1: Input parameters for MC simulation. Range in brackets indicates values assumed in the simulation.

Parameter	Value
Density ( $\text{g/cm}^3$ )	19.32
Atomic Number (g/mol)	196.97
Radius (mm)	20.0
Width (mm)	$[2.0 \times 10^{-4}, 2.0 \times 10^{-3}]$
Temperature (K)	$[300.00, 547.19]$

To generate the neutron flux with correct isotropic distribution and maximum sampling efficiency the following procedure was adopted.

- The incident position of each neutron on the target surface was randomly sampled according to a homogenous distribution;
- The initial position of the neutrons was sampled according to a spherical distribution with origin fixed at the neutron incident position;
- The two spatial points obtained in the previous items were used to define the initial direction of propagation of the neutrons.

The energy of the neutrons was defined within a range which allows analysis of the first resonance (1.0-10 eV). Each neutron had its energy sampled according to a homogeneous distribution defined in this range. Figures 1 and 2 show the trajectories of the neutrons. The trajectory of the neutrons before reaching the target material is shown as a side view on figure 1. For ease of exposition, only incident neutrons from the top hemisphere are shown. The trajectory of the neutrons which traversed the target is shown as a top view on figure 2. A validation procedure was implemented to verify and guarantee that the neutron flux generated was isotropic. To perform this test: the distribution of the incidence angles of the neutrons was obtained and found to be flat; and the number of events per unit area was calculated and found to be homogenous across the target surface.

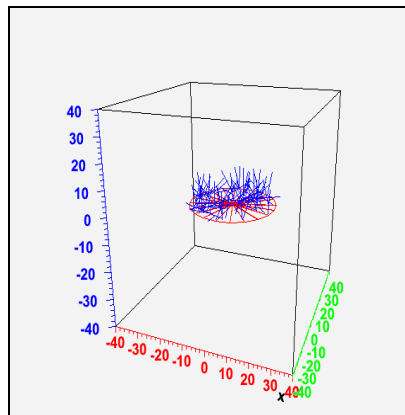


Figure 1: Isotropic neutron flux in the MC simulation. Incoming neutrons are shown. The axes scale is shown in mm.

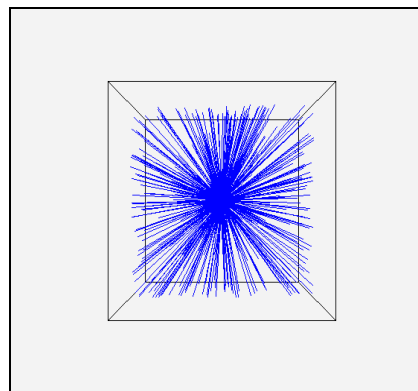


Figure 2: Isotropic neutron flux in the MC simulation. Outcoming neutrons are shown.

## 5. RESULTS

The results obtained for the variation of the self-shielding factors as a function of the controlled temperature are presented in this section. In all simulations the supercritical process in a PWR reactor were considered, using as fuel material  $^{235}\text{U}$  and assuming that  $\beta = 0.0065$ ,  $l = 0.0001\text{s}$ ,  $\lambda = 0.07741\text{s}^{-1}$ ,  $K_c = 0.05\text{K} / \text{MW}\cdot\text{s}$  and  $\rho_0 = 0.95\beta$ ,  $T(0) = T_0 = 300\text{K}$  and  $n(0) = n_0 = 10\text{MW}$ . The numerical method of finite differences was employed as the reference in the solution of point kinetics equations. Figure 3 shows the solution for the temperature of the reactor's core as a function of the time.

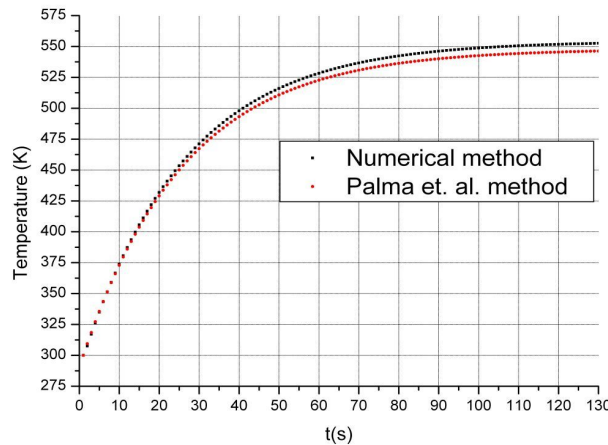


Figure 3: Temperature of nuclear core calculated by Eq. (11) and by the numerical method with  $\alpha = 5.0 \times 10^{-5}$ .

From fig. 3 it is reasonable to conclude that the expression proposed by Palma et. al. (2009) is adequate to estimate the temperature in the reactor's core where the gold disk used in the activation technique is placed. Using this result it was possible to estimate the maximum variation of the self-shielding factor as a function of time in a PWR reactor. These calculations were performed through the numerical approach described in section 2 and via the MC simulation described in section 3.

Figure 4 shows the effect of the temperature of the reactor core in the Doppler broadening, obtained by replacing Eq. (13) in Eq. (6):

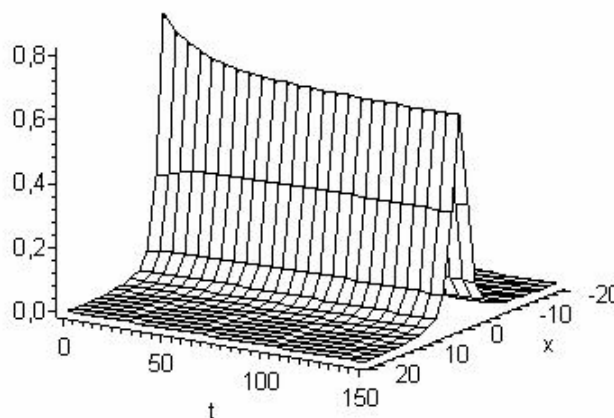


Figure 4: Doppler broadening function with temporal dependence.

In the MC simulation, each event generated contained one single neutron which was shot through the target volume. In order to evaluate the self-shielding factors it was necessary to simulate a huge number of events and then count those in which the neutron was captured. A total of  $2.5 \times 10^7$  events were simulated for each set of input parameters used in the analysis developed in this paper. Figure 5 shows an example of energy distribution of the captured neutrons in the target. The number of neutrons captured due to the resonance was estimated via a fit procedure that disentangled both the Breit-Wigner resonance distribution and the continuum  $1/v$  distribution. The fitted Breit-

Wigner was then used to evaluate the resonant self-shielding factors. The solid blue line represents the capture distribution due to the total cross section, the solid red line represents the resonant contribution to the total cross section and the dashed green line is the contribution of the continuum cross section.

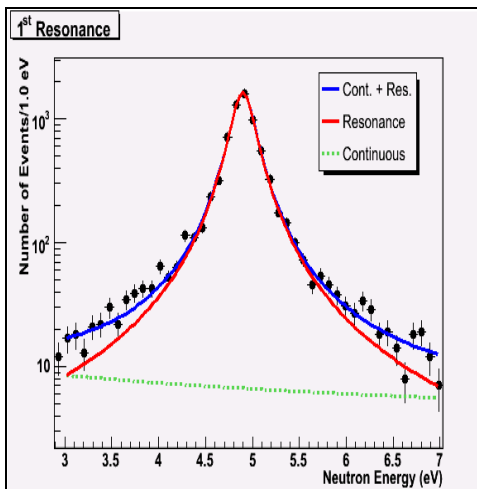


Figure 5: Energy distribution of the neutrons captured in the thin target. The different contributions to the cross-section are also indicated.

Figure 6 shows the self-shielding factor increase as function of the time for a 0.002 mm thin target. Very small variations of few percents were observed. The red dot markers indicate the values obtained by the method described in section 2. The blue squared markers indicate the values obtained through the MC simulation. The shapes of the curves obtained are quite similar. The values obtained for each curve differ by less than 30%. A perfect agreement was not expected since the assumptions used in section 2 usually do not hold for targets with widths higher than  $\sim 10^{-3}$  mm. On the other hand it was not possible to achieve satisfactory statistical uncertainties for the self-shielding factors using thinner targets in the MC simulation. Therefore, to perform this comparison the width of 0.002 mm for the gold target was used.

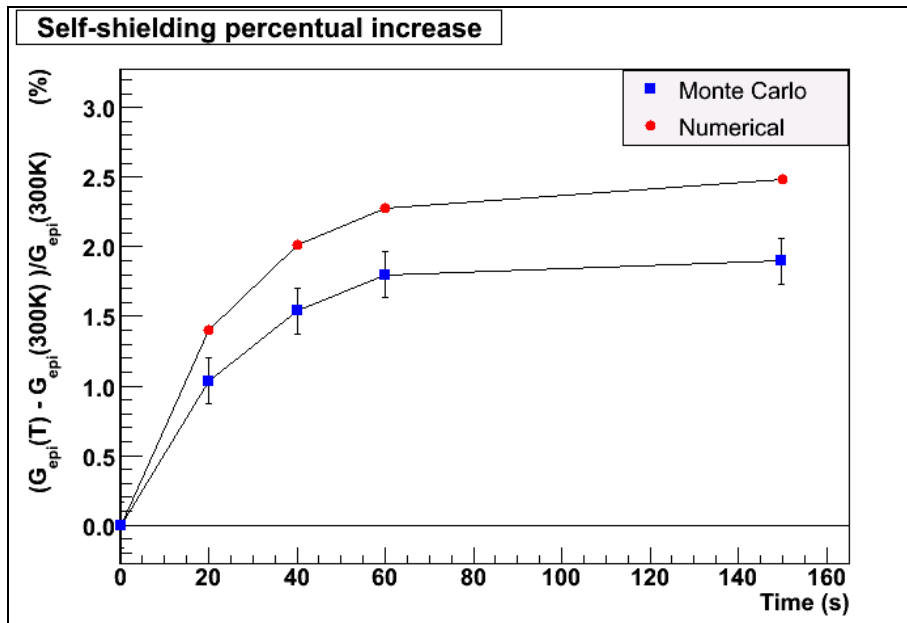


Figure 6: Variation of self-shielding factor as function of time calculated in percents. Red dots are the values obtained by the numerical method (section 2) and blue squares are the values obtained by the Monte Carlo method. In these calculations the coefficient of reactivity was  $\alpha = 5.0 \times 10^{-5}$  and the target width was 0.002 mm for the first resonance of  $^{197}\text{Au}$  isotopes.

## 6. CONCLUSIONS

This paper studied the behavior of self-shielding factors  $G_{epi}(\xi, \tau)$  with variations in the global temperature of the reactor core. As a practical application it was considered a transient near supercriticality where the temperature can be obtained analytically from the point kinetics equations with temperature feedback. A simple model shows that while the temperatures of the nuclear reactor changes during the process, the self-shielding factors vary little, corroborating with the practice of considering them constant in the technique of activation. The proposed method showed small deviations in relation to the values obtained from the Monte Carlo method, which demonstrates that both approaches are compatible.

## 7. ACKNOWLEDGEMENTS

The authors would like to acknowledge the support provided by FAPERJ and CNPq in the developing of this research.

## 8. REFERENCES

- Aboanber, A. E., Nahla, A. A., 2002. Solution of the point kinetics equations in the presence of Newtonian temperature feedback by Padé approximations via analytical inversion method. *J. Phys A: Math. Gen* 35, p. 9609 – 9627.
- Agostinelli, S. *et al.*, 2003. “Geant4 – A simulation toolkit”, *Nuclear Instruments and Methods A* 506, p. 250-303.
- Bitelli, U. D., Gonçalves, L. B., 2007, “The Self-shielding factors in activation detectors used in the IPEN/MB-01 reactor”, *International Nuclear Atlantic Conference (INAC)*, Santos.
- Bitelli, U. D., Gonçalves, L. B., Kuramoto, Y. R., 2007, “The Self-shielding factors in activation detectors used in the IPEN/MB-01 reactor”, *International Nuclear Atlantic Conference (INAC)*, Santos.
- Caldeira, A. D., 2007, “The self-shielding models used in the NJOY nuclear data processing system”, *International Nuclear Atlantic Conference*, Santos.
- Chen, W., Guo, L., Zhu, B., Li, H., 2007. Accuracy of analytical methods for obtaining supercritical transients with temperature feedback. *Progress in Nuclear Energy* 49, p. 290 – 302.
- Gradshteyn, I. S., Ryzhik, I. M., 2008, “*Tables of Integrals, Series, and Products*”, Academic Press Inc., New York.
- Jian, S., Cotta, R. M., 2000, “Improved lumped parameter formulation for simplified LWR thermohydraulic analysis”, *Annals of Nuclear Energy* 28, 1019 – 1031.
- Li, H., Chen, W., Zhang, F., Luo, L., 2007. “Approximate solutions of point kinetics equations with one delayed neutron group and temperature feedback during delayed supercritical process”, *Annals of Nuclear Energy* 34, 521 – 526.
- Nahla, A. A., 2009. An analytical solution for the point reactor kinetics equations with one group of delayed neutrons and the adiabatic feedback model. *Progress in Nuclear Energy* 51, p. 124 – 128.
- Palma, D. A., Martinez, A. S., Silva, F. C., 2006, “The Derivation of the Doppler Broadening Function Using Frobenius Method”, *J. Nucl. Sci. and Tech.* 6, p. 617-622.
- Palma, D. A., Gonçalves, A. C., Martinez, A. S., Silva, F. C., 2008, “New approximations for the Doppler broadening function applied to the calculation of resonance self-shielding factors”, *International Conference on Reactor Physics, Nuclear Power: A Sustainable Resource*, Interlaken.
- Palma, D. A., Silva, A. C., Gonçalves, A. C., Martinez, A. S., 2009. “An analytical method for prediction of transients with temperature feedback” Submitted to *Progress in nuclear energy*.
- Shcherbakov O., Harada H. 2002, "Resonance Self-Shielding Corrections for Activations Cross Section Measurements", *Journal of Nuclear Science and Technology, Japan* v. 39, n. 5, p. 548-553.
- Stacey, W. M., 2001. *Nuclear reactors physics*. Wiley–Interscience, New York.

## 9. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.