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Uncertainty analysis for the weighted least square fitted buildup factors in the point kernel module

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ABSTRACT

Point kernel method for nuclear power plant shielding analysis is widely used due to the simplicity of its application, implementation, and their fast solution. Point kernel method is mainly used to estimate an initial guess for the shielding design including material selection and shielding thickness. The buildup factor of point kernel method is of importance, which depends on photon energy and material attenuation parameter. In this paper, buildup factors of the point kernel method are put together from literature survey and a weighted least square fitting approach is used to provide more accurate results of the point kernel method. Uncertainties are evaluated when applying buildup factors based on the error propagation approach. Furthermore, a simple point kernel module is applied in the spherical geometry in order to test the fitted build up factors. Monte Carlo results are also used to validate the point kernel results with the least square fitted buildup factor in multi-layer test problems.

1. Introduction

The buildup factor is defined as the total flux including scattering and un-scattering events to un-scattered flux. And it is necessary to obtain reliable solutions of the radiation shielding analysis based on the point-kernel method. Dose absorption and energy absorption buildup factors are widely used in the shielding analysis, which are dependent of material, photon energy, and photon mean free path. The dose rate of the medium is main concern in the dose buildup factor, however energy absorption is of importance in the energy buildup factors (Trubey, 1996). Buildup factors begin with the empirical data by Goldstein and Wilkins. From then on lots of scientists have suggested several fitting approaches to obtain valid buildup factors and have tried to simulate the real application areas by utilizing advanced computational tools. ANSI/ANS-6.4.3-1991 standard data proposes both interpolation and extrapolation by means of an approximation method (Durani, 2009). Recently, Yoshida's geometric progression (GP) approach (Yoshida, 2006) is also proposed in a nonlinear fitted function and is widely used now. GP approach is also implemented in the QAD code (Broadhead and Emmett, 2009), which uses two kinds of buildup factors; DOSE for the standard air exposure response and ENG for the response of the energy absorbed in the material itself.

In the case of multilayer or stratified shielding problems, suitable buildup factors data is of main concern and many researches have been tried to generate the buildup factor data sets for certain configurations of multilayer shields (two layers or more) either as tabulated data or as figures (Bakos and Tsagas, 1994; Hirayama and Shin, 1998; Lin and Jiang, 1996; Shin and Hirayama, 2001).

In this paper, the weighted least square fitting method is taken into consideration to obtain a reliable uncertainty of buildup factor which is collected from several literatures proposed since 1991. The variances of the obtained buildup factors are used as a weight. Thus, the weighted least square fitting method provides an efficient result that makes good use of small data sets. It also provides different types of statistical intervals for estimation, prediction, calibration and optimization. And the main advantage of that weighted least squares is to handle regression where the data points are various qualities. When the variance of the random errors in the data is not constant across all levels of variables, the weighted least squares yields the most precise parameter estimates possible (NIST, 2012).

Total four datasets of air exposure buildup factors are analyzed for evaluation such as ANSI/ANS-6.4.3-1991, Taylor, Berger, and GP data (Chilton et al., 1984). And the uncertainty of buildup factor is derived from mainly based on the standard deviation of the fitted data and then it is combined by statistical and non-statistical results which are obtained from different methods. The dose rates of the point kernel method are also obtained and the uncertainties of the dose rate are evaluated by using the error propagation.

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Section 2 provides a brief review of the least square fitting methods and the fitted buildup factor for several materials are dealt with in Section 3. In order to verify the least square fitted results, a simple point kernel code is developed and its results are compared with those of the MCNP5 (X-5, 2003) code in Section 4. And finally, a summary and a conclusion of this work are given in Section 5.

2. Weighted least square fitting method

When buildup factors are distributed as a function of the mean free path for given photon energy, the weighted least square fitting method of the k-th order polynomial is expressed as follows

$$\begin{aligned} y_1 &= a_0 + a_1x_1 + a_2x_1^2 + a_3x_1^3 + \cdots + a_kx_1^k \\ y_2 &= a_0 + a_1x_2 + a_2x_2^2 + a_3x_2^3 + \cdots + a_kx_2^k \\ &\vdots \\ y_n &= a_0 + a_1x_n + a_2x_n^2 + a_3x_n^3 + \cdots + a_kx_n^k \end{aligned} \tag{1}$$

and their matrix form is easily obtained, too.

$$\begin{pmatrix} x_{10} & x_{11} & x_{12} & \cdots x_{1k} \\ x_{20} & x_{21} & x_{22} & \cdots x_{2k} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n0} & x_{n1} & x_{n2} & \cdots x_{nk} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_k \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \tag{2}$$

where a_j is a coefficient of x^j polynomial to be determined, and y_i is a buildup factor. In the case of the polynomial fitting method, mean free path, x_{ij} is expressed as $x_{ij} = x_i^j$.

The matrix equation with weighted least square method is written as in a simplified form such as

$$X^TWXA = X^TWY \tag{3}$$

where W is a weight matrix and it is a diagonal matrix of which term is $W_{ii} = 1/\sigma_i^2$. The variance of the buildup factor is defined as σ_i^2. It works as a weighting thus this least square fitting method is called as 'weighted least square method'. In this case, it is assumed that there are no correlations between buildup factors of y_i. For simplicity, when variances are not taken into consideration, the weight matrix is equal to the unit matrix.

Eq. (3) is solved easily by matrix inversion and the coefficients are obtained as (Chapra, 2013)

$$A = (X^TWX)^{-1}X^TWY \tag{4}$$

and their variances are also obtained as

$$V(a_j) = \sigma^2(a_j) \approx \frac{R}{n-m}(X^TWX)_{jj}^{-1} \tag{5}$$

where R is the total residue, $R = \sum_i (y_i - \hat{y}_i)^2$, $\hat{y}$ is an estimate of the given buildup factor of y, and m, n are the fitting polynomial order and number of data sets, respectively (Wikipedia, 2015). If we obtain the fitting coefficients, then the buildup factor ($\hat{y}$) is obtained given a mean free path (x). y is the provided raw data. In general, when evaluating the fitting variance, it is assumed that the variable of X has no errors. The standard deviation of the fitted buildup factor is easily expressed as follows when the third order polynomial is selected:

$$\begin{aligned} \sigma^2(\hat{y}(x_i)) = {} & \sigma^2(a_0) + x_i^2\sigma^2(a_1) + x_i^4\sigma^2(a_2) + x_i^6\sigma^2(a_3) \\ & + 2x_i\mathrm{cov}(a_0,a_1) + 2x_i^2\mathrm{cov}(a_0,a_2) + 2x_i^3\mathrm{cov}(a_0,a_3) \\ & + 2x_i^3\mathrm{cov}(a_1,a_2) + 2x_i^4\mathrm{cov}(a_1,a_3) + 2x_i^5\mathrm{cov}(a_2,a_3) \end{aligned} \tag{6}$$

where $\mathrm{cov}(a_i,a_j) \approx \frac{R}{n-m}(X^TWX)_{ij}^{-1}$. Depending on the distribution of raw data, the adequate fitting order can be chosen. In our test region, the data is smoothly distributed, thus the third order polynomial is selected to provide sufficient accuracy of fitted results.

3. Uncertainty of buildup factor

When a buildup factor (y) is a function of variables x (energy or mean free path), its combined uncertainty is expressed as follows:

$$\begin{aligned} & y = f(x_1, x_2, x_3, \cdots, x_n) \\ & U_y^2 = \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + \sum_{i=1}^n \sum_{j=1, j\neq i}^n \left(\frac{\partial f}{\partial x_i}\right)\left(\frac{\partial f}{\partial x_j}\right) u(x_i)u(x_j) \end{aligned} \tag{7}$$

where U_y is uncertainty of a buildup factor y and $u(x_i)$ is uncertainty of a variable of x_i. $\partial f/\partial x_i$ is the sensitivity coefficient of a variable x_i.

If there is no correlation between variables, the latter term of Eq. (7) will be neglected for evaluation of the combined uncertainty. For example, there are several useful ways for uncertainty evaluation such as additive and multiplicative rules:

$$\begin{aligned} & Y = cA + dB, \quad U^2(Y) = c^2u^2(A) + d^2u^2(B) \\ & Y = cA^2 - dB, \quad U^2(Y) = 4c^2A^2u^2(A) + d^2u^2(B) \\ & Y = cAB, \quad R^2(Y) = R^2(A) + R^2(B) \\ & Y = cA^2/B, \quad R^2(Y) = 2R^2(A) + R^2(B) \end{aligned} \tag{8}$$

where A, B: variables, c, d: constants, $U(Y)$: uncertainty of Y, $u(A)$: uncertainty of A, $R(Y)$: relative uncertainty of Y ($R(Y) = U(Y)/Y$), and $R(A)$: relative uncertainty of A ($R(A) = u(A)/A$).

Table 1
Buildup factors of concrete and lead for a 1 MeV photon source.

Normalized MFP	Concrete				Lead			
	ANSI/ANS	Taylor	Berger	GP	ANSI/ANS	Taylor	Berger	GP
0.5	1.45	1.733	1.645	1.450	1.20	1.158	1.149	1.195
1	1.98	2.488	2.311	1.982	1.38	1.312	1.296	1.367
2	3.24	4.069	3.708	3.233	1.68	1.612	1.582	1.675
3	4.72	5.746	5.194	4.711	1.95	1.900	1.860	1.952
4	6.42	7.524	6.774	6.405	2.19	2.176	2.130	2.206
5	8.33	9.409	8.452	8.308	2.43	2.441	2.392	2.444
6	10.40	11.406	10.233	10.412	2.66	2.697	2.645	2.670
7	12.70	13.520	12.122	12.713	2.89	2.942	2.891	2.886
8	15.20	15.757	14.124	15.202	3.10	3.178	3.129	3.095
10	20.70	20.624	18.490	20.718	3.51	3.626	3.582	3.495
15	37.20	35.402	31.786	37.287	4.45	4.616	4.593	4.426
20	57.10	54.690	49.171	57.153	5.27	5.462	5.445	5.275
25	80.10	79.676	71.661	79.966	5.98	6.200	6.155	6.014