

# MASTER

## PREDICTIVE MODELS BASED ON SENSITIVITY THEORY AND THEIR APPLICATION TO PRACTICAL SHIELDING PROBLEMS\*

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ABSTRACT

Two new calculational models based on the use of cross-section sensitivity coefficients have been devised for calculating radiation transport in relatively simple shields. The two models, one an exponential model and the other a power model, have been applied, together with the traditional linear model, to 1- and 2-m-thick concrete-slab problems in which the water content, reinforcing-steel content, or composition of the concrete was varied. Comparing the results obtained with the three models with those obtained from exact one-dimensional discrete-ordinates transport calculations indicates that the exponential model, named the BEST model (for basic exponential shielding trend), is a particularly promising predictive tool for shielding problems dominated by exponential attenuation. When applied to a deep-penetration sodium problem, the BEST model also yields better results than do calculations based on second-order sensitivity theory.

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INTRODUCTION

Because employing sophisticated shielding computer codes based on the Boltzmann transport equation incurs high costs and requires special expertise, relatively simple radiation shielding problems are usually solved by applying simplified models with which rapid and inexpensive calculations can be performed. For a number of years, the simple linear model has been the technique most frequently used. This model assumes that detailed transport calculations of the integral system performance parameter (that is, the desired response  $R$ ) have already been performed for a given shield, and that the impact on  $R$  due to changes in the material composition of the shield can be determined from sensitivity predictions based on first-order sensitivity theory. The required data base for the linear model calculations is a set of sensitivity coefficients  $P_{\Sigma}$ , also assumed to be available from previous calculations. Using the notation of Obloz,  $P_{\Sigma}$  can be expressed as

$$P_{\Sigma} = (\Sigma/R) (dR/d\Sigma), \quad (1)$$

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\*Worked performed while on assignment to Oak Ridge National Laboratory through the International Atomic Energy Commission.

where  $\Sigma$  is the data "field" and  $dR/d\Sigma$  is the functional derivative in an unperturbed system.

If only the change in the total response is desired, the linear model calculations can be performed on a desk calculator. If, however, changes as a function of energy are needed, a computer is required, and the calculations are facilitated by employing the SENTINEL code,<sup>2</sup> which uses as input the sensitivity coefficients and the fractional changes in the constituent cross sections, both as a function of energy.

When applied to reactor benchmark problems, the linear model and the SENTINEL code have been shown to predict changes in  $R$  that are in complete agreement with those obtained with the more sophisticated transport methods.<sup>3</sup> But when applied to shielding benchmark problems, large discrepancies have occurred, and these have raised questions as to the validity of a model based on sensitivity theory for shielding problems. To answer these questions, a program was initiated at ORNL to develop other, hopefully more satisfactory, predictive sensitivity models for shielding applications. To date, two models -- one an exponential model and the other a power model -- have been developed. This paper describes the models and shows how they compare with the linear model and with detailed transport calculations when applied to practical shielding problems.

#### DEVELOPMENT OF THE MODELS

The linear model can be deduced by considering the following formulation:

$$\frac{dR}{d\Sigma} = F \cdot P_{\Sigma^g}, \quad (2)$$

where the quantity

$$F = \frac{R^0}{\Sigma^0}$$

is constant, and the superscript zero refers to quantities evaluated in the original (unperturbed) system. In its most general form -- the form used by the SENTINEL code -- the solution is expressed as

$$R_L = R_0 \left[ 1 + \sum_g \sum_i P_{\Sigma_i^g} \left( \frac{\Sigma_i^g}{\Sigma_i^0} - 1 \right) \right], \quad (3)$$

where  $R_0$  is the response calculated for the original (unperturbed) shield,  $R_L$  is the response for the perturbed system, and the subscripts  $g$  and  $i$  denote the energy group and shield material constituent, respectively. For the case in which the variation in the macroscopic cross sections is not a function of the energy group, Eq. (3) reduces to:

$$R_L = R_0 \left[ 1 + \sum_i P_{\Sigma_i} \left( \frac{N_i}{N_i^0} - 1 \right) \right], \quad (4)$$

where

$$P_{\Sigma_i} = \sum_g P_{\Sigma_i^g}$$

is the total relative sensitivity for constituent  $i$ , and  $N_i$  and  $N_i^0$  are, for example, the perturbed and unperturbed number densities, respectively, for constituent  $i$ .

### Exponential Model

In the exponential model, the quantity  $F$  in Eq. (2) is defined as

$$F = \frac{R}{\Sigma^0}$$

and varies with  $R$ . The exponential model solution ( $R_E$ ), analogous to Eq. (4), is then

$$R_E = R^0 \prod_i \left\{ \exp \left[ \left( \frac{N_i}{N_i^0} - 1 \right) P_{\Sigma^0} \right] \right\}, \quad (5)$$

which can also be expressed as

$$R_E = R^0 \left( \exp \left[ \sum_i P_{\Sigma^0} \left( \frac{N_i}{N_i^0} - 1 \right) \right] \right). \quad (6)$$

### Power Model

In the power model, the quantity  $F$  in Eq. (2) is defined as

$$F = \frac{R}{\Sigma}$$

and varies with both  $R$  and  $\Sigma$ . From this, we obtain a power model solution ( $R_P$ ) for changes in the response function that are independent of the energy group:

$$R_P = R^0 \prod_i \left( \frac{N_i}{N_i^0} \right)^{P_{\Sigma^0}}. \quad (7)$$

### APPLICATION TO CONCRETE SLAB PROBLEMS

The linear, exponential and power models were compared by using each to calculate changes in the tissue dose rates emerging from 1- and 2-m-thick concrete shields that were exposed to a normally incident fission source and were perturbed with respect to (1) water content, (2) rebar content, or (3) concrete composition. The data base for the comparisons consisted of sensitivity coefficients for the following reference cases: 1- and 2-m-thick slabs of standard concrete (4.96 wt% water); and 1- and 2-m-thick slabs of rebar concrete. The compositions of these slabs are given in

Table 1. Slab Compositions Used in This Study

Element	Atomic Density ( $10^{24}\text{cm}^{-3}$ )			
	Standard Concrete	Rebar	Homogenized <sup>a</sup> Rebar Concrete	TSF Concrete
H	7.77 (-3) <sup>f</sup>		7.18 (-3)	8.88 (-3)
C	1.00 (-9) <sup>f</sup>	9.82 (-4)	7.46 (-5)	7.97 (-3)
O	4.39 (-2)		4.06 (-2)	4.20 (-2)
Na	1.05 (-3)		9.70 (-4)	2.73 (-5)
Mg	1.49 (-4)		1.38 (-4)	1.44 (-3)
Al	2.45 (-3)		2.26 (-3)	4.14 (-4)
Si	1.58 (-2)		1.46 (-2)	3.83 (-3)
S	5.64 (-5)		5.21 (-5)	1.015 (-4)
K	6.93 (-4)		6.40 (-4)	2.34 (-3)
Cn	2.92 (-3)		2.70 (-3)	1.00 (-2)
Mn		5.15 (-4)	3.91 (-5)	
Fe	3.13 (-4)	8.37 (-2)	6.65 (-3)	2.64 (-4)
Density (g/cc)	2.34	7.83	2.76	2.39

<sup>a</sup>Same as standard concrete at 0.924 volume fraction plus rebar at 0.076 volume fraction.

<sup>f</sup>Read  $7.77 \times 10^{-3}$ .

<sup>†</sup>Low concentration assigned to avoid distortion of answers.

Table 1, together with the composition of a concrete that has long been used in radiation shielding experiments at ORNL's Tower Shielding Facility. The TSF concrete was also used in the model comparisons.

Transport calculations for the reference cases performed with the ANISN disopete ordinates code in both the forward mode and the adjoint mode provided the tissue dose rates for the unperturbed systems and

also constituted the first step of the sensitivity calculations. The calculations used the VITAMIN-C cross-section library applied with  $P_3$  cross-section expansion and  $S_{16}$  angular quadrature. The quantity calculated was the dose equivalent rate per unit incident flux [ $(\text{rem}\cdot\text{h}^{-1})/(\text{cm}^{-2}\cdot\text{s}^{-1})$ ] due to fission neutrons penetrating through the slab to the detector and to secondary gamma rays produced within the slab and reaching the detector.

Table 2. Total Macroscopic Cross-Section Sensitivities Used as Reference Base for the Prediction Models

Constituent	$P_3$ Sensitivity <sup>a</sup>	
	1-m slab	2-m slab
Standard Concrete Slabs (4.96 wt% Water)		
Water	-2.00043	-2.81860
H	-1.7334	-2.32544
C	-9.63386-08	-1.50955-07
O	-3.0218	-5.57983
Na	-0.14651	-0.276091
Mg	-0.017964	-0.0332595
Al	-0.30203	-0.566342
Si	-1.9073	-3.79948
S	-0.007529	-0.0159036
K	-0.13386	-0.300728
Ca	-0.47229	-1.00945
Fe	-0.068398	-0.0987944
Rebar Concrete Slabs (7.6 vol% Steel)		
Concrete	-7.48073	-12.9769
Steel	-1.29088	-2.84410

<sup>a</sup>Relative dose rate change per relative density

The sensitivity coefficients were obtained with the JULIET module of the FORSS code system. In all cases, the sensitivities considered were the sensitivities of the total dose rate at the exit face of the slab to the total, absorption, and elastic-scattering cross sections. For the standard concrete slabs, these sensitivities were calculated for the individual constituents of the concrete, for the total mix, and for the water content of the slabs. For the rebar concrete, the sensitivities were calculated for the homogenized steel and for the homogenized rebar concrete. The results for both types of concretes are shown in Table 2. For the third concrete (the TSF concrete), the effect investigated was the effect of varying the total mix of constituents from that of standard concrete.

### Problem 1 -- Variation of Water Content of Standard Concrete Slabs

In this problem the cross-section change for water is not a function of energy, and thus it can be expressed as

$$\frac{\Sigma_{wR}}{\Sigma_{wG}^0} = \frac{\sigma_{wR} f_w}{\sigma_{wR} f_w^0} = \frac{f_w}{f_w^0}, \quad (8)$$

where  $f_w$  and  $f_w^0$  are the weight fractions of water for the perturbed and unperturbed cases, respectively. Using Eq. (8), the prediction models become

$$R_L = R^0 \left[ 1 + P_{\Sigma^0} \left( \frac{f_w}{f_w^0} - 1 \right) \right], \quad (9)$$

$$R_E = R^0 \left\{ \exp \left[ P_{\Sigma^0} \left( \frac{f_w}{f_w^0} - 1 \right) \right] \right\}, \quad (10)$$

and

$$R_P = R^0 \left( \frac{f_w}{f_w^0} \right)^{P_{\Sigma^0}}, \quad (11)$$

where  $P_{\Sigma^0}$  is the sensitivity due to water for the standard concrete reference (unperturbed) cases (see Table 2). Values of  $f_w$  varied from about 2 wt% to 8 wt%. The ratio of the total dose rate calculated with each model to the dose rate obtained from a corresponding ANISN calculation is plotted as a function of the water content of the perturbed concrete slab in Figs. 1a and 1b. Note that a value of unity for the ratio is the desired result.

### Problem 2 -- Variation of Rebar Content of Concrete Slabs

For this problem it was assumed that the concrete and steel could be homogenized and that equivalent number densities based on the volume fractions of steel and concrete could be used. Again, the cross-section changes considered (for steel and concrete) are not functions of energy and thus can be expressed as

$$\frac{\Sigma_{cR}}{\Sigma_{cG}^0} = \frac{\sigma_{cR} N_c}{\sigma_{cR} N_c^0} = \frac{N_c v_c}{N_c v_c^0} = \frac{v_c}{v_c^0}, \quad (12)$$

where  $v_c$  and  $v_c^0$  are the volume fractions of concrete in the perturbed and unperturbed slabs, respectively, and  $\Sigma$  and  $N$  represent equivalent quantities because of the assumption of homogenization of the slabs. In a similar expression for steel,  $v_s$  and  $v_s^0$  are, respectively, the perturbed and unperturbed volume fractions of steel in the slabs. Using Eq. (12), the prediction models in this case become

$$R_L = R^0 \left[ 1 + P_{\Sigma^0} \left( \frac{v_c}{v_c^0} - 1 \right) + P_{\Sigma^0} \left( \frac{v_s}{v_s^0} - 1 \right) \right], \quad (13)$$

$$R_E = R^0 \left[ \exp \left[ P_{\Sigma_c^0} \left( \frac{v_c}{v_c^0} - 1 \right) + P_{\Sigma_s^0} \left( \frac{v_s}{v_s^0} - 1 \right) \right] \right], \quad (14)$$

and

$$R_P = R^0 \left( \frac{v_c}{v_c^0} \right)^{P_{\Sigma_c^0}} \left( \frac{v_s}{v_s^0} \right)^{P_{\Sigma_s^0}}, \quad (15)$$

where  $v_c^0$  and  $v_s^0$  are 0.924 and 0.076, respectively, and  $P_{\Sigma_c^0}$  and  $P_{\Sigma_s^0}$  are the sensitivities due to concrete and steel for the reference (unperturbed) rebar slab cases (see Table 2). The results for the 1- and 2-m-thick rebar slabs are shown in Figs. 1c and 1d, respectively.

### Problem 3 -- Variation of Concrete Composition

In this problem we attempted to predict the dose rate response for slabs of concrete having the nonstandard composition of the TSF concrete. This problem tests the possibility of using the models for a concrete composition in which all the constituent elements are in different concentrations than those in the standard concrete used as the reference case. Here again the cross-section change (for each element) is not a function of energy and is simply represented by the ratio of number densities of each constituent, as indicated, for example, by Eqs. (4), (6), and (7). That is, the  $N_i$ 's are the atom densities of the constituent elements in the TSF concrete, and the  $N_i^0$ 's are the atom densities of the corresponding constituent elements in the standard concrete. In this case, the exponential model gives results 5% lower than the ANISN results for the 1-m-thick slab and 14% lower for the 2-m-thick slab. The power model gives answers much too large and the linear model gives answers much too small.

### Summary of Concrete Problems

For the case of the standard concrete slabs with variations in water content, the exponential model gives results for the 1-m-thick slab that are within 13% of the ANISN results for a water content of 3 to 8 wt%. For the 2-m-thick slab, the exponential model gives results that are within 21% of the ANISN results for a water content of 3 to 7 wt%. The power model does not perform quite as well for the 1-m-thick slab but gives better results (within 9%) for the 2-m-thick slab. The linear model does not work very well at all, especially for the 2-m-thick slab.

For the case of the rebar slabs, the exponential model gives results that agree within 9% with the ANISN results for the 1-m-thick slab for the entire range of rebar content (4 to 20 vol%) and within 13% for the 2-m-thick slab. The power model and the linear model both do reasonably well for the 1-m-thick slab and rebar contents below 10 vol%, but they give poor results for higher rebar contents. They also give poor results for the 2-m-thick slab over the entire range of rebar content.

For the TSF concrete case, only the exponential model yields acceptable results.

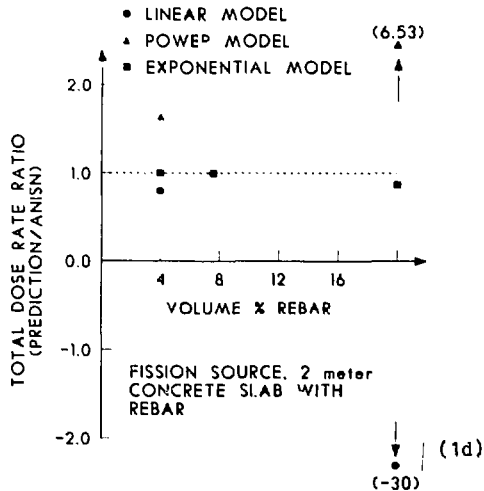
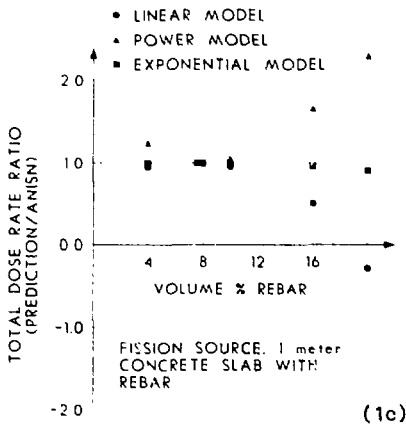
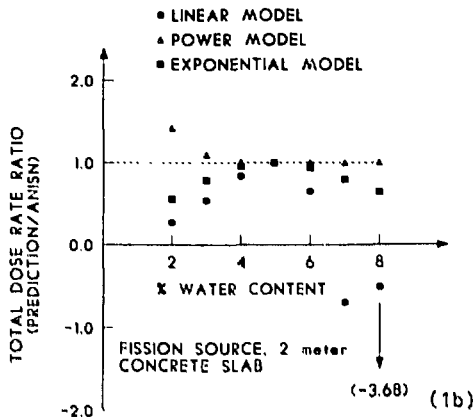
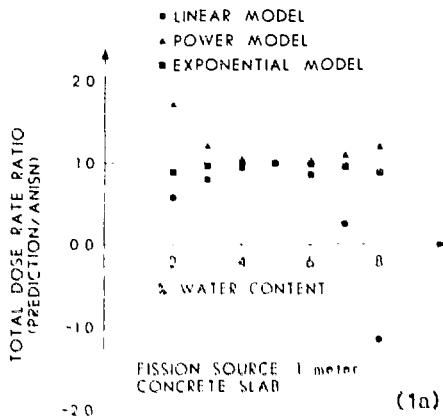


Fig. 1. Comparison of Dose Rates Predicted with Three Models. Plotted as ratio of model-predicted dose rate to ANISN-calculated dose rate.



## APPLICATION TO NEUTRON TRANSPORT IN SODIUM

In order to further investigate the applicability of the exponential model to shielding problems, we have applied it to a deep-penetration sodium problem for which results from other calculations were already available. Greenspan et al. <sup>10</sup> investigated higher order effects in cross-section sensitivity analysis for neutron transport through 260 cm of sodium. The energy of the neutron source was just above 297 keV, which is the energy of the major cross-section minimum in sodium, and the response of interest was the neutron fluence at an energy just below 297 keV. They developed a second-order sensitivity theory (SOST) and compared

results obtained with that theory with theory with results obtained with first-order sensitivity theory (FOST) (that is, the linear model). They also recalculated the problem with the perturbed cross-section set (exact). The variation studied was that of the cross section in the 297-keV minimum region, allowing the perturbed-to-initial-value ratio ( $\sigma/\sigma_0$ ) to vary from 0.5 to 1.5.

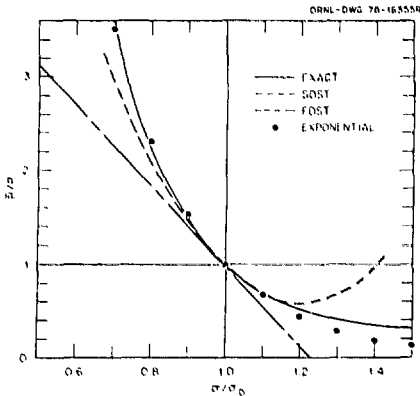


Fig. 2. Comparison of Predicted Dose Rates for Deep-Penetration Sodium Problem. All results except exponential model results are from ref. 10.

In applying the exponential model to the same problem, we used the sensitivity coefficient which Greenspan et al. had calculated for use in their linear (FOST) model. The results of the four methods (FOST, SOST, exact, and exponential) are compared in Fig. 2, which was taken from ref. 10 and our results added. It can be seen that the exponential model does as well as, or significantly better than, the SOST model for the entire range of cross-section variation considered.

### DISCUSSION OF RESULTS

For the range of problems considered, the exponential model gives, overall, the best results, consistently outperforming the linear model. The reason for this lies in the nature of deep-penetration problems dominated by large attenuation, which can make them very sensitive to cross-section changes. In the concrete slab examples chosen, the change in calculated responses induced by variations in the parameters studied varied from a factor of 4 for the 1-m-thick rebar slab to a factor of 42 for the 2-m-thick concrete slab. For the sodium problem, the responses varied by at least a factor of 10. Thus, the basic assumption required in the linear model, i.e., that the flux not change significantly, is obviously violated for these problems. Some insight into the success of the exponential model can be gained by looking at assumptions inherent in the models.

Referring to Eq. (2), the linear model suggests that the quantity  $R \cdot P_{\Sigma} / \Sigma$  vary slowly with cross-section change in the range of interest. The exponential model suggests that  $P_{\Sigma} / \Sigma$  vary slowly, while the power model suggests that  $P_{\Sigma}$  vary slowly. We have tested this by performing a sensitivity calculation for a 1-m-thick concrete slab with 3 wt% water and comparing the results with those calculated for our standard case (4.96 wt% water). The comparisons showed that:

$$\frac{P_{\Sigma} / \Sigma_w}{P_{\Sigma^0} / \Sigma_w^0} = \frac{P_{\Sigma} / f_w}{P_{\Sigma^0} / f_w^0} = 1.15, \quad (\text{Exponential})$$

$$\frac{R_{\Sigma} \cdot P_{\Sigma} / f_w}{R_{\Sigma^0} \cdot P_{\Sigma^0} / f_w^0} = 2.72, \quad (\text{Linear})$$

and

$$\frac{P_{\Sigma}}{P_{\Sigma^0}} = 0.69 \quad (\text{Power})$$

With the ideal value for the ratios being unity, the exponential model obviously gives the best results.

It is interesting to note that the exponential model can be represented as a Taylor series expansion with as many terms as desired. The linear model is obtained by retaining the first term with  $\Delta \Sigma$ . Viewed from this perspective, the exponential model can be thought of as higher order sensitivity theory in that terms of higher order in  $\Delta \Sigma$  are inherent in the function.

## CONCLUSIONS

For the range of problems considered, the exponential model gives the best results, the linear model gives answers that are too low and in many cases are negative, and the power model predicts answers that are, in general, too high and in many cases diverge. The power model does have the advantage of being conservative in most cases, however.

Because the exponential model works well for shielding problems dominated by attenuation, it has been denoted as the basic exponential shielding trend model -- or the BEST model. The BEST model is recommended for use as a predictive tool for studying the effect of cross-section changes for shielding problems.

A more detailed discussion of the models and of data bases developed for use with the models is given elsewhere.<sup>11</sup>

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