Design Optimization of a Neutron Activation Based Explosives Detection System

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INTRODUCTION

The use of neutrons for detection and characterization of explosives has been extensively studied [1-3] especially for their detection in vehicles [4], air cargo [5] and for humanitarian demining [6-8]. In an Explosives Detection System (EDS) based on thermal neutron activation (TNA), a neutron source is used to activate an unknown sample to detect the scattered neutron and gamma signals which are used as signatures for material identification as well as to estimate the quantity of a concealed explosive. Several design studies have been carried out [9-12] for portable systems capable of detecting small amounts (<300g) of TNT, RDX, etc. concealed as deep as 10-15cm in soil.

The design efficiency of a TNA based EDS depends on the neutron source and detectors (neutron and photon) in an optimal arrangement of moderating and absorbing materials to obtain 'good' signals. Moderators such as polyethylene, borated ethylene, and paraffin have been considered and neutron sources such as ^{252}Cf and ^{241}Am-^{9}Be on the performance of an EDS [10-15].

Explosives such as TNT consist of hydrogen, carbon, oxygen and nitrogen which can be detected by signature gamma rays, especially 2.22 MeV γ-rays from hydrogen and 10.83 MeV γ-rays from nitrogen. Sources producing ~10^7 neutrons/s stably have been shown to effectively detect gamma rays of 10.83 MeV from 800 g melamine (plastic) explosives over a measurement time of 1500 s. Detailed Monte Carlo simulations [10] have shown that a landmine system using neutron backscattering could detect a small cylindrical landmine distinguishing down to <300 g TNT explosive from other nearby substances until a burial depth of 15 cm in limestone with a scanning speed of 9.6 m^2/min.

Experiments have also been carried out for TNT of mass 1000, 520 and 200 g using ^{252}Cf for 900 s counting time [13] with a helium detector for neutrons and a NaI detector for gamma rays [12].

Design optimization issues crucial to an EDS based on TNA relate to (i) the moderation of fast source neutrons, since the radiation capture (n,γ) reaction varies inversely with neutron energy, and (ii) the selection and optimal placement of moderators for enhanced BF_3 detector efficiency as well as the radiation shielding. These issues are addressed in this paper by carrying out a simulation of an EDS with MCNP5 and discussing alternative optimization methods based on a variational formulation [16] in a two-group formulation [17] and on Monte Carlo (MC) perturbation theory based on derivative sampling [18-20]. Simulation is carried out for an EDS, with a californium ^{252}Cf source, to obtain estimates of the (n,γ) reactions, in a soil with a concealed explosive, and B (n,α) reaction rates in BF_3 detectors. This analysis extends existing work in the literature by modeling the source cavity to obtain an optimal source configuration so that, by minimizing direct source contribution to the detectors, a good signal (from a concealed explosive)-to-noise ratio (SNR) may be achieved.

MODELING AND SIMULATION

The model of the EDS, consisting of a point source S, with a schematic layout of the BF_3 and NaI detectors is shown in Fig. 1 and material compositions are listed in Table 1. The source spectrum for ^{252}Cf is modeled by the Watt spectrum in MCNP5 with a probability distribution function for energy: $f(E) = Ce^{-E/a}\sinh\sqrt{bE}$, a=1.025, b=2.926.

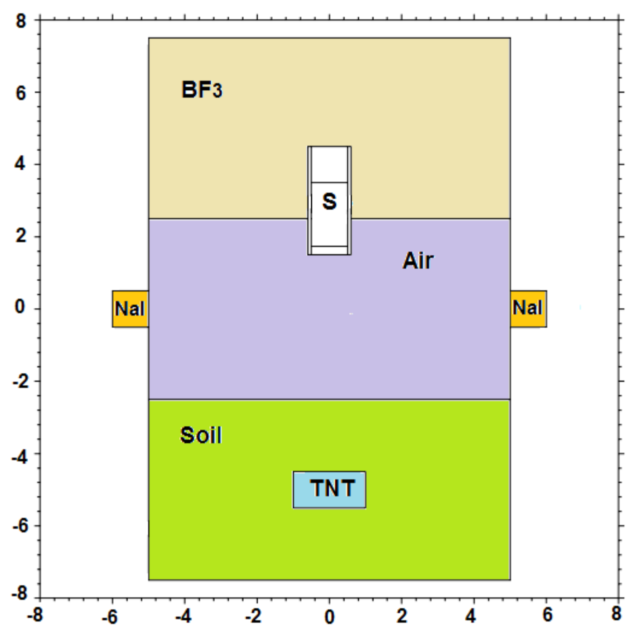

Fig. 1. Model of the Detection System (dimensions in *cm*).

For the simulation, the Monte Carlo code MCNP5 [18] is used. The candidate materials for moderator and absorber are polyethylene, borated polyethylene, paraffin wax and boron carbide. Estimates are made of the (n,α) reaction rates in the BF_3 counters and of the (n,γ) reactions in the explosive/soil region. All simulations were carried out for TNT explosive in a cylinder of radius 3 cm and height 3 cm (mass ~ 140.3 g) buried at a depth of 1 cm below the soil.

Table 1: Composition of materials (w_i = mass fraction)

Element and w_i			
Dry Air: $\rho = 0.0012$ g/cm^3			
$^{14}_{7}N$ 0.75519	$^{16}_{8}O$ 0.23179	$^{12}_{6}C$ .00014	$^{40}_{18}Ar$ .0129
Wax: $\rho = 0.930$ g/cm^3			
$^{1}_{1}H$ 0.148605	$^{12}_{6}C$ 0.85139		
Soil (Limestone): $\rho = 2.71$ g/cm^3			
$^{12}_{6}C$ 0.12	$^{16}_{8}O$ 0.48	$^{40}_{20}Ca$ 0.40	
BF_3: $\rho = 0.002567$ g/cm^3			
$^{10}_{5}B$ .143368	$^{11}_{5}B$ 6.568e-3	$^{19}_{9}F$ 0.850064	
TNT: $\rho = 1.654$ g/cm^3			
$^{1}_{1}H$ 0.022189	$^{12}_{6}C$ 0.37016	$^{14}_{7}N$ 0.185	$^{16}_{8}O$ 0.423

Design optimization by the variational formulation

For design optimization, two variational formulations can be considered viz the continuous and the discrete (Pontryagin's Maximum Principle PMP). In the 'continuous variational formulation', the Lagrangian is written as

$$\mathcal{L} = < u(x)\sigma_x^T, \underline{\phi} > + < \underline{\phi}^{+T}, \widehat{M}\underline{\phi} > \quad (1)$$

with an objective to obtain the optimal distribution $u^*(x)$ by taking first-order variations for a stationarity condition. With variations in $u(x), \underline{\phi}, \underline{\phi}^+$ and $\widehat{M}$ and requiring the variations in the trial functions be zero in the domain (excluding the boundary) the stationarity conditions can be obtained. These are solved to give the fluxes which are used to obtain the optimal distribution $u^*(x)$.

In the 'discrete variational formulation', the coupled second-order ODEs $\widehat{M}\underline{\phi} = 0$ are written in state space form with a defined performance index P.I. $= < u, \phi >$. The first-order equations are written as

$$\dot{y}_i = f_i\left(\underline{y}, u, x\right), i = 0,1,2,3,4 \quad (2)$$

with the P.I incorporated by setting $\dot{y}_0 = f_0\left(\underline{y}, u, x\right) = u y_3$ and with the associated Lagrange multiplier as $\lambda_0 = 1$, the Hamiltonian is written as

$$H = \sum_{i=0}^{4} \lambda_i f_i\left(\underline{y}, u, x\right) \quad (3)$$

to give the adjoint equations which can be solved using the transverse boundary conditions. The Hamiltonian is then written as a function separating the terms containing the control u as follows:

$$H = g(u, x) + h(x) \quad (4)$$

and thus the shape of $g(u)$, also refered to as the 'switching function', determines which of the admissible values of the control u are to be applied according to the PMP: $H(\underline{y}^*, u^*, x) \geq H(\underline{y}^*, u, x)$ where $u_{\min} \leq u \leq u_{\max}$. The discrete form simplifies the continuous form by permitting the control u to be a constant in a particular sub-domain of the problem. Thus where $g(u, x)$ is minimum (either sign), $u_{\max}$ is applied and *vice versa*. The number of zeros of the switching function will determine the number of controls applied. Both these formulations, can in principle, be used to obtain optimal material distributions.

Design optimization byMC perturbation theory

While the above 'deterministic' approach is applicable to regular geometries, the MC method is a 'natural' choice for realistic (often irregular) geometries and hence optimization techniques in MC simulation would be preferred if possible. However, optimization analyses require the ability to estimate the effect of small material density or geometry perturbations. A drawback of MC methods is that the uncertainty of an estimate may be of the same order of magnitude as the perturbation itself and thus the effect of the design or operational change may become masked. This implies that the difference of two MC simulations may be inadequate to estimate perturbations. Perturbation techniques were developed with 'correlated tracking' and 'derivative sampling' techniques by Rief [19] The techniques were extended by Watkins for material perturbations in a research reactor and demonstrated for two-group transport for fusion reactor neutronics optimization studies by Koreshi et al [20]. The perturbation feature is now part of several MC codes and is used extensively. The change in a response function such as dose D, due to a variation in an independent parameter, such as material density ρ, expressed as a Taylor series

$$D(\rho) = D(\rho_o) + D'(\rho_o)\delta\rho + \frac{1}{2!}D''(\delta\rho)^2 + \cdots$$

can thus be used with first- and second-order derivatives D' and D'' from a single run.

RESULTS

In this section, simulation results are presented to investigate the effect of (i) source energy on photons produced in a concealed explosive, (ii) effect of moderating the source neutrons, (iii) effect of a moderator on the BF_3 detection system, and (iv) the effectiveness of the radiation shielding in an EDS.

Effect of source energy

To investigate the effect of source energy on the (n,γ) reactions, MCNP5 simulations were carried out in the range 0.01 – 5 MeV for the model in Fig. 1. From simulations of 10^5 source neutrons with typical CPU times of ~0.3 minutes each and MCNP relative standard errors within 4%, it was seen that N(n,γ) reduced from 1.72269 X 10^{-6} reactions cm^{-3} per source neutron to 1.50811 X 10^{-8}, H(n,γ) reduced from 1.27126 X 10^{-5} to 4.24581 X 10^{-8}, C(n,γ) reduced from 1.82070 X 10^{-7} to 2.92567 X 10^{-8}, O(n,γ) reduced from 8.75284 X 10^{-9} to 1.86949 X 10^{-11} with a total reduction from 1.46262 X 10^{-5} to 1.42674 X 10^{-7} reactions cm^{-3} per source neutron i.e. the decrease is by a factor of ~100 over the energy range considered. Thus, a low energy spectrum is highly advantageous for an EDS. For source energies exceeding 5 MeV, there is a reversal in this trend as the (n,γ) reaction cross-section begins to increase – a doubling in the reaction rate was found with an increase of source energy from 5 MeV to 10 MeV.

Effect of moderating source neutrons

The effect of moderating the source neutron at emission was studied by varying the thickness of a moderator such as polyethylene. Fig. xxx shows the effect of the moderator on the energy spectrum of incident and emergent neutrons from the ground for a source of 0.5 MeV and a moderator cylinder of radius 0.5 cm and thickness 4 cm. The F1 tally results are shown for the incident and emergent currents J^{-}, J^{+} with and without moderator.

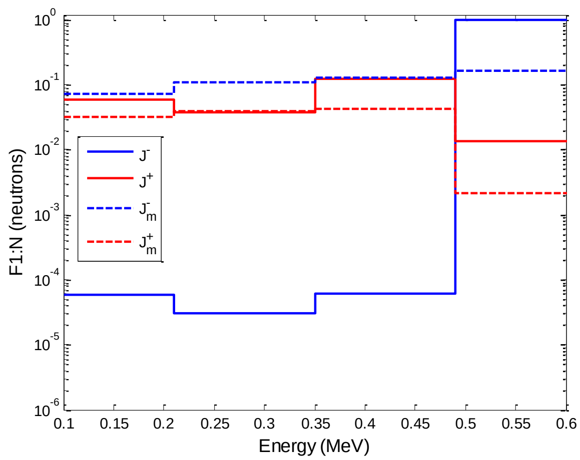

Fig.2. Effect of moderation of 'fast' source neutrons on Incident and emergent neutron currents from the soil.

Figure 2 shows an improved (i.e. softer) incident energy spectrum with moderation compared with only the fast neutrons. However, the emergent spectrum remains better without moderation of source neutrons. The reason for this is the attenuation of the source by the moderator, resulting in an incident fraction of 0.480 i.e. a reduction of over ~52% and an emergent fraction of 0.116.

Effect of moderator on BF_3 detection

As mentioned in an earlier section, the moderation of neutrons is important for efficient BF_3 detection due to the high $B^{10}(n,\alpha)$ reaction cross section as seen in Fig.3. Thus, a moderator layer before the BF_3 leads to an increase in the neutron flux till an optimum thickness is reached. For the case of borated paraffin wax, MCNP simulations showed that the optimal thickness is ~ 4 cm and thereafter, the reduction in intensity leads to a decrease in neutron slowing-down and subsequently in the overall detection efficiency.

Radiation shielding

In order to consider the radiation dose reduction from a number of moderators, MCNP5 simulations were carried out that for a shield of radius 5cm, with a 25μg ^{252}Cf point source for the following materials: SS316, water, polyethylene (P), borated polyethylene (B), and B_4C, lead with the combinations SBB, SWW, SWS, all B, all P, and all water. The neutron and gamma doses, calculated from the ICRP H*(10mm) ambient dose equivalent fluence-to-dose conversion factors, are shown in Fig. 4. For a water shield, the neutron dose is 6.75 rem/h while the photon dose is 5.87 rem/h compared with a SS316 shield giving a neutron dose 10.11 rem/h and a photon dose 0.0347 rem/h. It was found that the lowest neutron dose is from a polyethylene shield while B_4C gives the lowest photon dose.

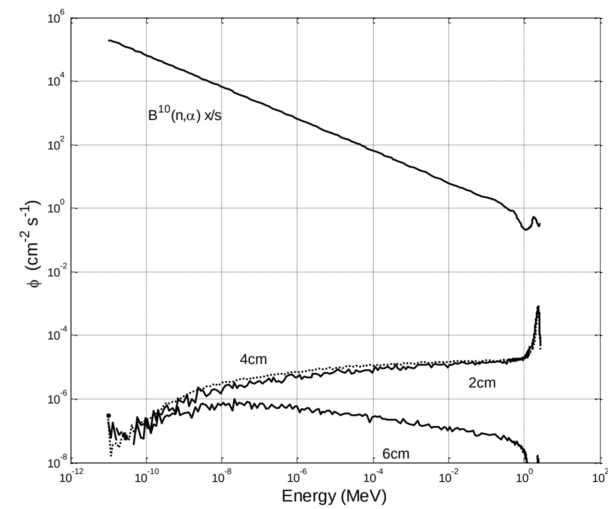

Fig.3. Neutron flux in BF_3 detector for varying B-paraffin wax moderator thickness shown with the B(n,α) cross-section.

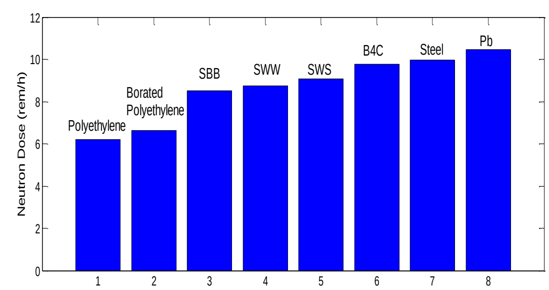

Fig. 4. Neutron dose (rem/h) with a shield of thickness 5cm.

Thus, an optimized configuration for the shield surrounding the source is estimated by a selection of the materials to minimize the direct neutron signal to the BF_3 detectors and the direct γ signal to the NaI detectors. Similarly, the effect of a hydrogenous moderator such as water on the source spectrum is shown in Fig. 5 for TNT and ammonium nitrate explosives in the presence of both air and water. The increased effect of the 'softening' of the neutron spectrum is seen for the ^{252}Cf source.

CONCLUSIONS

As discussed in earlier sections, three possible routes for optimization studies are (i) repeated simulations, (ii) variational formulation-based optimization, and (iii) MC perturbation theory based optimization.

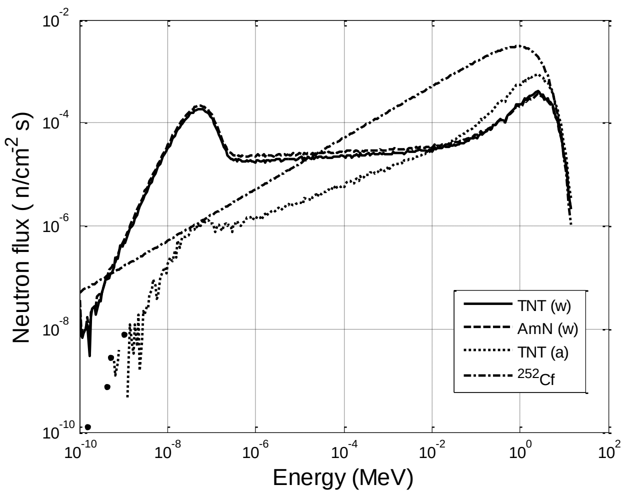

Fig. 5. Effect of water on the spectrum in TNT, Ammonium Nitrate.

In this work, the first approach was used, while the latter two can be demonstrated; especially MC optimization through the PERT feature of MCNP5. From the simulations carried out, it was concluded that low source energy is preferred while 'direct' moderation of the 'fast' source neutrons, though beneficial for radiative capture and subsequent activation of the concealed explosive, reduces the intensity of the incident signal to an extent that the overall detection efficiency is reduced.

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