THE NEUTRON MACROSCOPIC CROSS SECTIONS CALCULATION OF SOME MINERALS BY USING FLUKA MONTE CARLO METHOD

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Abstract: Because of neutrons are uncharged particles, they are powerful in terms of penetration into the material. Recently shielding is an important issue because of neutrons which have many applications today do not harm living tissue. Different compounds, alloys and composites are usually preferred against neutrons as shielding material. The aim of this project is to determine minerals (Veatchite(Sr₂B₁₁O₁₆(OH)₅*(H₂O)), Sussexite(Mn⁻²BO₃(OH)) and Vimsite(CaB₂O₂(OH)₄), based new shielding materials against neutron particles using by Fluka Monte Carlo method and then to obtain neutron total macroscopic cross sections and several shielding parameters by experimentally.

Key words: Neutrons, Macroscopic Cross Section, Fluka Monte Carlo

Introduction

Ordinary time, the neutron shielding effects of materials were examined for nuclear reactor shielding design and many shielding experiments and calculations were performed to obtain the removal cross sections of the materials. The neutron attenuations of materials were evaluated with the cross sections. After that, benchmark or mock-up experiments on the multi-layer problem to confirm the shielding characteristics or to evaluate analysis accuracy were reported recently, the need to transport spent nuclear fuels is increasing due to the current limited storage capacity. Considering that the existing storage facilities will be full by 2016, a national policy for spent fuel urgently needs to be established. Nowadays, the application field of neutron particles has increased and new scientific studies about discovering materials with higher performance that the material which are already used and can be used as a shield against neutrons has been prepared. A fast neutron loses their energy basically by the elastic crashes with atomic nucleus. In recent years, there has been rapid growth of electron accelerator based neutron sources for medical and industrial applications because of their compactness (Patil B.J., Chavan S.T, Pethe S.N., Krishnan R., Dhole S.D., 2010). In this study, neutron shielding for mineral appearance is seen in Figure-1(a,b,c) (http://www.mindat.org; http://webmineral.com/data).

A neutron can come to the thermal balance with the centre periphery of the atom by reaching 0.04 eV energy at ambient temperature after a lot of crashes. In these contributions, it is always valid as a simple and clear way to use Fluka Monte Carlo simulation techniques. It is possible to work intuitively on a neutron ray reaching the thermal balance.

Fig1. Neutron Shielding For Materials. (http://www.mindat.org; http://webmineral.com/data)
Methodology of the Monte Carlo FLUKA

Monte Carlo codes are extensively used for probabilistic simulation of various physical systems. These code are widely used in calculations of neutron radiation shielding and gamma ray transport in materials (Wielopolski L., Song Z., Orion I., Hanson A. L., Hendrey G., 2005). Monte Carlo methods are very different from deterministic transport methods. Deterministic methods, the most common of which is the discrete ordinates method, solve the transport equation for the average particle behavior. The other hand, Monte Carlo does not solve an explicit equation, but rather obtains answers by simulating individual particles and recording some aspects of their average behavior. Monte Carlo is well suited to solving complicated 3-D time-dependent problems (Bremister, J., 1993.). FLUKA code is a sub-program of the Monte Carlo code. It is a general purpose tool for calculations of particle transport and interactions with matter, covering an extended range of applications (Korkut, T., Karabulut, A., Budak G. et al., 2012). FLuka is a multipurpose transport Monte Carlo code, for calculations of particle transport and interactions with matter from electron and proton accelerator shielding to target design, calorimetry, activation, dosimetry, detector design, ADS systems, neutrino physics, radiotherapy, shielding design etc. Therefore, Fluka is a tool that is constantly employed in the majority of CERN applications where energy deposition has to be calculated through beam-matter interactions, as well as for radiation protection and shielding simulations. Fluka program works with Fortran Software written with machine code. The developments of Fluka program started with being used for Monte Carlo application for protons with high energy by J. Ranft and H. Geibel in 1962. Monte Carlo technique is randomly number selection technique from one or more probabilistic distribution in a special trial or simulation study (Hançerliogulları, A. 2006). The Mcnp code was used for reactor designs and calculations. The Monte Carlo simulation code Geant developed at CERN, allows the simulation of the particle shower generation and propagation inside a medium with a complicated geometry or composition. To follow hadrons inside matter, Geant is interfaced to Fluka, Gheisha and Micap codes. In particular, MICAP allows the simulation of neutron propagation and interaction within an energy region from 20 MeV down to 10⁻⁵ eV. The flux calculation has been completely carried out in the framework of the FLUKA Monte Carlo code (Battistoni, G., Ferrari A., Montraruli T., Sala P.R., 2003; Battistoni, G., Francesco, B., Markus, B., Mauro C., et al., 2011). The Fluka collaboration ensures the constant update of the code with the most advanced physics and features. Fluka is based, as far as possible, on original and well tested microscopic models. Due to microscopic approach to hadronic interaction modeling, FLUKA features a combinatorial geometry which is constantly enhanced in order to cope with new demands for more complex detector descriptions. The FLUKA simulations are carried out for a detailed description of an ideal calibration set up, exposing the detector only to direct collimated and monochromatic neutron beams avoiding any diffused radiation contribution (Borio di tigliole, A., Cesana, A., Dolfini R. et al., 2001).

Shielding Applications and Material

The development of medical technology and medical equipment using radiation has played a key role in the diagnosis and treatments of many diseases. In particular, the utilization of radiation for invasive procedures, such as angiography, has been expanded so that the exposure of patients and medical staff to radiation also tends to increase, making individual radiation protection a very important issue (Seon-ichi K., Kyung-Rae D., Woon-Kwan C., 2012). Shielding must be provided around a reactor to protect both personnel and material. Shielding that is adequate for neutrons and gamma rays will also stop alpha and beta particles. The weight of shielding to be used is almost independent of the shielding material itself. This study aims to evaluate the neutron shielding effects of tree materials, Veatchite, Sussexite and Vimsite by using a neutron source. Properties of minerals are shown in Table 1. The attenuation effects through shielding materials were investigated for various thicknesses of the materials. Neutrons are uncharged particles and are powerful in terms of penetration into the material. Neutrons, which has many applications today. In shielding design it is often useful to perform a first assessment of the required shielding thickness by using a simplified approach based for example on a point source line of sight model, to be verified at a more advanced stage of the project with a Monte Carlo simulation in a more realistic geometry of the facility (Agosteo S., Magistris M., Mereghetti, 2007). Neutron sources are more important in neutron shield measurements. The neutrons originate from spontaneous fission and from some (a, n) reactions in the source materials. The spontaneous fission and (a, n) neutron source terms are dependent on the kind of isotope and the decay time. For the prevent harm living tissue, shielding is an important issue. There are different compounds, alloys or composites are preferred against neutron particles using like shield. The purpose of this study was to shield against neutron radiation can be used as a material in three different mineral containing boron and hydrogen, and the evaluate of interaction these minerals with 4.5 MeV energy neutron using Monte Carlo simulation method. Neutron shielding is most effective is the nucleus of the shield material has about the same mass as the neutron. This makes hydrogen rich materials excellent neutron shits. It needs also to be something to absorb the neutrons, boron being the poison of choice. Conversely gamma shielding requires neutrons with very high mass. Were it not for the presence of the neutrons, depleted or native uranium would be the best choice (in fact depleted uranium is commonly used as shielding material for X-ray machines and radiography sources), but since neutrons and uranium shielding would
be counterproductive, lead is used instead. This nuclear code enables the use of possibility for particles from thermal energy neutrons to all other particles having energy and extensive radiation ranges.

Table 1: Properties of minerals (http://www.mindat.org; http://webmineral.com/data).

<table>
<thead>
<tr>
<th>Properties</th>
<th>Vimsite</th>
<th>Sussexite</th>
<th>Veatchite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>(CaB₂O₄(OH)₂)</td>
<td>(Mn₂BO₂(OH)₁₁)</td>
<td>(Sr₂B₂O₁₆(OH)₅(H₂O)₅)</td>
</tr>
<tr>
<td>Color</td>
<td>Colorless</td>
<td>white, green, pink, straw yellow</td>
<td>Colorless, Pearl White</td>
</tr>
<tr>
<td>Density</td>
<td>2.54 gr/cm³</td>
<td>3.12 gr/cm³</td>
<td>2.62 gr/cm³</td>
</tr>
<tr>
<td>Diaphaneity</td>
<td>Transparent</td>
<td>Translucent</td>
<td>Transparent</td>
</tr>
<tr>
<td>Hardness</td>
<td>4-Fluorite</td>
<td>3-Calcite</td>
<td>2-Gypsum</td>
</tr>
<tr>
<td>Luster</td>
<td>Glassy</td>
<td>Pearly</td>
<td>Vitreous-Pearly</td>
</tr>
<tr>
<td>Streak</td>
<td>White</td>
<td>White</td>
<td>White</td>
</tr>
<tr>
<td>Cleavage</td>
<td>Perfect</td>
<td>Perfect</td>
<td>Perfect</td>
</tr>
<tr>
<td>Locality</td>
<td>Siberia-Russia, Buriatia</td>
<td>South Africa, Kalahari</td>
<td>USA, Tick Canyon, Los Angeles, California</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>CaO % 34.67, B₂O₃% 43.05, 22.28 % H₂O</td>
<td>MnO % 61.82, B₂O₃ % 30.33, H₂O % 7.85</td>
<td>SrO % 31.73, B₂O₃ % 9.65, H₂O % 58.62</td>
</tr>
<tr>
<td>Magnetism</td>
<td>no</td>
<td>no</td>
<td>no</td>
</tr>
<tr>
<td>Radioactivity</td>
<td>no</td>
<td>no</td>
<td>no</td>
</tr>
</tbody>
</table>

General Equation for calculating shielding

In simplest form shielding involves interposing distance and materials between the source and recipient of radiation. Design considerations and the calculation of resultant dose complicate the problem. To gain some insight into shielding calculations we shall consider an oversimplified situation which involves a point source of radiation (National Council on Radiation Protection and Measurements, 1977).

According to the inverse-square law, the intensity of radiation on the surface of a sphere of radius R will be

\[ I = \frac{P}{4\pi R^2} \]  \hspace{1cm} (1)

If we place enough distance between ourselves and the source, the intensity of radiation will be reduced to safe levels. However, if we place material between ourselves and the source, we can take advantage of a collimated beam of gammas. The intensity of radiation follows an exponential curve

\[ I = I_0 e^{-\mu x} \]  \hspace{1cm} (2)

where \( \mu \) is linear absorption coefficient and has dimensions of reciprocal centimeters. A mass absorption coefficient may be defined by \( \mu_m = \gamma_0 \mu \), Equation -2 then becomes where D is the absorber thickness.

\[ I = I_0 e^{-\mu_m D} \]  \hspace{1cm} (3)
For a sphere of radius $R$, if put $X=R$, equation-2 will became

$$I = I_0 e^{-\mu R} \quad (4)$$

applies strictly to a collimated beam and only when scattered radiation is removed from the beam. In a thick shield such as that equation -4 would give a low result because some of the radiation is backscattered into the path. When primary neutrons dominate the shielding situation, the shielding transmission ratio for neutrons, $B_n$, can be derived from the neutron fluence rate, $\Phi_0$. The various types of interactions of neutrons with matter are combined into a total macroscopic cross sections value (Korkut, T., Karabulut, A., Budak, G. et al., 2012; Korkut, T., Korkut, H., Karabulut, A., Budak, G. 2011).

$$\sum_{TOTAL}^{} = \sum_{fission}^{} + \sum_{capture}^{} + \sum_{scatter}^{} + \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldotted

The fundamental purpose of radiation shielding is to reduce the dose-equivalent index from all sources of radiation that converge on a particular reference point, so that the dose-equivalent index rate at the reference point does not exceed the applicable $H_m$ or dose-limit value mathematically, this can be stated as follows:

$$\bar{H}_{Ld} \leq H_m \quad (6)$$

Where, $\bar{H}_{Ld}$ is the sum of dose-equivalent index rates at the reference point, $H_m$ is the applicable $H_m$ or dose-limit rate and $F_j$ is the maximum absorbed dose rate or particle fluence rate from the $j$th source, $B_j$ is the shielding transmission ratio for the radiation from the $j$th source, $T$ is the occupancy factor of the area represented by the reference point, $K_j$ is dimension-converting constant pertaining to radiation from the $j$th source, $D_j$ is the distance between the $j$th radiation source and the reference point.

$$\bar{H}_{Ld} = \sum_{j} F_j B_j T_{K_j D_j} \quad (7)$$

Monte Carlo methods can calculate directly the self-shielding factor taking into account the multiple scattering. The resonance self-shielding factor, $T_{res}(R)$, in wires of radius $R$, is defined as the ratio between the reaction rates per atom in the real sample and in a similar and infinitely diluted sample.

$$T_{res}(R) = \frac{\int_{C_2}^{C_1} \Phi_0(C) \sigma(C) dE}{\int_{C_2}^{C_1} \Phi(C) \sigma(C) dE} \quad (8)$$

where $\Phi_0(C) \propto C_1^{-1}$ is the original no-perturbed, epithermal neutron flux per unit energy interval inside the infinitely diluted sample, $\Phi(C)$ represents the perturbed epithermal neutron flux inside the real sample, $\sigma(C)$ denotes the $(n,\gamma)$ cross-section, and $C_1$ and $C_2$ are, respectively, the lower and the upper limits around the resonance energy $C_{res}$ (Gonçalves, I.F., Martinho, E., Salgado J., 2001; Gonçalves, I.F., Martinho, E., Salgado J., 2001).
Calculations
In this study the effects of cross section for high performance materials such as Veatchite, Sussexite and Vimsite were calculated, and also the parameters of the neutron armor of these materials were measured. There are many advantage using materials having hydrogen and boron in terms of neutron shielding technology because the neutron shielding capability.

![Fig2](image1.png)

**Fig2.** Isotope production for mineral Veatchite

depends heavily on the hydrogen concentration. As a shield material against neutron the interactivities with neutron particles with 4.5 MeV by the Fluka simulation method of three different minerals containing boron and hydrogen. A Comparison of double differential fluency predicted by FLUKA at various at a neutron energy. The Isotope production are shown in Fig 2–4. The effectiveness of different types of neutron shielding for the ATLAS forward region has been studied by means of Monte Carlo simulations and compared with the results of an experiment performed at the CERN PS (Štekl,J.,Pospsil S.,Kovalenko, V.K et al.,2000.)

![Fig3](image2.png)

**Fig3.** Isotope production for mineral Vimsite
Fig 4. Secondary radiation curve for mineral Vimsite

Fig 5. Compared neutron absorption cross sections minerals and concrete
Results and Conclusions

In our working, we have investigated fast neutron shielding properties of Vimsite, Sussexite and Veatchite samples simulation process. The results of this investigation have provided new information about the total macroscopic cross sections, secondary radiation, neutron flow absorbed doses and deposited energies by low energy neutron interaction of fast neutrons through materials including different amounts of boron and hydrogen atoms per unit volume. Absorbed dose per primary particle (in GeV/g) by samples calculated over Fluka. Simulation results are shown Fig-5. According to these results, the highest performance among the minerals is vimsit for the neutron shielding. Interaction of three different boron-containing mineral particles and 4.5 MeV energy neutron were simulated by Monte Carlo techniques. As a result of simulation studies minerals isotope production rates for the neutron radiation, flows and secondary curves were obtained. As a result of interactions has not found radioactive isotopes. It also was not detected in the secondary radiation with high stream. Evaluation of the total macroscopic cross sections for neutron shielding minerals (μ) and the stored energy values were determined. For frequently used in studies of neutron shielding concrete were calculated of the same values. All three minerals has been identified as a better neutron shield material than concrete.

References

http://www.minadat.org; http://webmineral.com/data
Korkut, T., Karabulut, A., Budak, G. et al., 2012. Investigation of neutron shielding properties depending on number of boron atoms for colemanite, Ulexite and tincal ores by experiments and Fluka Monte Carlo simulations. Applied Radiation and Isotopes. 70, 341-345
Štekli, J., Pospisil, S., Kovalenko, V.K et al., 2000. Monte-Carlo simulations of neutron shielding for the ATLAS forward region. Nuclear instruments and methods in physics research A. 452,458-469