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Study for the Development of a Biosensor Oriented at the Interaction-Response of Chemical War Agents and Ionizing Radiations

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1. Introduction

The development of technologies has always been gaining prominence due to its great potential in meeting demands closely linked to exposed weaknesses. These needs may be related to applications in energy, medicine, radiopharmaceuticals and curative, interventional and diagnostic health, applications in the areas of security and defense, food technologies, academic development, among others. The use of applied nuclear physics opens up a set of great possibilities due to the capacity for interaction between the development of new instrumentation and what our imagination allows us to do. The combination of applied nuclear physics and integrated biological systems allows us to convert one form of energy into a different one, based on the reading of a transduced biological signal, for example, an initial purely chemical signal into an electrical signal.

The ability to detect or sense chemical warfare agents and ionizing radiation in the same device is something new, there are no records about a device or tool. In addition to increasing national autonomy on the topic, with a view to minimizing costs as an essential engineering parameter, it corroborates ideas of nuclear safety, microstructure applications, nuclear engineering applications, efficiency, quality (sensitivities) and others. The development of new biosensors with versatile applications shows new possibilities, being capable of acting in the characterization of chemical warfare agents (such as detection of organophosphates) and ionizing radiations.

Keywords: Biotechnology; Biosensor; Organophosphate; Nuclear; Radiation

2. Methodology

In this work, the biosensor with potential application for detecting organophosphate compounds and ionizing radiation will be developed in three stages: the first stage through theoretical studies, the second stage through molecular modeling studies (docking) between a biological receptor (molecular target) and the compounds of interest, using molecular mechanics, in the case of chemical warfare agents, and quantum calculations, in the case of ionizing radiation using computer simulation with the MCNPX code (general purpose Monte Carlo radiation transport code, continuous energy, geometry generalized, time-dependent) and Vised software which is a visual editor for MCNPX. The results of the *in silico* studies will serve as a starting point for the construction of the biosensor (which is the third stage of this study).

Creation of systems: Figures 01, 02 and 03 related to some organophosphates created for molecular modeling and Figures 04, 05 and 06 visual geometries for simulation in MCNPX.

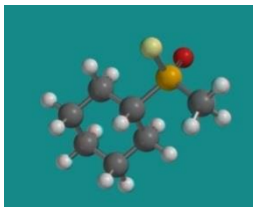

Fig. 01: Cyclo-Sarin

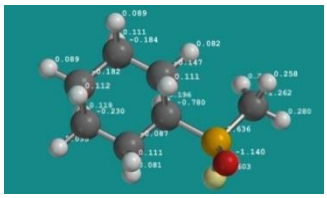

Fig. 02: Cyclo-Sarin with charge

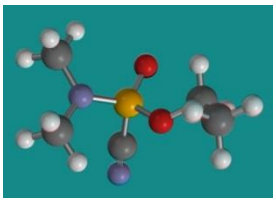

Fig. 03: Tabun

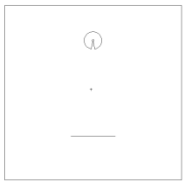

Fig. 04: VISED 2D System

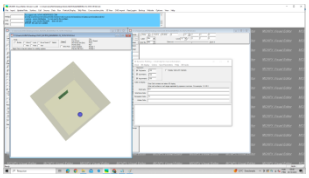

Fig. 05: VISED 3D System

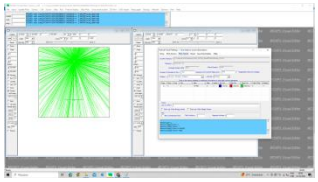

Fig. 06: VISED System Simulation

3. Results and Discussion

It is possible to address the agreement of results obtained through computational simulations, from the creation of organophosphate molecules, such as chemical warfare agents, in addition to simulations via MCNPX resulting in information that characterizes a representative model. By focusing on the schematic representation, it is possible to verify a certain trend among the resulting data, from the dispersion of energy around a given target, the absorbed energy, the energy due to the Compton effect, scattering and other properties. The graphs in Figures 07 and 08, below, show the number of particles generated, the number of particles that escape (do not collide with the target) and those that are captured:

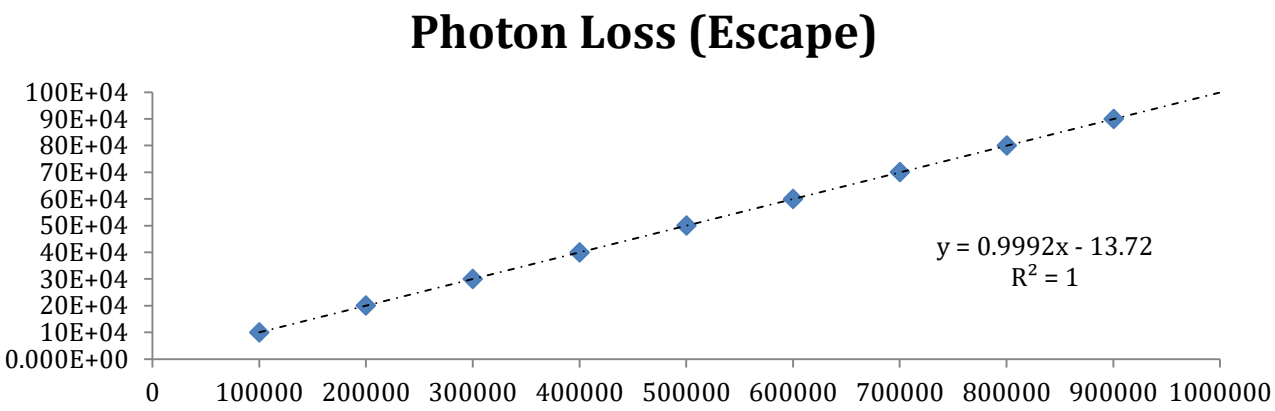

Fig. 07: Particles that do not reach the target (plate under study).

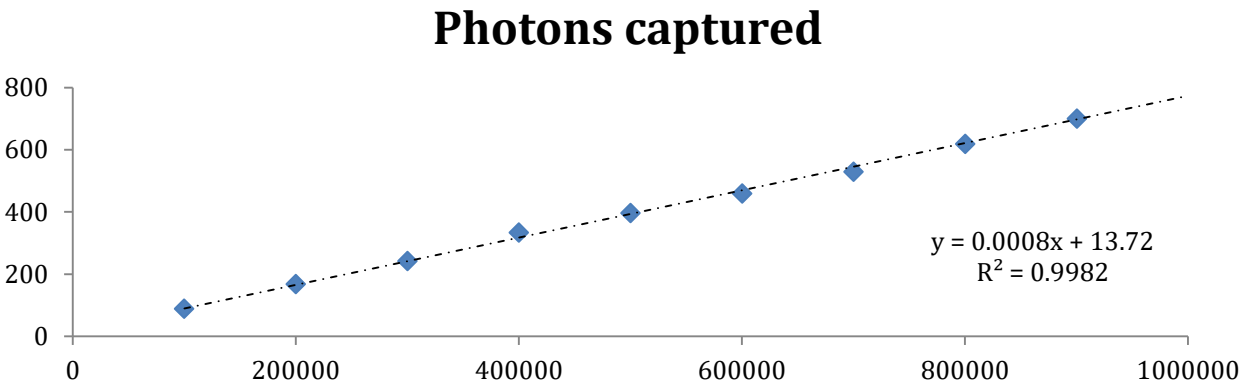

Fig. 08: Particles that reach and are captured by the target (plate under study).

In this way, when dealing with statistical phenomena, it is possible to relate the behavior of the system in relation to the amount of energy deposited on the study plate (target) that represents the biosensor interface, whether with this energy deposited in the medium it will be possible to be quantified, how this interaction will emit a response signal, the proportionality of the signal, which are materials and notes for an empirical evaluation, but partially predictable with the well-modeled and representative study system, once the amount of energy of the particles is known, the other variables corroborate to outline the entire system.

4. Conclusions

The research and data guide the formalization and materialization of the prototype, since a subtle variation in the electrical potential can be measured, conclusions and inferences can be made. This can generate significant impacts, both due to its innovative potential and as a resource to be used in the field compared to systems that use radionuclides for other studies. It is expected that the proposed equipment will be able to perform detection quickly, accurately and at a lower cost, contributing to the development of a national product.

Acknowledgements

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