

# Radiation Damage in Scintillator Detector Chemical Compounds: A New Approach Using PPO-Toluene Liquid Scintillator as a Model

C. H. Mesquita, J. M. Fernandes Neto, C. L. Duarte, P. R. Rela, and M. M. Hamada

**Abstract**—The effect of radiation damage was evaluated in PPO-Toluene liquid scintillator solution. Samples containing PPO (1% w/v) diluted in toluene were prepared and irradiated at different doses, using a  $^{60}\text{Co}$  irradiator at 1.8 Gy/s. The effect of radiation on transmittance, light output, and chemical modification in the PPO were evaluated before and after irradiation. Transmittance loss at 360 nm decayed exponentially with the dose. The light output decreased as the radiation dose increased. PPO degraded biexponentially with the dose, whereas PPO degradation products, such as benzoic acid, benzamide, and benzyl alcohol, increased with the dose.

**Index Terms**—Compartmental analysis, liquid scintillation detector, PPO, radiation damage, target theory.

## I. INTRODUCTION

THERE is a continuous effort to develop detectors capable to resist high radiation dose in order to survey the environment in nuclear reactors, in particle accelerators, and in industrial irradiation plants.

Organic scintillators are used in several applications, mainly in nuclear physics, astrophysics, and particle accelerators research. Vasilchenko *et al.* [1] reported that the interest for new radiation-resistant organic scintillators has increased due to a new generation of high-energy accelerators. The search for new radiation-resistant plastic scintillators was renewed in many scientific centers. In particular, polystyrene-based scintillators attracted the attention of researchers due to their high light yield and comparatively low cost. These searches have resulted in the discovery of a number of new radiation-resistant scintillators [1]–[3].

Although these detectors are composed of several chemical elements, studies evaluating radiation damage have emphasized its overall aspects [1], [4]–[6]. This kind of study is adequate when the resistance to the radiation damage is used to compare the quality among different types of detectors or to evaluate the suitability of their use in inhospitable environments. Otherwise, this approach is not suitable to infer the causes of the quality loss

of the detector. For instance, in organic detectors, the damage can occur due to 1) disarrangement in the polymeric chain matrix (e.g., polystyrene), as can be inferred from Chong *et al.* [3], or 2) the break or degradation of the scintillator component (e.g., PPO). Furthermore, degradation of the organic detector is a complex matter that needs study, including of the kernel of the detecting system, i.e., the scintillator.

In physicochemical studies, gamma- and X-ray radiations are used to detect interactions between free radicals (radiolytic) and substrates [7]–[9]. Among free radicals, solvated electron ( $e_s^-$ ) has special interest because it is the main radiolytic product of the irradiated materials, as inferred from Getoff [7] and Haofang *et al.* [8], [9].

The radiation interaction is intrinsically similar to chemical reactions. The prompt radiolytic concentration is proportional to the dose rate, i.e., it depends on the number of photons that interact with the material, and then the studies carried out with radiation would be formulated as the chemical reaction. Studying irradiated ethanol, Haofang *et al.* [9] described the chemical kinetics using

$$\frac{d[e_s^-]}{dt} = k_i \cdot D^* - k_3 \cdot [e_s^-] \cdot [\text{CH}_3\text{CHO}] - k_2 \cdot [e_s^-] \cdot [\text{C}_6\text{H}_5\text{COCH}_3]$$

where  $e_s^-$  is the concentration of solvated electron,  $D^*$  is the dose rate, and  $k_i$  is the initial chemical yields of  $e_s^-$ . Reactions have been considered as a second-order type, and the dose as a “compound.”

Few studies detailing the radiation damage in chemical constituents of the detector have been described, although this knowledge could be valuable to developing optimized radiation-resistant detectors and to understand the origin of the damage mechanism. For example, one scintillator can produce a good physical response in its radiation interaction. However, it can be unstable from the energetic point of view, reducing the mean life of the detector. In fact, Chong *et al.* [3] observed that a detector doped with 0.7% primary scintillator 2,5-bis-(styryl-4)-oxadiazole + 0.025% of POPOP was able to provide a high level of scintillation light output. However, detectors based on these dopants do not resist high radiation dose.

Hamada *et al.* [4] has reported that in detectors under strong radiation field, the light conversion yield and the transparency decrease. Loss of these properties is affected differently by several factors, such as the absorbed dose intensity, dose rate, temperature, and environmental gas composition during the irradiation.

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C. H. Mesquita is with the Instituto de Pesquisas Energéticas e Nucleares IPEN-CNEN/SP, Sao Paulo, Brazil, and the Faculdade de Ciências Farmacêuticas, Universidade de Sao Paulo, Brazil (e-mail: chmesqui@usp.br).

J. M. Fernandes Neto, C. L. Duarte, P. R. Rela, and M. M. Hamada are with the Instituto de Pesquisas Energéticas e Nucleares IPEN-CNEN/SP, Sao Paulo, Brazil.

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Pla-Dalmau *et al.* [6] carried out several studies of radiation damage using different dose rates and pressure conditions. They state that understanding of the complete mechanisms on the polymeric chain degradation is necessary in order to develop new techniques for construction of detectors, capable of increasing the stability of the materials when submitted to strong irradiation.

When a radiation-resistant detector is required, knowledge of the activation energy can be an important parameter to select among the scintillator options. Furthermore, damage studies are capable of explaining some physical and chemical properties of the radiation detectors [4]. "Target theory" is an interpretative model to explain radiation-induced cell killing. This model has been extended to other fields of interest, especially to biological molecules and chemical reactions [5], [10], [11]. It is known that target theory is not applicable under water irradiation conditions, and this is a major limitation of the method. In liquid solutions, so-called indirect effects can occur. For example, water irradiation results in the formation of  $H^+$ ,  $OH^-$ , peroxide, and other radiolytic products, which can diffuse at appreciable distances before reacting. Thus, the inactivation can occur by the direct action of radiation and by secondary chemical inactivation induced by the free radicals.

Kempner and Schlegel [5] used the target theory to determine the molecular weight of enzymes. Empirically, enzymes are at least two times more sensitive to radiation in solution than in dry state. So far, this subject has been studied in dry state, where direct action of radiation occurs on matter and the damage is caused entirely by primary ionization.

This paper evaluates the effects of radiation damage on an organic detector, using the target and the compartment theory. The damage effects in liquid solution were focused on PPO and on toluene. The damage caused by the radiation was evaluated by the following measurements: a) light-output yield (pulse-height analysis), b) optical transmission, and c) analysis of the chemical modifications in the detector. For analysis of these parameters, a predictable mathematical model, based on the compartment theory, was designed to estimate the degradation of PPO, and a sigmoid model was applied to predict the transmittance as a function of dose  $D$ .

## II. MATERIAL AND METHODS

Although plastic scintillators have been frequently chosen for high-energy physics studies [1], the liquid scintillator was chosen in this study due to the facility of discriminating the effect of damage in the scintillator component. Toluene was used as the solvent because it is not polymerized by radiation and can be easily separated from the solid scintillator PPO and non-volatile residues by evaporation.

Twenty samples were irradiated in duplicate containing toluene and PPO. Twenty more samples in duplicate containing only the toluene were irradiated in a Gammacell-type irradiator containing  $^{60}Co$  source of 334 TBq (9021 Ci), at a dose rate of 1.8 Gy/s. The doses were extended up to 1000 kGy to accentuate the production of damage and for better definition of the concentration curves for the resulting chemical products. After irradiation, the toluene contained in

the flasks was evaporated in an oven at 40 °C. Subsequently, nonirradiated toluene (10 mL) was added to restore the sample. A small source of  $^{137}Cs$  was used to study the light yield of the irradiated samples. The source was fixed in the bottom of the flask (external face) and placed in the measurement chamber of the Beckman Liquid Scintillator model LS150. This procedure was repeated for each sample. The signal generated from the two phototubes processed by the coincident and sum circuit was connected to an amplifier (Ortec 450). The output signal from this amplifier was connected to a multichannel analyzer ADCAM (Ortec 918), and the spectra of the source  $^{137}Cs$  were used for pulse-height analysis. An aliquot of 1  $\mu$ L from each sample was taken for gas chromatograph mass spectrometer (GCMS) analysis (Shimadzu GCMS-QP5000), and 1 mL was used to measure transmittance (Shimadzu spectrophotometer UV-1601 PC).

Fig. 1 displays the outline of the compartment model adopted to explain the degradation of PPO in the liquid scintillator. This model is represented mathematically by the system of differential equations

$$\frac{df_1}{dD} = -(k_{1,3} + k_{1,4}) \cdot f_1 \quad f_1(0) = I_1 \quad (1)$$

$$\frac{df_2}{dD} = -(k_{2,3} + k_{2,4}) \cdot f_2 \quad f_2(0) = I_2 \quad (2)$$

$$\frac{df_3}{dD} = k_{1,3} \cdot f_1 + k_{1,4} \cdot f_2 - k_{3,0} \cdot f_3 \quad f_3(0) = I_3 \quad (3)$$

$$\frac{df_4}{dD} = k_{1,4} \cdot f_1 + k_{2,4} \cdot f_2 - k_{4,5} \cdot f_4 \quad f_4(0) = I_4 \quad (4)$$

$$\frac{df_5}{dD} = k_{4,5} \cdot f_4 \quad f_5(0) = I_5 \quad (5)$$

where

- $f_1$  concentration of PPO degraded by secondary processes of damages (i.e., reactions with free radicals produced in the irradiated solution);
- $f_2$  concentration of PPO degraded by the primary process of radiation ( $\gamma$  photons hitting PPO directly);
- $f_3$  concentration of benzamide produced by irradiation;
- $f_4$  concentration of benzoic acid produced by irradiation;
- $f_5$  concentration of benzyl alcohol;
- $f_i(0) \equiv I_i$  is the initial value for the  $i$ -compartment function;
- $k_{i,j}$  fractional probability of conversion ( $kGy^{-1}$ ).

The AnaComp [12] software was used to estimate the unknown parameters of the model showed in Fig. 1.

The  $w$  and  $G$  parameters were calculated using the equations

$$w \left( \frac{J}{mol} \right) = \frac{MM \left( \frac{g}{mol} \right)}{k_{i,j} (kGy^{-1})} \quad (6)$$

$$w \left( \frac{eV}{hit} \right) = w \left( \frac{J}{mol} \right) \times 1.036 \times 10^{-5} \quad (7)$$

where  $MM(g/mol)$  is the molecular mass of the target and  $k_{i,j}(Gy^{-1})$  is already defined; its values are shown in Table I. The factor  $1.036 \times 10^{-5}$  is the ratio of

$$\frac{joule \rightarrow eV \text{ convorsor Factor}}{\text{Avogadro number}} = \frac{6.2415 \times 10^{18} \left( \frac{eV}{J} \right)}{6.0225 \times 10^{23} \left( \frac{\text{Target}}{\text{mol}} \right)} \quad (8)$$

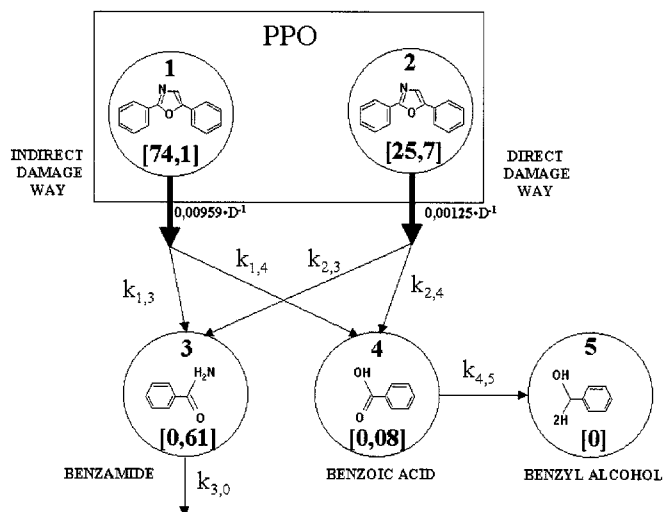


Fig. 1. Compartmental model used to explain the degradation of PPO (2,5-Dipheniloxazole) and its radiation damage products. The values between square brackets represent the initial concentrations (%), determined experimentally in the nonirradiated sample. The compartments represent, respectively, 1) the PPO destroyed indirectly or secondarily by actions of radiolytic in toluene, 2) the PPO damaged directly or primarily by the radiation, 3) benzamide, 4) benzoic acid, 5) benzyl alcohol, and (0) other compounds not identified. The constant  $k_{i,j}$  represents the fractional probability of conversion ( $\text{kGy}^{-1}$ ).

The radiation chemical yield  $G$  value was calculated as

$$G \left( \frac{\text{hit}}{100 \text{ eV}} \right) = \frac{100}{w \left( \frac{\text{eV}}{\text{hit}} \right)} \quad (9)$$

$$G \left( \frac{\text{mol}}{\text{J}} \right) = \frac{100}{w \left( \frac{\text{J}}{\text{mol}} \right)}. \quad (10)$$

The sigmoid model was used to fit the light output yield based on the photopeak position in function of dose  $D$

$$\text{Photopeak Channel} = A_2 + \frac{(A_1 - A_2)}{\left[ 1 + \left( \frac{D}{D_{1/2}} \right)^p \right]} \quad (11)$$

where  $A_1$  and  $A_2$  are the upper and the lower asymptotic values for zero and high dose  $D$ ,  $D_{1/2}$  is the dose (kGy) that reduces the light output yield to half, and  $p$  is an exponential parameter associated with the curve slope.

### III. RESULTS AND DISCUSSION

The photopeaks of liquid scintillator using irradiated PPO and excited under a  $^{137}\text{Cs}$  source is attenuated as a function of the dose. This can be seen in Fig. 2.

The loss of the energetic resolution after 40 kGy was so intense that the photopeaks could not be observed because they merged in the Compton area. This kind of analysis was useful until the value of 40 kGy. On the other hand, the results presented in Fig. 3 represent another way to improve this analysis.

As observed in Fig. 3, displacement of the photopeak fits to a sigmoid curve, i.e., it presents a plateau for doses in the range from 0 to 10 kGy, followed by a fast slope in the range from 10 to 40 kGy and a bottom plateau after 60 kGy. It was concluded from the  $D_{1/2}$  parameter that a dose of approximately 31.7 kGy is required to decrease the detector performance by half.

TABLE I  
NONLINEAR LEAST SQUARE PARAMETERS, MOLECULAR MASS,  
AND QUANTITIES DETERMINED WITH GAS CHROMATOGRAPH  
MASS SPECTROMETER

PARAMETER	VALUE $\pm$ ERROR ( $\times 10^{-3}$ )
$k_{1,1}$ ( $\text{kGy}^{-1}$ )	9.590 $\pm$ 1.240
$k_{1,3}$ ( $\text{kGy}^{-1}$ )	4.210 $\pm$ 1.400
$K_{1,4}$ ( $\text{kGy}^{-1}$ )	5.380 $\pm$ 1.870
$K_{2,2}$ ( $\text{kGy}^{-1}$ )	1.250 $\pm$ 0.205
$K_{2,3}$ ( $\text{kGy}^{-1}$ )	1.700 $\pm$ 0.680
$K_{2,4}$ ( $\text{kGy}^{-1}$ )	0.453 $\pm$ 0.710
$K_{4,5}$ ( $\text{kGy}^{-1}$ )	0.100 $\pm$ 0.148
$K_{3,0}$ ( $\text{kGy}^{-1}$ )	1.160 $\pm$ 0.791

INITIAL CONDITIONS	CONTENT	
	(%)	(g)
$I_1$ PPO* ( $\text{C}_{15}\text{H}_{11}\text{NO}$ )	74.3 $\pm$ 4.57	0.0743
$I_2$ Molec. Mass: <b>221.26</b> g/mol	25.7 $\pm$ 4.13	0.0257
$I_3$ Benzamide ( $\text{C}_8\text{H}_9\text{CONH}_2$ ) Molec. Mass: <b>121.14</b> g/mol	0.61 <sup>s</sup>	0.00061
$I_4$ Benzoic Acid ( $\text{C}_7\text{H}_5\text{CO}_2\text{H}$ ) Molec. Mass: <b>122.12</b> g/mol	0.08 <sup>s</sup>	0.00008
$I_5$ Benzyl Alcohol ( $\text{C}_7\text{H}_9\text{O}$ ) Molec. Mass: <b>108.14</b> g/mol	0.0 <sup>s</sup>	0.0

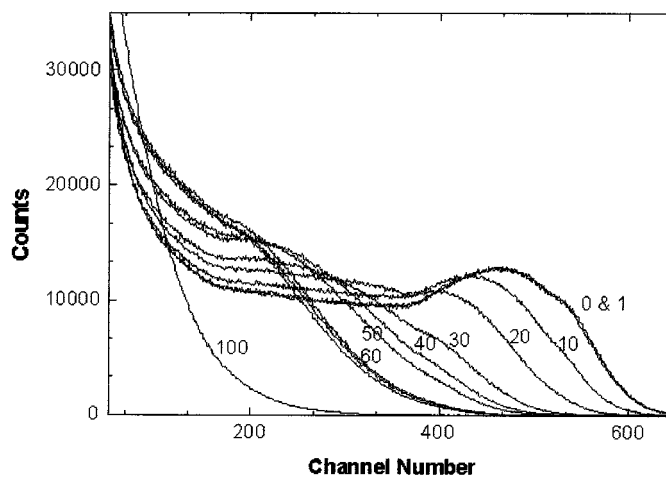


Fig. 2.  $^{137}\text{Cs}$  spectra. Liquid scintillator containing 1% (w/v) of PPO (2,5-Dipheniloxazole). Numbers beside each curve represent the respective dose (kGy).

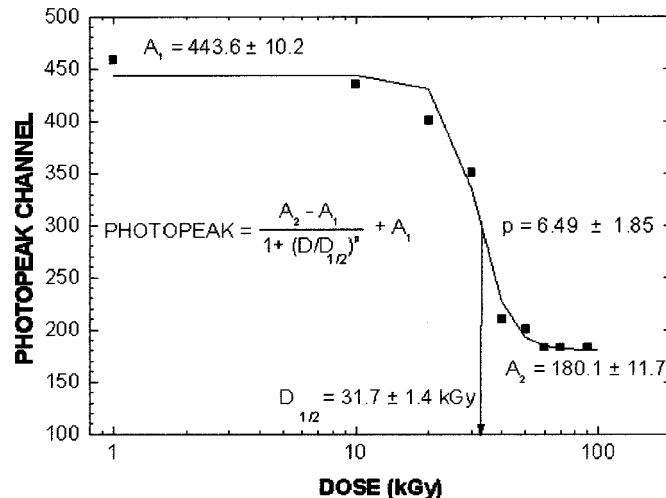


Fig. 3. Light output yield based on the photopeak position.  $A_1$  and  $A_2$  are the upper and lower asymptotic parameters, respectively,  $D_{1/2}$  is a balance value, and  $p$  is an exponential parameter associated with curve slope.

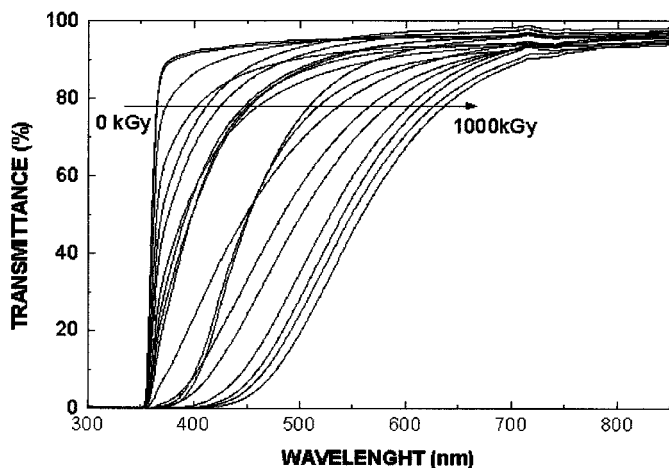


Fig. 4. Transmittance of the samples irradiated with different doses. Samples containing 1% of PPO in 10 mL of toluene were irradiated. Irradiated toluene was evaporated and resuspended with no irradiated toluene.

The transmittance curves as a function of dose in the range from 320 to 800 nm are exhibited in Fig. 4.

As can be observed, the transmittance decreased as a function of dose. Similar results were described by Hamada *et al.* [4] and Chong *et al.* [3]. Considering that the peak of PPO fluorescence occurs at 360 nm, the transparency was evaluated in that value, as shown in Fig. 5. The transmittance decreased exponentially with the dose, showing a strong correlation ( $r = 0.9989$ ).

The transparency loss and/or the light yield decreased, i.e., the degradation of the detector performance may be ascribed to the increase in optical absorption and scattering by the new molecular species and gases produced by gamma photons [3]. As shown in Tables I and II, at least three other products were generated in the irradiated PPO-toluene solution: benzyl alcohol, benzoic acid, and benzamide. Probably, there are various minor products, which are difficult to detect with our instruments. All of these substances can generate color and/or chemical quencher, and they should be responsible for the transmittance loss.

Fig. 6 displays the behavior of the PPO scintillator and its degradation products as a function of the dose. As can be inferred, the same concentration of PPO, benzoic acid, and benzamide was found around 200 kGy. The curves showed that PPO is degraded in a biexponential function with the subsequent growth of the benzoic acid and benzamide (Table II and Fig. 6).

The biexponential degradation can be explained by two damage processes that lead PPO to degrade. Therefore, the curve was split into two exponentials.

The fast slope ( $74.1 \bullet e^{-0.00959 \bullet D}$ ,  $D_{1/2} = 72.3$  kGy) can be explained as indirect damage. First, the gamma photons interact with the molecules of toluene, which generate radiolytic subproducts. Photoelectric and Compton interactions generate a primary electron  $e^-$  that loses its energy by excitation and ionization (secondary electrons). Subsequently, these electrons are energetically thermalized and combine electrostatically with ions and polarized molecules, forming the solvated electrons  $e_s^-$ . This sequence of events acts as a major role in the radiolytic products, as can be inferred from the literature [7]–[9], [13].

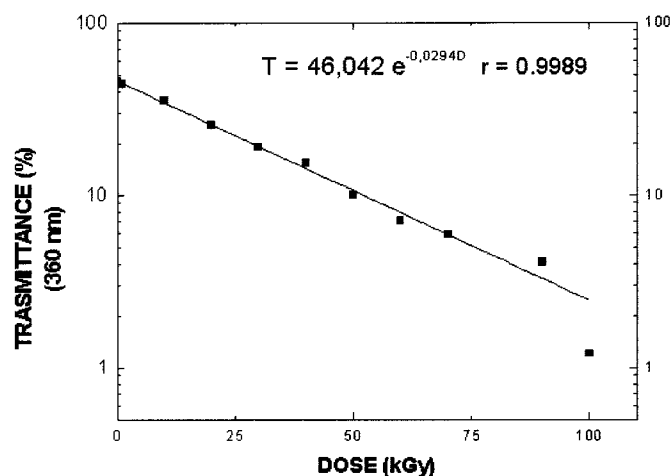


Fig. 5. Transmittance at 360 nm for irradiated samples and reconstituted with no irradiated toluene.

TABLE II  
CONCENTRATIONS OF CHEMICAL COMPOUNDS: MEASURED AND CALCULATED VALUES

Dose (kGy)	CONCENTRATION (%)							
	PPO (2,5-Dipheniloxazole)		BENZAMIDE		BENZOIC ACID		BENZYL ALCOHOL	
	Observ	Calc*	Observ	Calc*	Observ	Calc*	Observ	Calc*
0	98.61	99.80	0.61	0.61	0.08	0.08	0.00	0.00
1	97.88	99.06	0.25	0.96	0.10	0.47	0.06	0.00
10	92.10	92.70	5.07	3.99	1.76	3.77	0.08	0.00
20	86.38	86.23	10.25	7.06	2.24	7.10	0.09	0.01
30	81.33	80.33	8.54	9.83	7.18	10.12	0.10	0.02
40	76.10	74.94	14.43	12.35	7.69	12.85	0.13	0.03
50	74.19	70.02	16.31	14.63	7.97	15.32	0.20	0.04
60	70.69	65.52	10.33	16.70	9.47	17.55	1.17	0.06
70	63.36	61.42	16.28	18.57	14.17	19.56	0.25	0.08
90	50.30	54.22	10.70	21.79	19.46	23.02	0.52	0.12
100	47.60	51.08	24.44	23.17	20.55	24.50	0.51	0.14
200	28.53	30.90	29.89	31.23	30.38	33.07	0.80	0.44
300	26.32	21.84	29.54	33.58	30.16	35.64	1.08	0.78
400	17.62	17.19	28.96	33.61	32.99	35.98	1.76	1.14
500	14.79	14.37	30.97	32.67	33.81	35.51	1.79	1.50
600	12.13	12.37	32.06	31.31	34.05	34.78	1.82	1.85
700	10.18	10.80	30.45	29.76	34.75	34.01	2.65	2.19
800	8.25	9.49	30.20	28.13	35.57	33.25	3.09	2.53
900	9.39	8.36	30.64	26.48	37.32	32.53	2.58	2.86
1000	7.83	7.37	32.54	24.83	36.24	31.85	1.65	3.18

\*AnaComp software [12]

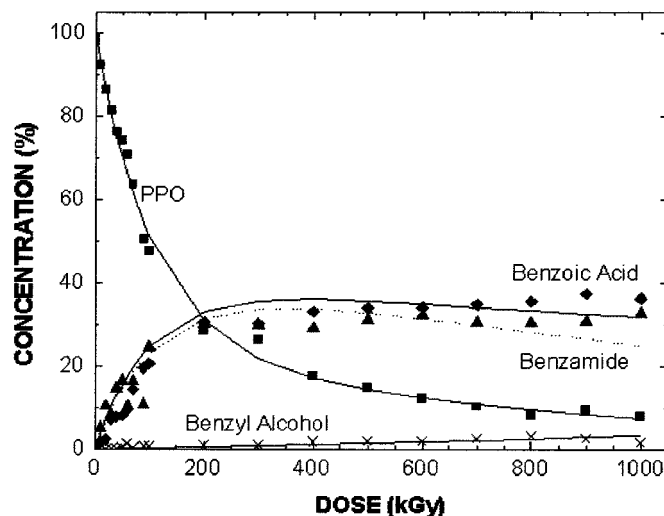


Fig. 6. Concentration of PPO (2,5-dipheniloxazole) and its degradation products as a function of dose. The continuous curves were generated by AnaComp [12] using the model described in Fig. 1.

TABLE III  
THE ENERGY W EQUIVALENT OF A "HIT" TO PRODUCE DAMAGE IN THE PPO (2,5-DIPHENYLOXAZOLE) MOLECULE AND THE G VALUE, WHICH IS THE BASIC UNIT OF RADIATION CHEMICAL YIELD

DAMAGE PROCESS	w value		G value	
	(eV/hit)	(J/mol) × 10 <sup>3</sup>	(Hit/100eV)	(mol) × 10 <sup>-3</sup>
Indirectly, by radiolytic reactions (total)	0.24 ± 0.03	23	3	418 ± 54
Indirectly, PPO → Benzamide	0.54 ± 0.18	53	17	184 ± 61
Indirectly, PPO → Benzoic Acid	0.43 ± 0.15	41	14	235 ± 82
Directly, $\gamma$ -ray "hits" the PPO (total)	1.84 ± 0.30	177	29	54 ± 9
Directly, PPO → Benzamide	1.35 ± 0.54	130	52	74 ± 30
Directly, PPO → Benzoic Acid	5.06 ± 7.94	488	766	20 ± 31
Benzoic Acid → Benzyl Alcohol (total)	12.7 ± 19.8	1224	1815	8 ± 12
Benzamide → Others (total)	1.06 ± 0.74	104	71	92 ± 63

The electron vacancy and the excitation process generate other free radicals such as H, H<sub>s</sub><sup>+</sup>,  $\dot{\text{O}}\text{H}$ , and OH<sub>s</sub><sup>-</sup> [7]. The lifetime of radicals in the organic solutions ranges to picoseconds [13]. Therefore, the instantaneous concentration of the primary radicals is extremely dependent on the dose rate.

Why can't high doses contribute to a substantial diminishing on the PPO concentration? In the dose-response curve, why is the slope decreased for high doses? A probable explanation may be that some radiolytics act as an effective e<sub>s</sub><sup>-</sup> scavenger.

Gases dissolved in the solution, such as O<sub>2</sub>, can contribute to the enhancement of the radiolytic products, as demonstrated by Chong *et al.* [3]. In our work, samples were irradiated by <sup>60</sup>Co under oxygen-free atmosphere at an environment of approximately 40 °C (104 °F). Consequently, the parameters shown in Tables I and III are restricted to these conditions.

On the other hand, the slow slope ( $25.7 \bullet e^{-0.001 25 \bullet D}$ ;  $D_{1/2} = 554.5$  kGy) can be interpreted as the damage caused by primary interaction of the  $\gamma$ -radiation with targets, i.e.,  $\gamma$  photons directly hit PPO molecules. As the dose increases, the amount of radiolytic products tends to saturation or reaches equilibrium by the neutralizing action of scavengers. Thus, high-absorbed dose increases the probability of the gamma photon to hit the PPO molecule directly. Above 97.7 kGy, the direct damage in PPO, at 1% (mass/vol in toluene), becomes predominant. The direct hit of  $\gamma$  photon in the scintillator molecule gives us information about the process of detector damage. As can be seen in Table I, parameters  $k_{2,3}$  and  $k_{2,4}$  represent the fractional rate of PPO damage in benzamide and benzoic acid. From these values, we calculated the G value for direct interaction between the  $\gamma$ -ray from <sup>60</sup>Co source and the PPO molecule, as shown in Table III. The G and w-values calculated from ( $25.7 \bullet e^{-0.001 25 \bullet D}$ ;  $D_{1/2} = 554.5$  kGy) could be assumed as an estimate from the irradiation of PPO in powder form.

Table III shows the energy necessary for each reaction (parameter w) and the chemical yield (G-value). The energy involved in the reactions produced by free radicals by an indirect process on the solvent ranged from 0.24 to 0.54 eV/reaction or "hit." As the  $\gamma$  photon of <sup>60</sup>Co has approximately  $1.25 \times 10^6$  eV, it has enough energy to produce damage in at least 2 million PPO molecules. With regard to G-parameters, values similar to that described in the literature were found. As can be seen from the literature, free radicals such as H, H<sub>s</sub><sup>+</sup>, OH, and OH<sub>s</sub><sup>-</sup> seem to have larger G than complex molecules.

The indirect action of  $\gamma$  radiation is approximately 2.5–12 times more efficient to produce damage compared to the direct mode (ratio between G values from indirect and direct modes, as can be seen in Table III).

Although a liquid scintillator was used in this study, it is important to consider that the most important facts of this work can

be extended for other types of detectors, since they have some compound that can be quantified and that changes with the dose.

#### IV. CONCLUSION

The damage of the radiation on the liquid scintillating system (PPO + toluene) showed that the main damage occurs in PPO, insofar as samples irradiated without PPO did not generate the products benzamide, benzoic acid, and benzyl alcohol. The liquid scintillating system has reasonably low sensitivity to radiation damage, but doses larger than 30 or 40 kGy cause severe damage in the detector and practically turn it useless. Pulse-height analysis showed that doses from 30 to 40 kGy generated a substantial loss of the quality of the sensor (liquid scintillating) and reduced it after to half, by 31.7 kGy. The transparency of the solution for photons produced in the liquid scintillator decreased monoexponentially. The compartmental model with five compartments (PPO indirectly damaged, PPO directly damaged, benzamide, benzoic acid, and benzyl alcohol) was satisfactory as a predictive model to estimate the products as a function of the dose. The coefficient  $r^2 = 0.985636$  shows that the model is capable of explaining 98.6% of the experimental variations among the experimental points of concentration.

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