Simulation of dose distribution with PUFFIn® software on hydrogels for environmental applications

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Abstract

PUFFIn® software was used to make simulations of the Dose Uniformity Ratio (DUR) in hydrogels cross-linked with radiation. The results showed optimal DUR when E beam energy of 5 MeV to 10 MeV was applied from the thinner side. In conclusion, PUFFIn® software allows analysis of dose distribution simulations, although is affected by product composition, geometry, energy and beam direction.

Introduction

The use of adsorbent materials is of interest to reduce the environmental impact of industrial dyes. Hydrogels can be cross-linked with ionizing radiation and functionalized with materials such as clays, with the ability to bind organic and inorganic molecules.

The hydrogel was made with deionized water, polyvinyl alcohol (PVA), bentonite clay and agar (Fig.1). The solution requires doses between 15 and 30 kGy with 7-10 kGy/h using a ^{60}Co source for an optimum synthesis . The objective of this work is to evaluate whether they can be cross-linked with E-beam, so simulation studies were performed using PUFFIn software.

Material / Methods

The software PUFFIn® (version 4F) was used for simulations. The hardware used was Intel i5 10300H, 16Gb ram and 500 Gb SSD.

Parameters:
Hydrogel: PVA (5%), bentonite clay (4%), agar (1%) (Fig.2)
Container: polycarbonate (1.5 mm layer).
Volume: 4 x 4.5 x 1 cm (Fig. 3)
e-beam energy between 2 - 10 MeV
geometry 10x10 cm
10e^{6} particle number
beam applied in Y and Z axis

Figure 1. Hydrogel after irradiation.

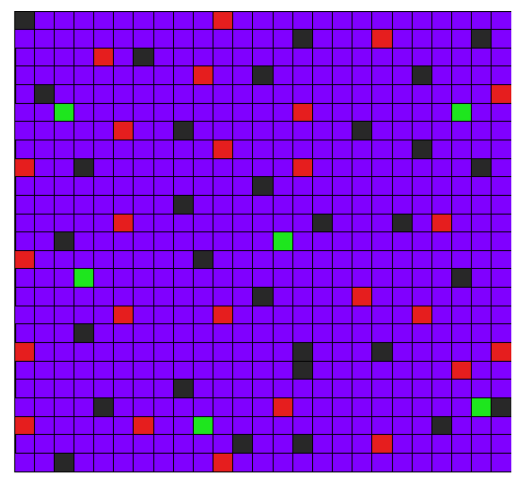

Figure 2. Surface mesh.

Water
Agar
PVA
Bentonite

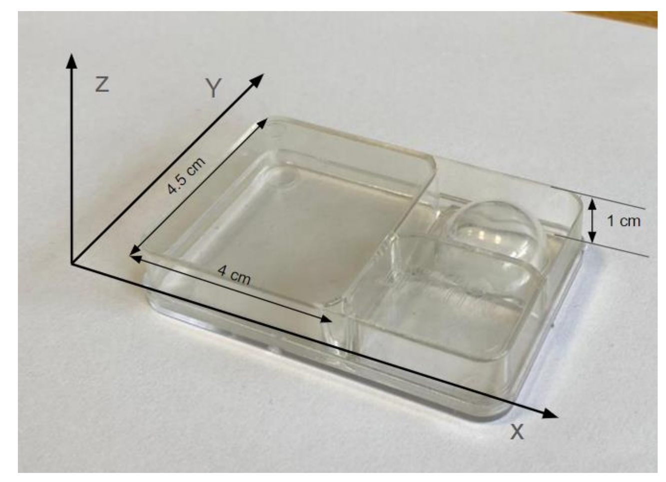

Figure 3. Polycarbonate container

Results / Discussion

The results with the source coming from Z axis (table 1) showed low DUR values, from 1.25 to 1.06, with energy beams from 5 MeV to 10 MeV. For 2 MeV e-Beam coming from Z axis, the DUR was higher and this means that a homogeneous hydrogel would not be obtained.

Table 1. Simulated DUR obtained. Source oriented in Z axis

Energy (MeV)	2	5	7	10
DUR	33.12	1.25	1.12	1.06

In the case of irradiation applied from Y direction (table 2), a penetration greater than 40 mm was obtained with the energy beam of 10 MeV, with 5 MeV this value decreases to 20 mm. In these cases, a large dose dispersion is observed, so the cross-linking of the polymers would not be homogeneous and a modification of the dimension, or the rotation of the sample during the irradiation process, should be considered (Fig.4).

Table 2. Simulated DUR and penetration obtained. Source oriented in Y axis.

Energy (MeV)	2	5	7	10
DUR	16.3	7.9	6.4	4.7
Penetration (mm)	5	20	30	42

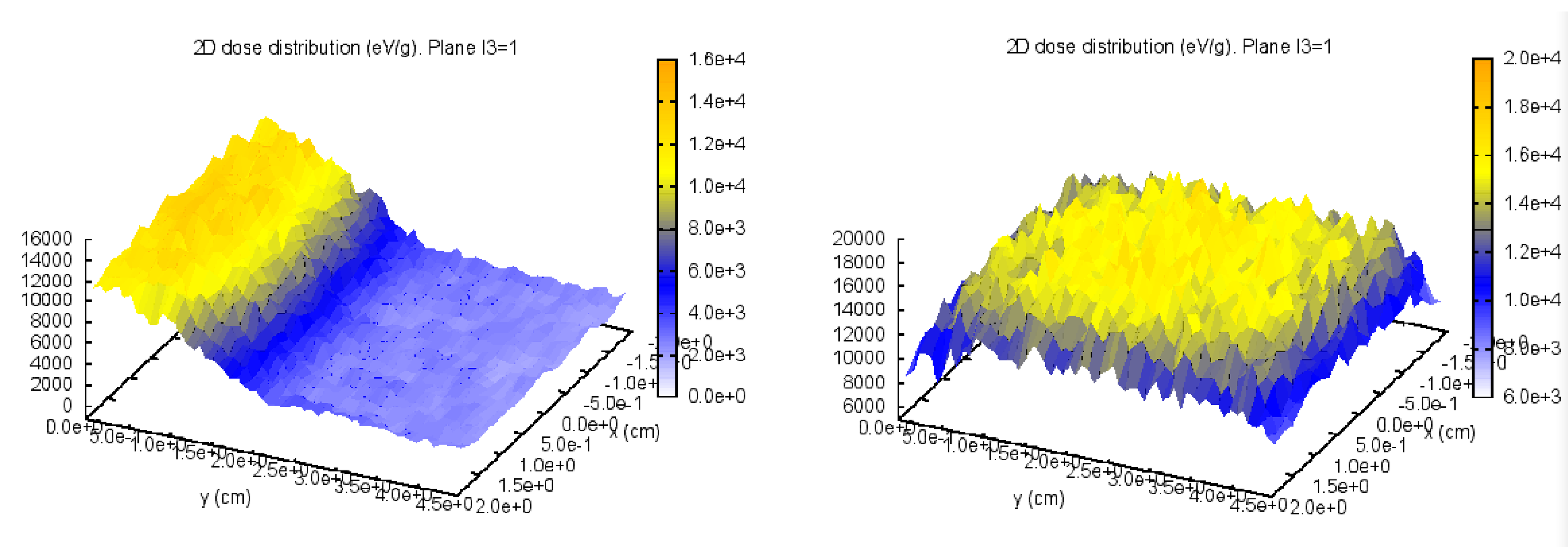

Figure 4. Dose distribution along axis Y (left) and Z (right) with 5 MeV.

Conclusions

The PUFFIn® software proved to be a versatile tool that can be used to analyze dose distribution with different irradiation parameters, product , compositions and geometries. In addition, it could be a useful tool for both: industry and research activities. However, simulations must be confirmed with laboratory tests.