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SIMULATION STUDIES ON THE INTERACTIONS OF ELECTRON BEAM WITH WASTEWATER*

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Abstract

High energy electron beam irradiation is capable of removing harmful organic compounds from industrial manufacturing, which are hard to be degraded by the conventional wastewater treatment methods. This paper utilizes FLUKA code to evaluate the electron beam-wastewater interaction effects with different energy, space and divergence distributions of the electron beam. With 8 MeV average energy, the electron beam exits from a 0.0127 cm thick titanium window, travels through a 4.3 cm distance in air and through a second 0.0127 cm thick stainless sample container window with 2.43 cm radius, and finally is injected into the wastewater sample container, which has a volume of around 75 cubic cm. The distributions of the electron beam are obtained from the GPT (General Particle Tracer) simulations for the UITF (Upgraded Injector Test Facility) in Jefferson lab. By varying the parameters of the electron beam, the dose distributions through the water, the contributions from the electrons and bremsstrahlung photons are scored and compared. It is found that a spatially uniform electron beam results for the case of the most uniform dose distribution and the electrons are the main source for the dose. In addition, the electron differential fluence through the multiple planes of the has been modelled, which provides the base for the further electron beam requirements study.

INTRODUCTION

With their wide use in the industry nowadays, organic compounds, like 1,4-dioxane and PFAS (per- and polyfluroralkyl substances), which are manufacturing products, are found in the ground water or municipal water. These organic compounds have become the new pollutants of high concern and brought big challenges to the wastewater treatment, because they are miscible in water and are extremely difficult to be removed by the conventional wastewater treatment methods, like the adsorption and chlorination [1-4].

It has been reported that the following methods are capable to remove the organic compounds include UV (Ultraviolet) light with hydrogen peroxide, gamma irradiation and EB (electron beam) irradiation. However, UV light has a treatment limit of the compound concentration and doesn't always work for different kind of organic pollutants [3, 5-7], the gamma irradiation needs strong shielding and is not appliable for the large-scale treatment [6], and usually the former two methods take more treatment time. It has been proven that EB irradiation on wastewater is a successful approach with many advantages, such as high efficiency, non-selectivity, sustainability and large-scale treatment [7].

In general, the beam energy of EB irradiation is less than 10 MeV to avoid the radioactive material. Therefore, in an aqueous environment the main treatment reaction is indirect irradiation [8]. In that process the high energy electrons interact with water molecules to produce very reactive radicals including the aqueous electron ${e^-}_{aq}$, hydrogen $\cdot H$ and hydroxyl $\cdot OH$, which subsequently break down the organic target compounds with Redox reactions. The former two radicals are reducers and the last one is an oxidant, so it is a redox process that results in the non-selectivity of EB irradiation. The produced radicals are proportional to the absorbed energy or dose (energy per unit mass) and they can be described by Eq. (1) [8].

$$\begin{aligned} \mathrm{H_2O} \;&\rightarrow \cdot OH(2.7) + {e^-}_{aq}(2.5) + \cdot H(0.55) \\ &+ \mathrm{H_2}(0.55) + \mathrm{H_2O_2}(0.71) + \mathrm{H_3}O^+(2.7) \end{aligned} \tag{1}$$

The number in the brackets is the radicals per absorbed 100 eV, or G value.

In practical applications, the wastewater is designed to be a thin sheet of wastewater flow in front of the electron beam, for the electrons in water will be stopped after a certain distance determined by its energy [9]. The electron penetration affects the dose distribution through the wastewater flow depth and in turn the radical distribution, which are the key to the consequent chemical reactions. Therefore, it is important to make a uniform dose distribution through the water depth. One way for that is to construct a relevant electron beam, including the appropriate space and energy distributions, which is still an open question.

With the UITF in Jefferson lab, we have designed the 1,4-dioxane wastewater treatment experiment with 8 MeV electron beam, where the wastewater sample is inside a container with up to 4 cm depth and 75 cubic cm volume. By applying FLUKA [10], which is a particle and matter interaction Monte-Carlo code, we will state the dose distribution under different electron beam parameters, the contributions of different particles to the dose, the electron differential fluence spectrum through the pure water. The

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energy spread and divergency of the electron beam are obtained from the GPT [11] simulations for the UITF wastewater treatment beamline design.

SIMULATION SETUP

The sample container is designed with 4 cm depth based on the optimum depth under 10 MeV [9] which is the maximum electron energy of UITF, and its corresponding cross section diameter is 2.43 cm, which requires a 0.8 cm to 0.9 cm standard deviation radius for the Gaussian electron beam. With the 8 MeV energy and 100 nA current of the electron beam, the UITF wastewater treatment beamline was designed with the GPT simulations, where the simulated beam energy spread is less than 75 keV standard deviation energy and the divergency is less than 10 mrad standard deviation angle.

The simulation schematic is shown in Fig. 1. The electron beam traverses from the left vacuum region, through the accelerator Ti (Titanium) exit window with 0.0127 cm thickness, through an air region with 4.3 cm distance, through the container stainless steel window with 0.0127 cm thickness and then into the water region. Along the water is longitudinal direction z, for the transverse space there is horizontal direction x and vertical direction y, it is a right-hand cartesian coordinate system. The accelerator Ti exit window is at z = 50 cm, the water surface is at z = 55 cm.

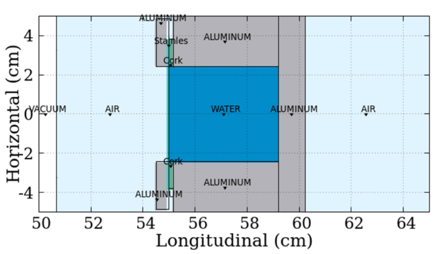

Figure 1: Schematic of the treatment simulations.

For the FLUKA simulation settings, the applied primary electron number is 500, 000. Except for the above electron beam parameters, the smaller beam sizes are also considered.

DOSE PROFILE

The absorbed dose is not always the same everywhere through the depth direction of the target matter [9], it increases to a peak dose due to the production of secondary electrons and then decreases due to the electrons consumed. The lower the peak dose is, the more uniform the dose distribution is. In addition, the optimum depth, R_{opt}, where the dose is equal to that at the entrance of the target matter, is usually used as the target depth design.

RESULTS AND DISCUSSIONS

All of the dose measurements are converted to the equivalent dose rate at 100 nA. The doses at the z locations are the integration over the radial and angular directions within the water sample. Similarly, the doses at the radial locations is the integration over z and angular directions.

Dose Distributions

The beam radius, beam shape, energy spread, divergency and energy are all considered.

Beam transverse size Without energy spread and divergency, three transverse rms beam radiuses of 4, 8, 9 mm were applied, which is shown in Fig. 2. The electron energy is 8 MeV.

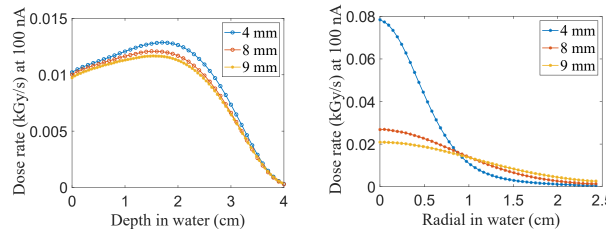

Figure 2: Dose distributions under 4, 8, 9 mm standard deviation beam radiuses.

With the beam size increasing, the dose distribution along both longitudinal and radial directions is being more and more uniform.

Beam shape The different Gaussian shapes and uniform shape are compared by setting different ratios of direction x to direction y, which is shown in Fig. 3. The 8 MeV electron beam energy is with 8 mm rms beam size, without energy spread and divergency.

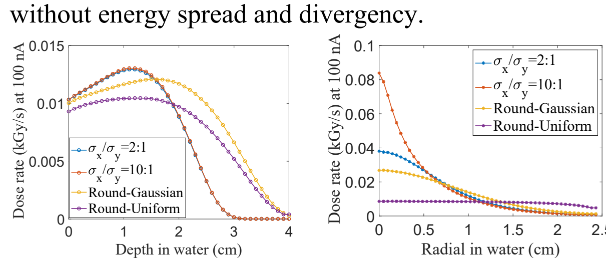

Figure 3: Dose distributions under different beam shapes.

It is clear that the spatially uniform beam results in the most uniform dose distribution for both longitudinal and radial directions. Compared to the non-round beam, the dose penetration of the round beam spreads more widely on both longitudinal and radial directions in the water.

Energy spread and divergency The 8 MeV electron beam is with 8 mm rms beam size, 0, 75 keV rms energy spreads and 0, 5, 10 mrad rms divergencies, the corresponding results are shown in Fig. 4. It can be seen that within these investigating ranges, they don't have too much influence on the dose distribution.

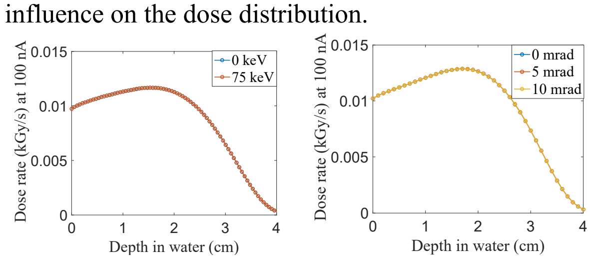

Figure 4: Dose distributions under different energy spreads (left) and divergencies (right).

Beam energy In addition to 8 MeV, the other two energies 6 MeV, 10 MeV are applied, which is shown in

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Fig. 5. All of them has an 8 mm rms beam size, no divergency and no energy spread.

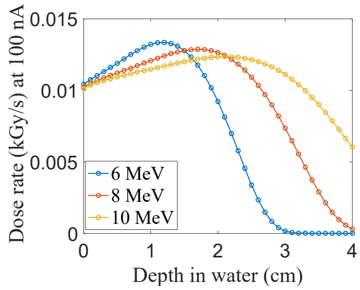

Figure 5: Dose distributions under different beam energies.

With the beam energy increasing, the dose distribution curve is being flatter and the dose through the water depth is being more uniform. With higher electron beam energy, the electrons lose less energy in the water surface range and travel deeper inside the water sample to produce more secondary electrons, which results in a more uniform dose distribution. This is why the depth of water sample should be designed according to the electron beam energy to make sure that all the internal area are irradiated.

Based on the above results, the dose distribution in this case depends more on the transverse space distribution of the electron beam, and it is not affected too much by the investigated energy spreads and beam divergencies. The main reason is that the energetic electrons travel with the relativistic speed of light, free of the low energy spread and divergency, to penetrate through the water sample. Consequently, the uniform space distribution leads to the most uniform dose distribution. In addition, the higher electron beam results in the more uniform dose distribution. As an alternative, the shorter depth of the container can also be considered.

Particle Contribution to Dose

After the electrons have been injected into the water sample region, they induce two types of collisions, one is the inelastic collision to produce secondary or even tertiary electrons, the other one is to produce the bremsstrahlung photons. Both of them contribute to the energy deposition or dose in the water. To construct the required optimum electron beam, we have to investigate the relative contributions of these two processes. Figure 6 shows the longitudinal dose distributions under different particles.

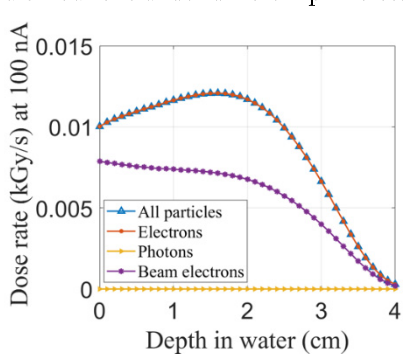

Figure 6: Dose contributions resulting from the electrons and bremsstrahlung photons.

The electrons from the beam are absorbed more in the water than in the air before z = 55 cm, which induces the secondary electrons that are included in the red curve. It can be seen that the dose curve of the electrons is overlapping with that of the whole particles, while the yellow curve of the photons is so low that we can ignore its contribution. With the set electron beam energy, we shall pay more attention to the electron properties through the water.

Electron Differential Fluence Spectrum

In order to investigate the characteristics of the electrons through the water sample depth, the electron differential fluence with respect to the energy is simulated through every imaginary plane in the water with a 0.1 cm interval, which is shown in Fig. 7.

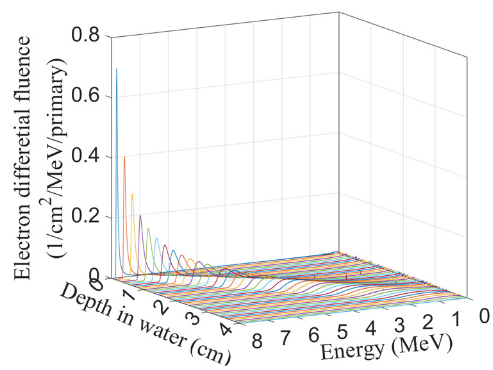

Figure 7: Electron differential fluence at different positions through the water sample container.

There is a high peak of electron differential fluence right on the water surface at the moment the electrons enter the water sample container. With the water depth increasing, the peak decreases to almost a flat plateau after 1 cm depth and before around 3 cm depth. After 3 cm, the peak decreases gradually to very low level. The dose is proportional to the electron fluence, which should be a good research direction for further uniform dose distribution study.

CONCLUSIONS AND OUTLOOK

With the electron beam parameters of the UITF wastewater treatment beamline design, we have acquired the dose distributions, electron differential fluence spectrum by the FLUKA code. This simulation study demonstrates that the electron beam energy and its transverse space distribution are the main factors affecting the uniform dose distribution. The contribution to the dose stems results mainly from the electrons including the primary beam electrons and the secondary electrons, which shows that more efforts should be taken on the electrons. Finally, the electron differential fluence spectrum, related to the dose, through the water is obtained, which is of importance to gain a better understanding of the electron property.

These simulation studies have provided valuable insights into the interactions of electron beam with wastewater and revealed the main factors determining the dose distribution in the wastewater sample container. We will continue this work to elucidate further theoretical electron beam requirements.

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