Simulation Studies on the Interactions of Electron Beam with Wastewater *

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Abstract

High energy electron beam irradiation is capable of removing the manufactured organic compounds 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 air and a second 0.0127 cm thick stainless sample container window with 2.43 cm radius, and finally is injected into the sample area, where the volume of container is around 75 cubic cm. The distributions of the electron beam are 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 the spatial uniform electron beam results in 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 water are carried out, which provides the base for the further electron beam requirements study.

INTRODUCTION

With their wide use in the industrial areas nowadays, the manufactured organic compounds, like 1,4-dioxane and PFAS (per- and polyfluroralkyl substances), found in the ground water or municipal water have become the new pollutants and brought big challenges to the wastewater treatment, for they are miscible in water and difficult to be removed by the conventional wastewater treatment methods, like the adsorption and chlorine [1-4].

It has been reported that the methods able to remove the organic compounds include UV (Ultraviolet) light with hydrogen peroxide, gamma irradiation and EB (electron beam) irradiation. However, the 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 successful 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, so in aqueous environment the main treatment reaction is indirect irradiation [8]. In that process the high energy electrons interact with water molecules to produce reactive radicals including the aqueous electron $e^{-}{}_{aq}$, hydrogen $\cdot H$ and hydroxyl $\cdot OH$, which are then to break down the target compounds. 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 equation 1[8].

$$\mathrm{H_2O} \rightarrow \cdot OH(2.7) + e^{-}{}_{aq}(2.5) + \cdot H(0.55) + \mathrm{H_2}(0.55) + \mathrm{H_2O_2}(0.71) + \mathrm{H_3}O^{+}(2.7) \qquad (1)$$

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

In reality the wastewater is designed to be a thin flow in front of the electron beam, for the electron 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 then the radicals which are the key to the consequent chemical reactions, so it is of importance to make a uniform dose distribution through the water depth. One way for that is to construct a relevant electron beam, including the 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, the wastewater sample is inside a container with up to 4 cm depth and 75 cubic cm volume. By applying the FLUKA [10], 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 energy spread and divergency of the electron beam are 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

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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 Figure 1. The electron beam is from the left vacuum region, through the accelerator Ti (Titanium) window with 0.0127 cm thickness, air region with 4.3 cm distance, 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 window is at z = 50 cm, the water surface is at z = 55 cm.

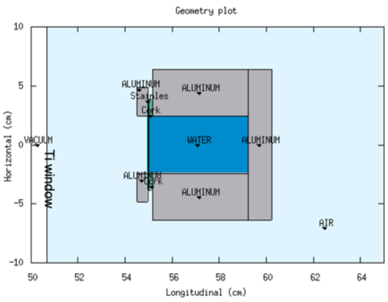

Figure 1: Schematic of the treatment simulations.

For the FLUKA simulation settings, the applied primary electron number is 500, 000 with 5 cycles in total. Except for the above electron beam parameters, the smaller beam sizes are also considered.

DOSE PROFILE

The typical longitudinal dose distribution through the treated target is shown in Figure 2 [9], where the EB irradiation is on one side of the target.

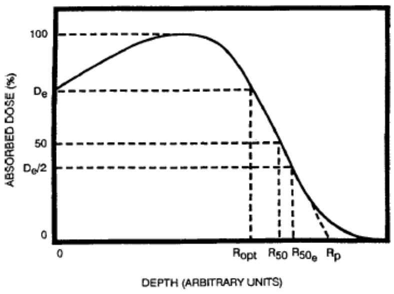

Figure 2: Dose profile of one-sided EB irradiation [9].

The absorbed dose is not always same everywhere through the depth direction, it increases to a peak dose due to the secondary electrons producing and then decreases with the electrons consuming. 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, is usually used as the target depth design.

RESULTS AND DISCUSSIONS

This section states the dose distributions under different electron beam parameters, the contributions of the electrons and bremsstrahlung photons to the dose distributions, and the electron fluence spectrum through different positions of the water. All of the dose measurements are converted to the equivalent dose rate at 100 nA or normalized dose per incident primary beam electron.

Dose distributions

The beam radius, beam shape, energy spread, divergency and energy are considered for the dose distribution comparison.

Beam transverse size The real beam is generally close to a gaussian transverse space distribution, here three transverse standard deviation beam radius, 4, 8, 9 mm are applied, which is shown in Figure 3.

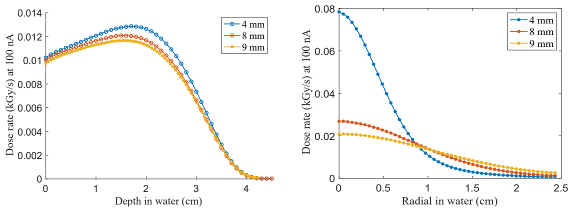

Figure 3: Dose distributions under 4, 8, 9 mm standard deviation beam radiuses.

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

Beam shape The round gaussian and uniform beam are compared, and the different gaussian beam shapes are compared by setting different ratio of direction x to direction y, which is shown in Figure 4.

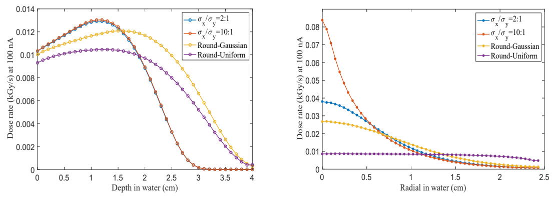

Figure 4: Dose distributions under different beam shapes.

It is clear that the spatially uniform beam results in the most uniform dose distribution for both longitudinal and radial directions.

Energy spread and divergency Based on the GPT simulations, the standard deviation energy 0, 75 keV and the standard deviation divergency 0, 5, 10 mrad are applied, which is shown in Figure 5. It can be seen that within these investigating ranges, they don't have too much influence on the dose distribution.

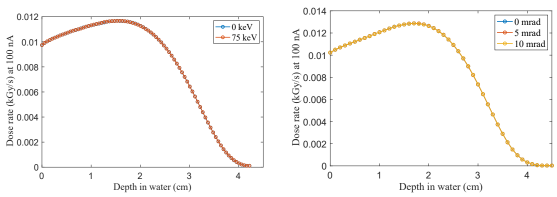

Figure 5: Dose distributions under different energy spreads (left) and divergencies (right).

Beam energy Except for the investigated 8 MeV, the other two energies 6 MeV, 10 MeV are applied, which is shown in Figure 6.

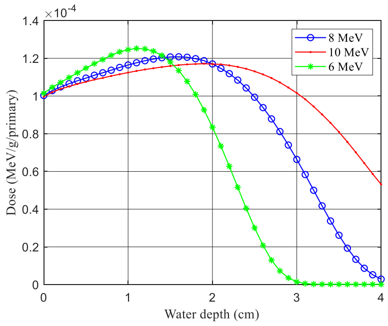

Figure 6: Dose distributions under different beam energies.

With the beam energy increasing, the curve is being flatter, the dose through the water 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 to produce more secondary electrons, which results in the more uniform dose distribution.

Based on the above results, the dose distribution in this case depends more on the transverse space distribution of the electron beam, while is not affected too much by the investigated energy spreads and beam divergencies. The main reason is that the energetic electrons are in the relativistic speed of light, free of the low energy spread and divergency, to penetrate through the water, so 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 injected into the water region, there 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 electron beam, we have to investigate the contributions of them. Figure 7 shows the longitudinal dose distributions under different particles.

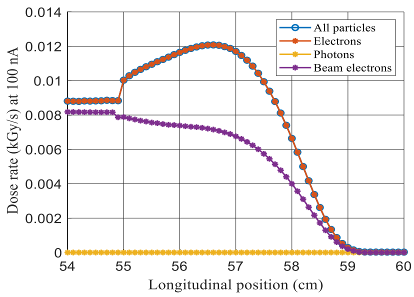

Figure 7: Dose contributions from the electrons and bremsstrahlung photons.

The electrons from the beam are consumed 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 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 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 Figure 8.

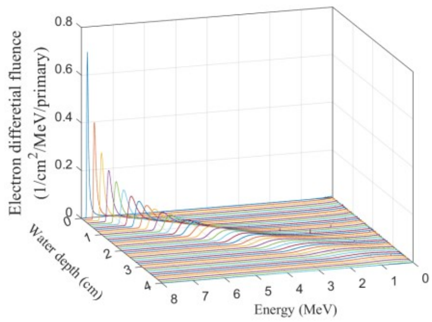

Figure 8: Electron differential fluence at different positions through the water.

There is a high peak electron differential fluence on the water surface at the moment the electrons injected. With the depth increasing, the peak decreases to almost a flat 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 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. It demonstrates that the electron beam energy and its transverse space distribution are the main factors to the uniform dose distribution. The contribution to the dose is mainly from the electrons including the 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 more understandings of the electron property.

The simulation studies have provided the prospective of the dose distribution and the main factors. We will continue this work for the further theoretical electron beam requirements.

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