Simulation research on wastewater treatment with the Upgraded Injector Test Facility e-beam irradiation

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Introduction and Motivation

With the increasing industrialization affecting the quality of human life, more and more varieties of harmful industrial **organic compounds** are found in the wastewater. These toxic organic compounds like 1,4 dioxane are extremely difficult to be removed by existing conventional treatment methods, which **challenges** the wastewater treatment before it is discharged to the surroundings or reused for the replenishment of ground water. **EB (electron beam) irradiation** has been proven to be a sustainable approach for the wastewater treatment, since it is capable of removing efficiently and effectively the most harmful pollutants including the toxic chemicals, metal, bacteria, viruses, pathogens, and especially the organic compounds from industrial manufacturing.

SWIFT (sustainable water initiative for tomorrow) is a local program conducted by HRSD (Hampton roads sanitation district) to slow down and ultimately restore the land subsidence of the Chesapeake Bay with the replenishment of the treated wastewater to the Potomac aquifer, where the wastewater is treated to reach drinking water standard level before recycling it to replenish groundwater lost by excessive use. The remediation of the pollutants is usually affected by a lot of factors, such as the **electron beam parameters**, the pH of the wastewater, the target compounds, and the degradation pathways of different chemicals are also different. 1,4-dioxane, a common toxic organic compound in the wastewater, has been designated as the initial target chemical. Instead of using flow water, the sample wastewater is going to be irradiated in a special designed sample container to investigate the degradation mechanism of harmful organic pollutants.

The electron beam is utilized with the UITF (Upgraded Injector Test Facility) in Jefferson lab. After we have investigated research scenarios under several different electron beam energies, 8 MeV electron beam has been designed and used as the initial wastewater e-beam irradiation experiment study.

Mechanism of e-beam irradiation on wastewater

$$H_2O \rightarrow \cdot OH(2.7) + e^-_{aq}(2.5) + \cdot H(0.55) + H_2(0.55) + H_2O_2(0.71) + H_3O^+(2.7)$$

Energetic electrons

Oxidants | Reducers → Reactions → 1,4 dioxane, etc.

Radical numbers per 100 eV absorbed energy.

kJ/kg

Uniform Dose → Uniform radicals → Uniform treatment

The electron energy is less than 10 MeV to avoid the radioactive material. Then the main treatment reaction is indirect irradiation. The high energy electrons interact with water molecules to produce very reactive radicals including the reducers and the oxidants, which subsequently break down the organic target compounds.

Simulation setup

- The absorbed electron energy is not always uniform everywhere through the depth direction of the water container. Therefore, there is a specific depth to make sure the dose distribution is relative uniform.
- The initial volume of the cylinder water container is 75 mL and its depth is 4 cm according to the referred Monte Carlo simulations, the corresponding radius 2.43 cm, as Fig.1 shows.
- The beamline is designed by the GPT (General Particle Tracer) to aim to a transverse beam radius around 2.4 cm, then the corresponding beam parameters are acquired.
- The Dose distribution are investigated by the Monte-Carlo simulations to optimize the water depth to be 3.3 cm.

Beam transverse radius: 2.4 cm.

Volume: 61 mL.
Depth: 3.3 cm.
Radius: 2.43 cm.

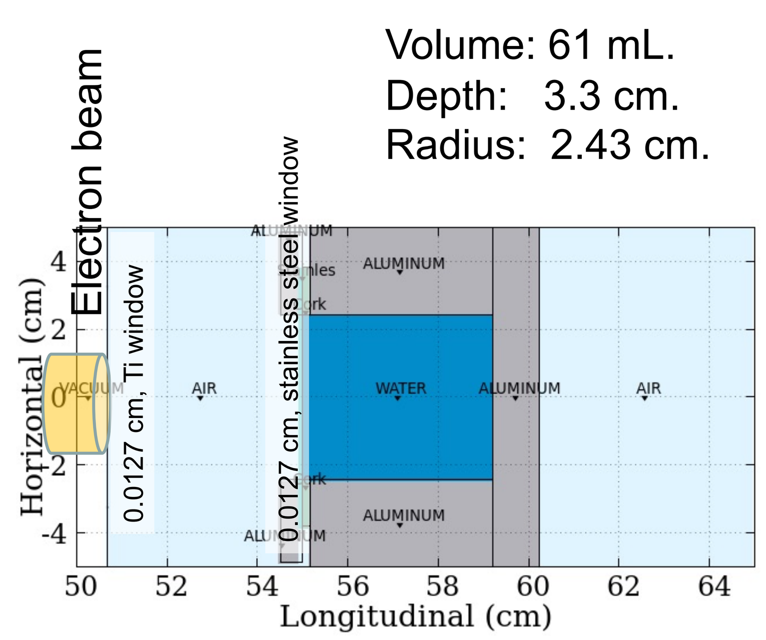


Fig. 1 Schematic of the initial water container.

Beamline design

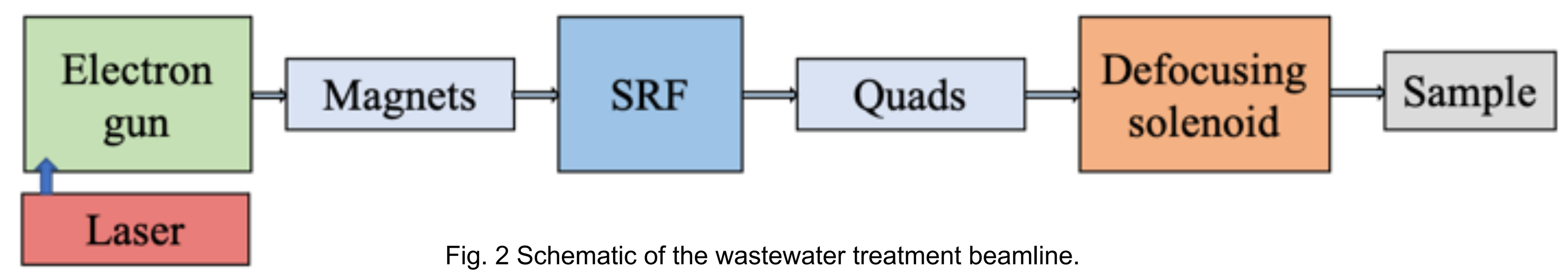
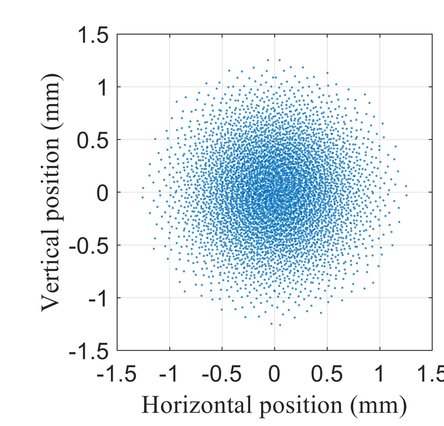


Fig. 2 Schematic of the wastewater treatment beamline.

Table 1. Initial properties of the electron beam.

Photocathode	GaAs	
MTE	0.04 eV (@780 nm)	
Kinetic energy	3/2 * MTE	Uniform distribution
Bunch charge	-1.33e-16 C	100 nA, CW mode.
Beam size	0.425 mm (σ_x)	3 cutoff, Gaussian.
Bunch length	~14.86 ps (σ_t)	4 cutoff, Gaussian.

Gaussian distribution



- The laser pulses with **780 nm** wavelength are getting absorbed by the photocathode to emit the electrons, which are then accelerated to **200 keV** energy by the electric field in the DC gun and transported through the solenoids, chopper cavity and buncher cavity before reaching the SRF cavities of 1.5 GHz.

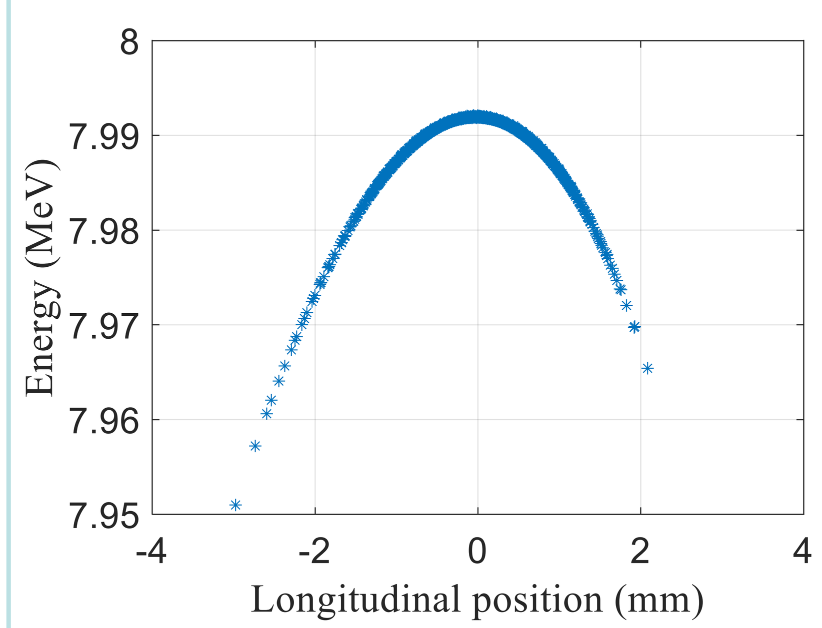


Fig. 3 Longitudinal phase distribution after the SRF accelerating.

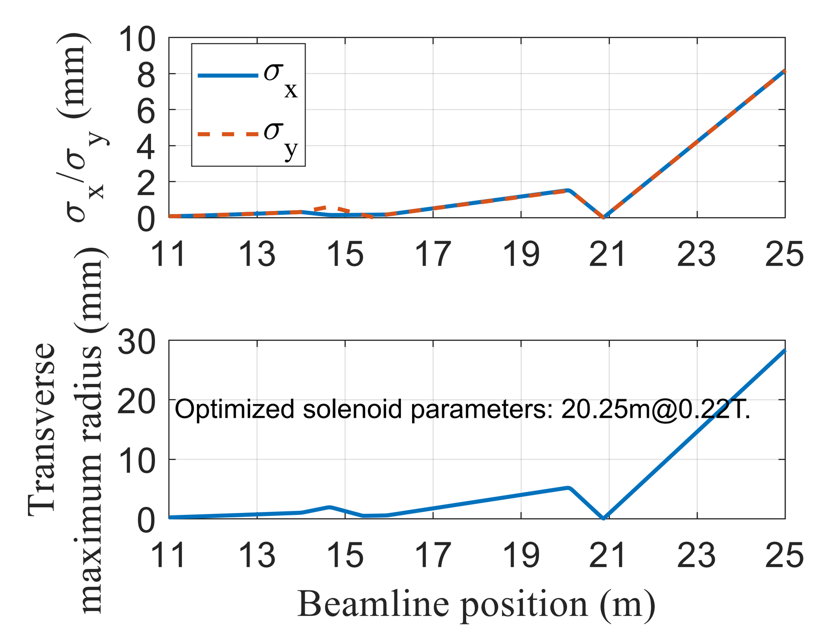


Fig. 4 Beamline envelope through the quadrupoles and defocusing solenoid.

- The electric fields and phases of the two SRF cavities are optimized by setting the phase at **the crest energy gain**. Fig. 3 shows the longitudinal phase distribution after the acceleration in that case. The highest investigated σ_E is around 75 keV when they are not at the crest energy gain, as table 2 shows.
- The following four quadrupoles are not sufficient to expand the electron beam to a big round beam size within the existing beamline distance less than 10 m. Therefore, **a solenoid**, with peak on axis magnetic strength of 0.23 T, is applied to **over-focus** the beam to achieve it. Fig. 4 shows one solution of the beam envelope.
- The **space charge effects** with 1000 times higher beam current are investigated under the highest energy spread 75 keV, as Fig 5 shows. The beam size increases with the bunch charge increasing, so decreasing the solenoid strength can cancel it.

Table 2. Electron beam parameters at the exit of the accelerator.

Parameters of the achieved e-beam	
Electron energy	8 MeV
Energy spread	< 75 keV (σ_E)
Transverse maximum radius	~25 mm
Beam size	8 - 9 mm (σ_x)

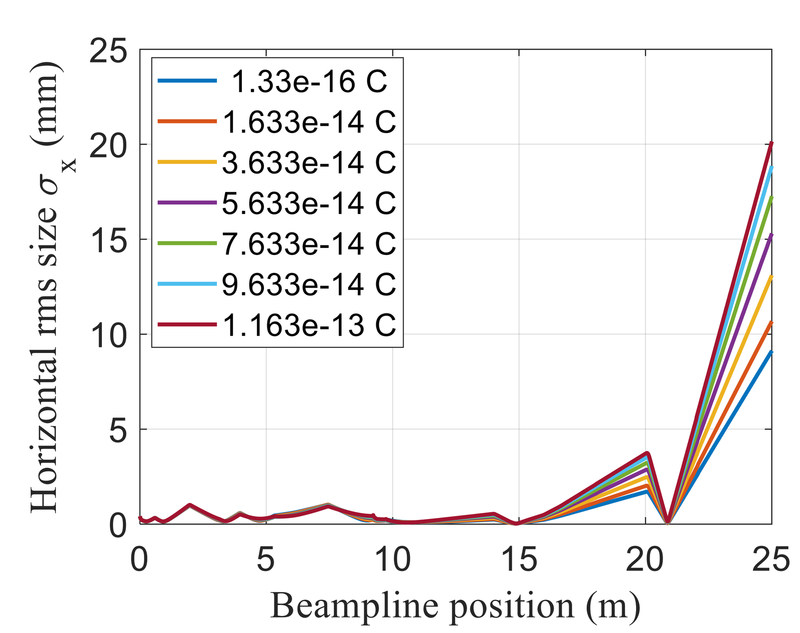


Fig. 5 Beam envelope under higher bunch charges with the space charge effect considered.

Dose (deposited energy) distribution in water

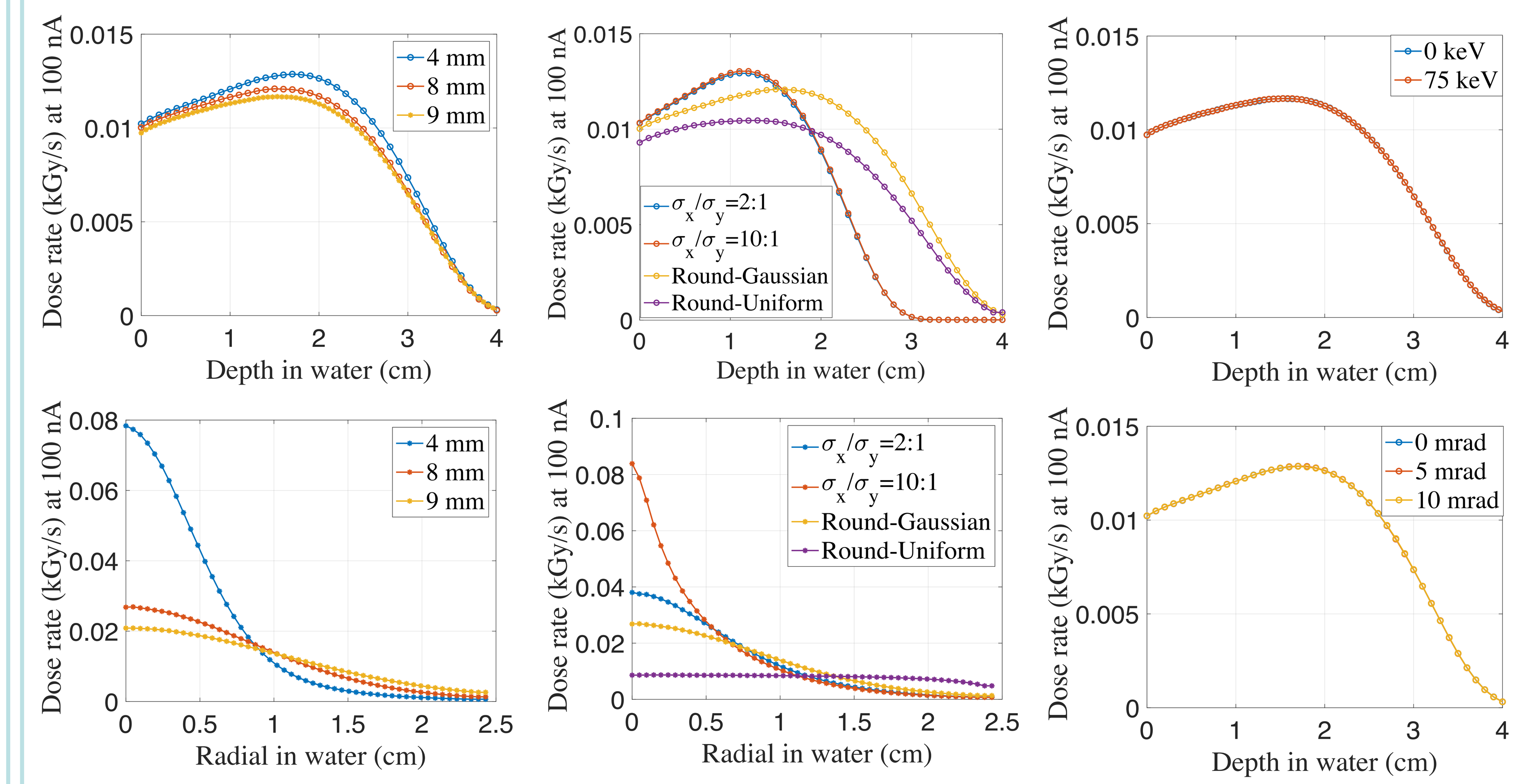


Fig. 6 Dose distribution inside the water container under different electron beam parameters.

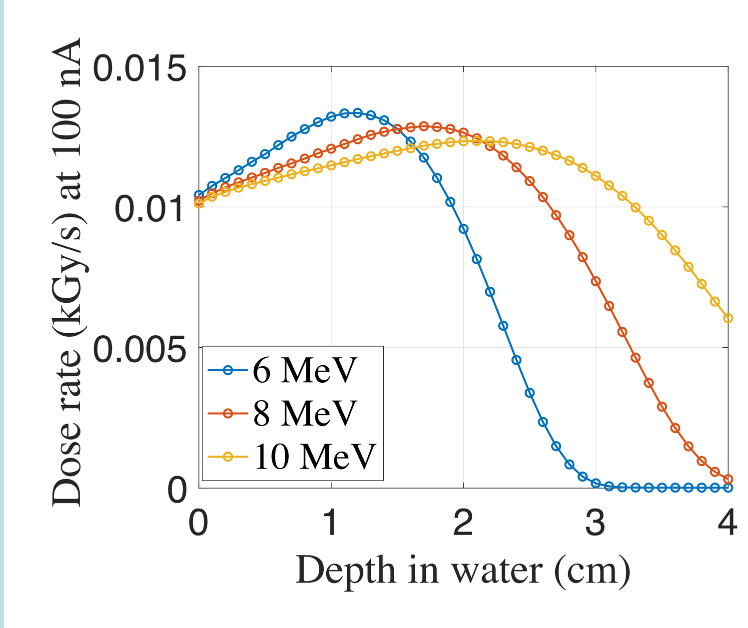


Fig. 7 Dose rate at 100 nA electron beam current under different electron beam energy.

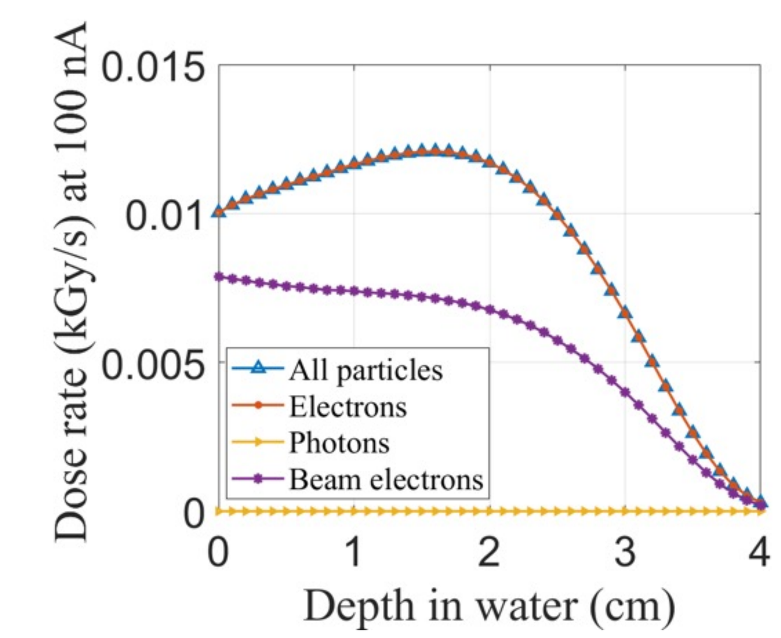


Fig. 8 Dose contributions resulting from the electrons and bremsstrahlung photons .

- With the electron beam parameters acquired from the beamline design, the dose distributions are investigated by the Monte-Carlo simulations.
- The electron beam energy and its transverse space distribution are the main factors affecting the dose uniformness, as shown in Fig. 6 and Fig. 7.
- The uniformness along the depth in water is more important, since the water is flowing in front of the electron beam in real applications. The **round transverse uniform** electron beam achieved the **most uniform** distribution, the energy spread and the beam divergencies within the considered ranges don't affect the dose distribution.
- With the energy increasing, the dose distribution is being more uniform. For 8 MeV electron energy, the depth of 3.3 cm is good for a more uniform dose distribution.
- The electrons during the deposition process contribute most to the deposited energy into the water while the bremsstrahlung photons are very low, so it is a safe method.

Conclusions and outlook

- The electron beam irradiation beamline is designed and achieved successfully with 8 MeV electron energy and 0.8 cm to 0.9 cm rms transverse beam radius.
- The depth of the water container is optimized to be 3.3 cm after the investigation of the dose distribution simulations, where the electron energy and the transverse space distribution domain the dose uniformness through the water depth.
- For next stage and further study, the beamline will be installed, commissioned and run for the wastewater sample irradiation.