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JUSTIFICATION OF A HIGH-ENERGY REGIME FOR WATER DISINFECTION BY AN ELECTRON BEAM

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The challenge of providing safe and clean drinking water requires reliable disinfection methods. Electron beam processing is a promising technology, but its industrial application is often limited by regulatory constraints, which typically cap the electron energy at 10 MeV to prevent induced radioactivity. This paper presents a theoretical justification for the radiological safety of using a higher, sub-threshold energy regime. This paper proposes operating in the 10–15.6 MeV range (using 14.9 MeV as a case study) and demonstrate that this approach allows for the treatment of significantly thicker water layers compared to the standard 10 MeV regime, while ensuring radiological safety. A comprehensive numerical model was used to simulate the process, calculating the bremsstrahlung photon spectrum and the induced activity from potential photonuclear reactions. A quantitative analysis of induced activity was performed for the main components of water (^{16}O , ^{2}H) and typical trace impurities according to Ukrainian standards (DSanPiN 2.2.4-171-10). The analysis proves that the induced radioactivity is negligible. The primary activation channel on oxygen is energetically forbidden, and the activity from trace elements is short-lived and falls far below the intervention levels set by Ukrainian radiation safety norms (NRBU-97). This work provides a strong physics-based rationale that a high-energy, sub-threshold regime is radiologically safe, which allows for a reconsideration of existing energy limitations in the design of electron beam water treatment facilities.

Keywords: Water disinfection; Electron beam; Bremsstrahlung; Induced activity; Photonuclear reactions; Computer simulation; Sub-threshold energy

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1. INTRODUCTION

Providing access to clean and safe drinking water is one of the key global challenges of our time and a cornerstone of public health. Traditional disinfection methods, such as chlorination, while widespread, can lead to the formation of potentially toxic and carcinogenic organochlorine by-products. Alternative methods, like ultraviolet (UV) irradiation, are safe but their effectiveness drops sharply in turbid media, limiting their application. In this context, radiation processing using accelerated electron beams appears to be a promising, fast, and highly efficient technology capable of achieving a high degree of water sterilization regardless of its optical properties.

A major factor limiting the widespread adoption of radiation processing is the concern over induced radioactivity in the treated products. For this reason, international and national standards typically limit the maximum energy of electron beams used for processing food and water to 10 MeV. This limitation ensures the absence of photonuclear reactions in most light and medium nuclei. However, from a physics standpoint, the penetration depth of electrons is directly dependent on their energy. At the same time, the primary disinfecting agent in direct electron irradiation is the electron beam itself, through the formation of highly reactive radiolytic products caused by the ionization and excitation of water molecules. A detailed description of these processes can be found in foundational texts such as Spinks and Woods [1]. The key products include hydrated electrons (e_{aq}^-), hydroxyl radicals (·OH), and hydrogen peroxide (H₂O₂), which effectively destroy microorganisms by damaging their DNA and cell membranes. The secondary bremsstrahlung radiation, however, is the source of photons that can induce radioactivity, creating a conflict between the desire for greater penetration depth (high energy) and the strict requirement for radiological safety (low energy).

The purpose of this work is to provide a theoretical justification and quantitative proof, by means of computer simulation, that using an electron beam with an energy higher than 10 MeV but strictly below the threshold of the main water activation reaction $^{16}\text{O}(\gamma, n)^{15}\text{O}$ (15.66 MeV) allows for a significant increase in the treatment depth without creating radiologically significant induced activity in the water. This paper presents a calculation of the absorbed dose and a quantitative analysis of possible activation channels for water that complies with the Ukrainian standards DSanPiN 2.2.4-171-10 [2].

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2. NUMERICAL MODEL AND METHODS

To quantitatively assess the efficiency and safety of the proposed irradiation regime, a numerical model was developed using the Python programming language (version 3.x) [6]. All mathematical calculations and array manipulations were performed using the NumPy library [7], and the results were visualized using the Matplotlib library [8]. The model allows for the calculation of the bremsstrahlung spectrum, absorbed dose, and induced activity in water for a given experimental configuration.

2.1. General simulation setup

The model utilizes a one-dimensional geometry, representing the dose distribution along the central axis of the beam. In a practical application, a beam scanning system would be employed to distribute the dose uniformly over the width of the treatment channel. The simulation follows the passage of a monoenergetic electron beam sequentially through three media: 1) the accelerator exit window (100 μ m thick titanium foil); 2) an air gap (10 cm); and 3) the water target. The baseline parameters for the calculations were an initial electron beam energy of $E_0 = 14.9$ MeV and a current of I = 1 μ A, normalized to a cross-sectional area of S = 1 cm². The water composition was assumed to comply with DSanPiN 2.2.4-171-10 [2].

2.2. Calculation of physical quantities

The simulation is based on a step-by-step calculation of three key physical quantities: the absorbed dose, the bremsstrahlung photon spectrum, and the induced activity.

Absorbed Dose. The absorbed dose distribution was estimated using a simplified one-dimensional model. The calculation is based on the energy deposited by the electron beam, E_{dep} [J], in a given mass layer, m_{layer} [kg]. For this first-order approximation, the fundamental definition of absorbed dose was used [11], with energy loss, dE/dx, based on stopping power data from the NIST ESTAR database [9]:

$$D = \frac{E_{dep}}{m_{layer}} = \frac{(dE/dx) \cdot \Delta x \cdot N_e \cdot t_{irr}}{m_{layer}}$$

where N_e is the number of electrons per second, and Δx is the thickness of the water layer. We acknowledge that this linear model is an approximation valid for thin absorbers and does not account for electron scattering effects. For precise dosimetry in a thick target, more advanced methods like Monte Carlo simulations are required. However, for the primary purpose of this paper—the safety analysis—this model is sufficient for a general estimation.

Bremsstrahlung Spectrum. The bremsstrahlung photon flux, $\Phi_{\gamma}(E_{\gamma})$, was calculated to assess the potential for photonuclear activation. For this purpose, a conservative estimation approach was adopted. The calculation was based on the Schiff theory [10], which accurately describes the spectrum from a thin target. This model was applied using the initial electron energy ($E_0 = 14.9$ MeV), effectively assuming the entire photon flux is generated in a thin layer without prior energy loss of the electrons.

This approach is intentionally conservative for a safety analysis involving a thick target, such as the water layer. In a thick medium, electrons lose energy as they penetrate, which "softens" the resulting bremsstrahlung spectrum, reducing the fraction of high-energy photons. By using the thin-target Schiff formula for the maximum initial energy, the model overestimates the flux of high-energy photons responsible for activation. Therefore, if the calculated induced activity is found to be negligible under this conservative assumption, the actual activity in a real-world scenario will be even lower.

Induced Activity. The rate of formation of the i-th radionuclide, R_i [nuclei/s], was calculated based on the fundamental activation equation, as described in standard texts like Krane [12]:

$$R_i = n_i \int_{E_{th}}^{E_0} \Phi_{\gamma}(E_{\gamma}) \sigma_i(E_{\gamma}) dE_{\gamma}$$

where n_i is the number of target nuclei of type i, $\Phi_{\gamma}(E_{\gamma})$ is the calculated photon flux spectrum, $\sigma_i(E_{\gamma})$ is the cross-section for the specific photonuclear reaction, and the integration is performed from the reaction threshold energy E_{th} up to the initial electron energy E_0 . The cross-section data were obtained from the TALYS code [4] and international nuclear data libraries. The time-dependent activity, A(t), was then calculated using the standard activation and decay equation.

3. RESULTS AND DISCUSSION

Based on the developed model, calculations of the absorbed dose and induced activity were performed for the baseline configuration of the facility ($E_0 = 14.9 \text{ MeV}$, $I = 1 \mu\text{A}$, $S = 1 \text{ cm}^2$).

3.1. Absorbed Dose Distribution and Penetration Depth

A key indicator of the radiation processing capability is the absorbed dose distribution as a function of depth in the target. The calculations, based on the model described in the Methods section, indicate a significant difference in penetration depth for electron beams with initial energies of 10 MeV and 14.9 MeV.

The model shows that the 10 MeV beam is completely absorbed within a \sim 5.2 cm layer of water, whereas the 14.9 MeV beam provides effective treatment through a layer of \sim 7.8 cm. This demonstrates the technical advantage of the higher-energy regime: it allows for the treatment of significantly thicker water layers in a single pass. It is important to clarify that this increase in penetration and treatable volume is a direct consequence of the higher beam power (for a given current) and does not imply a higher energy efficiency per unit mass of treated water. The value of this approach lies in a significant expansion of technological capabilities. The ability to treat a thicker water layer in a single pass simplifies the hydraulic engineering of the flow system, potentially eliminating the need for complex weirs or thin-film flow designs that are necessary for lower-energy beams. This simplifies the overall design and operation of the treatment facility.

The calculated surface dose rate (\approx 2 kGy/s) indicates that a sterilizing dose of 10 kGy, recommended by the IAEA, can be delivered to the water in a matter of seconds, confirming the high-throughput nature of the electron beam method.

3.2. Radiological safety analysis

To illustrate the underlying principle of the sub-threshold safety regime, the calculated bremsstrahlung photon spectrum is superimposed with the cross-section of the dominant photonuclear reaction, ${}^{16}O(\gamma, n){}^{15}O$, in Fig. 1.

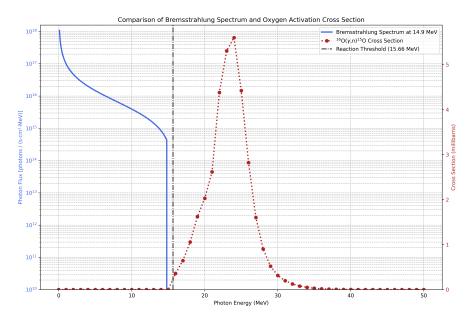


Figure 1. Comparison of the calculated bremsstrahlung photon spectrum with the experimental photonuclear reaction cross-section for $^{16}O(\gamma, n)^{15}O$.

The photon spectrum was calculated using the Schiff theory based on the simulation parameters outlined in the Methods section: an initial electron beam energy of 14.9 MeV, a current of 1 μ A, and a cross-sectional area of 1 cm², after passage through a 100 μ m titanium accelerator window and a 10 cm air gap. The cross-section data were obtained from international nuclear data libraries. The lack of significant overlap between the two curves visually demonstrates the principle of the sub-threshold safety regime.

As can be seen from Fig. 1, the reaction rate, which is determined by the overlap region of the two curves, is negligible because the photon spectrum effectively ends before the reaction cross-section becomes significantly non-zero. A quantitative analysis confirms this:

- Activation of Oxygen-16: The induced activity from the formation of 15 O is theoretically zero, as the maximum energy of the electron beam (14.9 MeV) is below the 16 O(γ , n) 15 O reaction threshold (15.66 MeV). This primary activation channel, which is dominant at above-threshold energies, is physically forbidden in the proposed regime.
- Photodisintegration of Deuterium. The ${}^2{\rm H}(\gamma,n){}^1{\rm H}$ reaction (threshold ≈ 2.225 MeV) does occur, generating a fast neutron flux of approximately $10^7 10^8$ n/(s·cm²). It is important to emphasize that this process does not produce radioactive isotopes in the water (the products are stable protium and a neutron) and thus does not create residual

radioactivity after the beam is turned off. The resulting prompt neutron field is a standard engineering consideration for the shielding design of any high-energy accelerator facility.

• Activation of Impurities: A comprehensive safety assessment requires a multi-step analysis of trace elements present in the water according to DSanPiN standards [2]. Such an analysis involves calculating the absorbed dose and the resulting time-integrated photon flux, followed by the calculation of radionuclide production for each potential impurity. The final step is to determine the total and spectral activity at the end of the irradiation cycle and predict its decay over time.

Following this methodology, a preliminary conservative analysis was performed. It shows that for all relevant photonuclear reactions, such as $^{35}\text{Cl}(\gamma, n)^{34}\text{Cl}$ (product $T_{1/2} = 32 \text{ min}$) or $^{14}\text{N}(\gamma, n)^{13}\text{N}$ (product $T_{1/2} = 9.97 \text{ min}$), the half-life of the produced radionuclide is orders of magnitude longer than the typical water irradiation time (which is on the order of seconds). Because the irradiation time t_{irr} is much shorter than the half-life $T_{1/2}$, the activity cannot build up to a significant level, reaching only a minuscule fraction of its potential saturation value. This comprehensive analysis confirms that for all likely impurities, the induced activity falls many orders of magnitude below the intervention levels established in the national standard NRBU-97 [3].

4. CONCLUSIONS

Based on the performed theoretical analysis and computer modeling, the following conclusions can be drawn:

- 1. A high-energy, sub-threshold approach to radiation-based water disinfection has been proposed and theoretically justified. It involves using an accelerated electron beam with an energy higher than the standard 10 MeV limit but strictly below the threshold of the main water activation reaction, ${}^{16}O(\gamma, n){}^{15}O$ (15.66 MeV).
- 2. It has been demonstrated through the developed computer model that operating in the proposed regime (using 14.9 MeV as an example) allows for the treatment of significantly thicker layers of water (7.8 cm) compared to the standard 10 MeV regime (5.2 cm). This represents an expansion of the technological capabilities for designing single-pass water treatment systems, rather than an increase in energy efficiency per unit mass.
- 3. A quantitative analysis of radiological safety has proven that the induced activity in the water is negligible in the proposed regime. The activation of the main water component, oxygen, is physically forbidden by selecting an energy below the reaction threshold. The prompt neutron flux from deuterium photodisintegration is a standard shielding design consideration and does not cause residual radioactivity. The induced activity from trace impurities is short-lived and rapidly decays to levels several orders of magnitude below the intervention levels set by the Ukrainian Radiation Safety Norms.
- 4. Thus, the proposed approach is physically justified and has been shown to be radiologically safe. It offers an expanded technological capability for water disinfection and provides a strong basis for reconsidering the current 10 MeV regulatory limit in the design and modernization of advanced water treatment facilities.
- 5. It is established that for a more detailed assessment of the induced activity in treated water samples, a separate comprehensive study is required. This future work should include: a) calculation of the absorbed dose and the corresponding time-integrated photon flux for the specific irradiation regime; b) analysis of the complete list of potential impurities according to DSanPiN standards; c) calculation of the production rate for each possible radionuclide; and d) determination of the total and spectral activity at the moment the irradiation is complete, followed by a forecast of its decay over time.

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ОБҐРУНТУВАННЯ ВИСОКОЕНЕРГЕТИЧНОГО РЕЖИМУ ДЕЗІНФЕКЦІЇ ВОДИ ЗА ДОПОМОГОЮ ПУЧКА ЕЛЕКТРОНІВ

Степан Г. Карпусь^{а,b}, Олег О. Шопен^b, Дмитро А. Захарчук^а, Тетяна О. Нарожна^c

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^ьНаціональний науковий центр «Харківський фізико-технічний інститут», вул. Академічна, 1, Харків, 61108, Україна ^сЗіньківський опорний ліцей № 1 Зіньківської міської ради, вул. Соборності, 62, Полтавська область, 38100, Україна Завдання забезпечення безпечною та чистою питною водою вимагає надійних методів дезінфекції. Електронно-променева обробка є перспективною технологією, але її промислове застосування часто обмежене нормативними обмеженнями, які зазвичай обмежують енергію електронів на рівні 10 МеВ для запобігання індукованій радіоактивності. У цій статті представлено теоретичне обгрунтування радіологічної безпеки використання вищого, підпорогового енергетичного режиму. У статті пропонується робота в діапазоні 10-15,6 МеВ (на прикладі 14,9 МеВ) та демонструється, що цей підхід дозволяє обробляти значно товстіші шари води порівняно зі стандартним режимом 10 МеВ, забезпечуючи при цьому радіологічну безпеку. Для моделювання процесу було використано комплексну числову модель, розраховано спектр гальмівного фотона та індуковану активність від потенційних фотоядерних реакцій. Було проведено кількісний аналіз індукованої активності для основних компонентів води (16O, 2H) та типових мікроелементів відповідно до українських стандартів (ДСанПіН 2.2.4-171-10). Аналіз доводить, що індукована радіоактивність є незначною. Первинний канал активації на кисні енергетично заборонений, а активність від мікроелементів є короткочасною та значно нижчою за рівні втручання, встановлені українськими нормами радіаційної безпеки (НРБУ-97). Ця робота надає вагоме фізичне обгрунтування того, що високоенергетичний підпороговий режим є радіологічно безпечним, що дозволяє переглянути існуючі енергетичні обмеження при проектуванні електронно-променевих водоочисних установок.

Ключові слова: дезінфекція води; електронний промінь; гальмівне випромінювання; індукована активність; фотоядерні реакції; комп'ютерне моделювання; підпорогова енергія