Computer simulation of chloroquine degradation in aqueous solution under electron beam irradiation

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1. Background and goal of this work

Chloroquine (CLQ) is popularly used as anti-malarials, autoimmune disease, skin disorders and also studied for therapeutic purposes for early COVID-19. CQ is also prescribed as a potential anticancer drug. It is persistence, bioaccumulation , it is important to understand its fate and eventual removal in the environment.

Aim of this work is to evaluate possibility of EB technology application to degradate CLQ using computer simulation.

2. Model description

The chemical model for transformation CLQ in aqueous solution under ionization radiation includes 68 reactions involving 29 species . The integration of the complete system of first order ordinary differential equations was performed by use of the computer code KINETIC employing a Gear algorithm especially suited for stiff systems. Initial concentration of CLQ in aqueous solution was 125mg/L if it is not specially pointed out, oxygen concentration in the solution was 1.22 × 10^{-3}mol/L. Temperature, pressure and water concentration were 298 K, 1 atm. and 55.35 mol/L, respectively. Pulse accelerator was applied, a pulse 10 MeV electron accelerator with a mean beam power of 10 kW was used, pulse duration was 6 microseconds and pulse repetition rate was 300 per second, one pulse delivered 4 Gy dose.

3. Results and Discussion

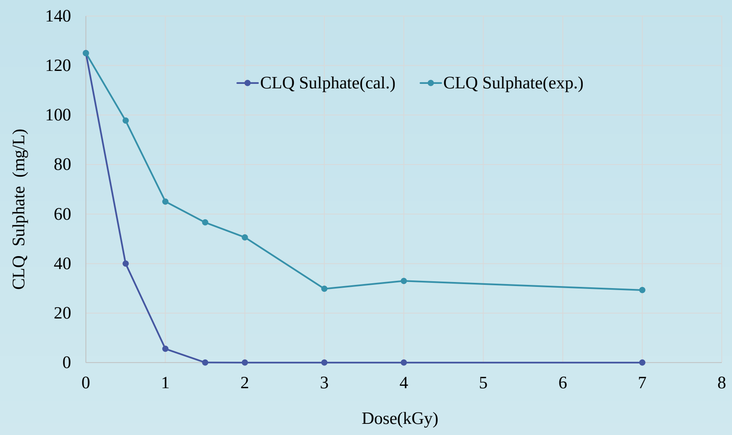

Fig.1 Comparison of calculated and experimental results of 125 mg/L CLQ sulphate degradation in aqueous solution under EB irradiation

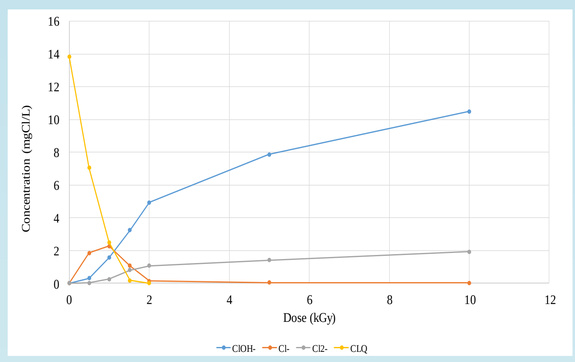

Fig.3. Changes of Cl versus dose under EB irradiation on 125 mg/L CLQ aqueous solution

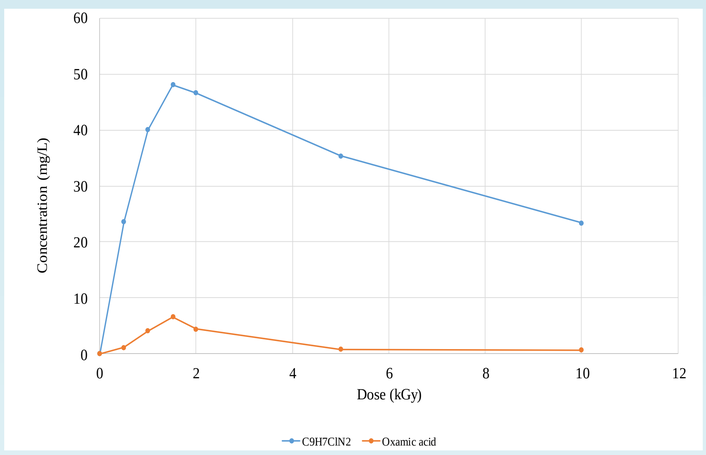

Fig.2 Organic products of CLQ decomposition versus dose under EB irradiation on 125 mg/L CLQ aqueous solution

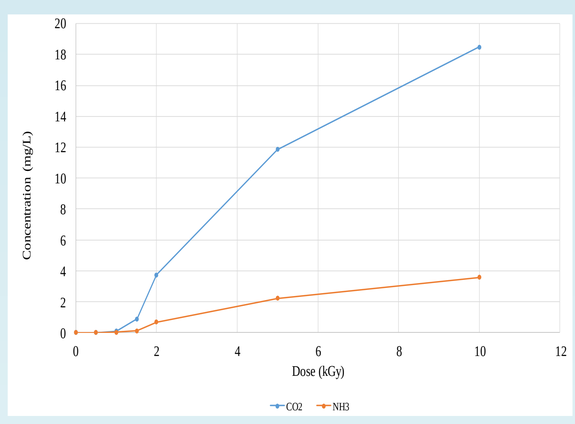

Fig.4 Formation of CO_2 and NH_3 versus dose under EB irradiation on 125 mg/L CLQ aqueous solution

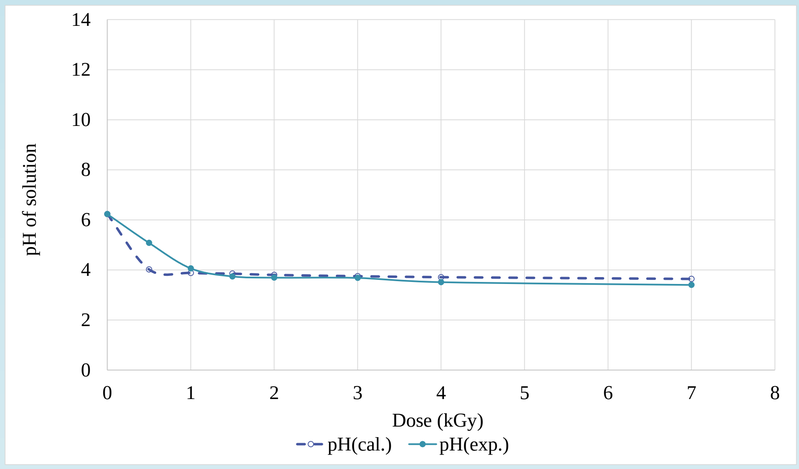

Fig.5 pH of the solution versus dose under EB irradiation on 125 mg/L CLQ sulphate aqueous solution

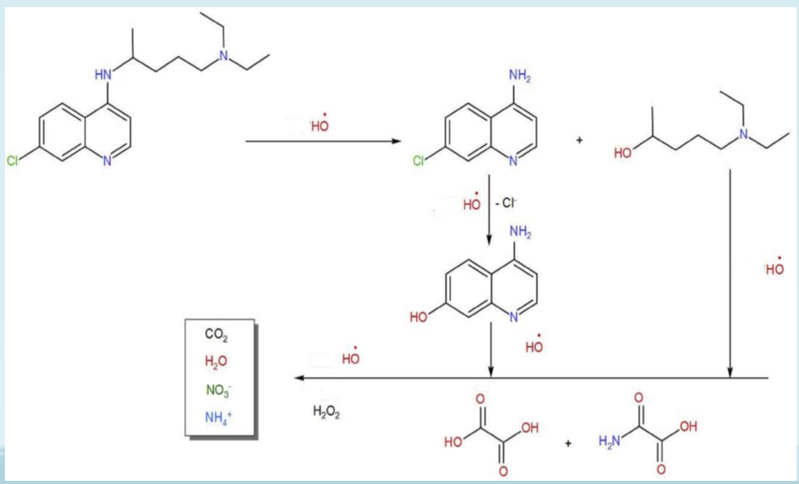

Fig.6 Simplified mechanism of CLQ degradation

$C_{18}H_{26}ClN_3 + e_{aq}^- = Cl^- + \bullet C_{18}H_{26}N_3$ $k=4.8 \times 10^{10}$ $[dm^3.\ mol^{-1}.\ s^{-1}]$

$\bullet OH + C_{18}H_{26}ClN_3 = \bullet C_{18}H_{26}ClN_3\text{-}OH$ $k=7.3 \times 10^{9}$ $[dm^3.\ mol^{-1}.\ s^{-1}]$

Conclusions

CLQ is easily decomposed under EB irradiation , more than 99.9% CLQ was decomposed at 2 kGy absorbed dose. Decomposition efficiency of CLQ increases with increasing the dose, while decreases with increasing the inlet concentration of CLQ. pH of the solution decreases with increasing the absorbed dose, from 7 reduced to 3.94 at 2 kGy absorbed dose. 4-amino-7-chloroquinoline and oxamic acid are predicted as organic degradation products, concentration of inorganic products , such as CO_2, NH_3 and chlorides etc. increases with increasing the absorbed dose, the mineralization of CLQ was predicted by the formation of chloride and inorganic nitrogen. Chloride dissociation hydrated electrons attachment and hydroxyl radicals addition reaction cause CLQ degradation.

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