

Supporting Information

Inactivation of *E. coli*, Bacteriophage MS2 and *Bacillus* Spores under UV/H₂O₂ and UV/Peroxydisulfate Advanced Disinfection Conditions

Peizhe Sun,^{*,a,b} Corey Tyree,^b Ching-Hua Huang^{*,a}

^aSchool of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332, United States

^bDivision of Energy and Environment, Southern Research Institute, Birmingham, Alabama 35205, United States

*Corresponding Authors.

Phone: 404-894-7694. E-mail: ching-hua.huang@ce.gatech.edu

Phone: 404-358-4858. E-mail: sunpeizhe@gatech.edu

Text S1. Chemicals and reagents

Text S2. Preparation of the culture stock of microbial surrogates

Text S3. Conversion between UV fluence and area-metric light intensity

Text S4. Model validation

Text S5. Estimation of diffusion-controlled limits

Text S6. Unit conversion of H₂O₂ and PDS

Text S7. Demonstration of EE/O calculation

Table S1. Characteristics of the Water Samples

Table S2. Elementary reactions

Table S3. Radical concentrations determined by experiments and kinetic model

Table S4. UV fluence (Einstein·L⁻¹) for experiments in Figure 2.

Figure S1. Illustration of collimated beam photoreactor.

Figure S2. Light spectra of low pressure UV lamp.

Figure S3. Inactivation of MS2 in the UV/H₂O₂/NaHCO₃ system with or without PNA.

Figure S4. Inactivation of *E. coli*, bacteriophage MS2 and *Bacillus subtilis* spores versus *CT* values of different radicals.

Prepared Date: March 22, 2016

Text S1. Chemicals and reagents

H₂O₂ (wt. 30%) was purchased from Fisher Scientific Co. (Pittsburgh, PA). PDS (98%) was purchased from Alfa Aesar (Ward Hill, MA). TBA (99.5%) was purchased from Sigma Aldrich Inc. (St. Louis, MO). NaHCO₃, K₂HPO₄, KH₂PO₄ and MgSO₄ were obtained from Fisher Scientific Co. Nutrient broth, agar, tryptone, yeast extract, and glucose were obtained from VWR International Inc. (West Chester, PA).

Text S2. Preparation of the culture stock of microbial surrogates and experimental setup

E. coli (ATCC 15597) was inoculated in nutrient broth (VWR BD 234000) and grown for 18 h at 37°C. The culture was then transferred into a 50-mL tube, which was centrifuged at 1,000 g for 10 min. The supernatant was discarded. The bacteria pellet was washed two more times with 50 mL of phosphate-buffered solution (PBS) (3 mM phosphate at pH 7). Stock suspension of *E. coli* was prepared by resuspending the final pellet in 2 mL PBS and stored at 4 °C prior to use. To achieve an initial density of *E. coli* around 4×10^6 CFU/mL for each disinfection experiment, the stock suspension of *E. coli* was spiked in reaction solution by a dilution factor of 1,000–10,000. Disinfection experiments were initiated by placing the petri dish (containing 3.0 mM PBS (pH 7), 0.3 mM oxidant and microbial surrogates, with or without scavengers) under UV exposure. Preliminary test showed that the pH was stable during the disinfection experiments. For each condition, at least triplicate experiments were conducted. For each sample, a ten-fold serial dilution was performed up to 1/10,000 dilution ratio using 30 mM PBS at pH 7.1. 0.1-mL aliquot of each

diluted solution was inoculated onto each of three replicates of 47-mm sterile Petri dishes containing nutrient agar (8 g/L nutrient broth + 15 g/L agar,). Colony forming units (CFU) were counted after incubation at 37 °C for 24 h.

The stocks of bacteriophage MS2 (ATCC 15597-B1) were prepared using *E. coli* (ATCC 15597) as the host. *E. coli* host was grown and assayed in a medium containing 1% tryptone, 0.05% glucose, 0.8% NaCl, 0.03% CaCl₂·2H₂O and 0.1% yeast extract. Quantification of MS2 employed double-agar layer method of plaque assay. The incubation temperature was 37°C. MS2 stocks were prepared from the top agar layer, which was transferred into a 50-mL centrifuge tube and vigorously mixed with 10 mL of phosphate-buffered saline (PBS) (150 mM sodium phosphate plus 150 mM sodium chloride). After centrifugation at 3,000 g for 15 min, the supernatant containing MS2 was saved. To achieve an initial density of bacteriophage MS2 around 3×10^6 PFU/mL for each disinfection experiment, the stock suspension of MS2 was spiked in reaction solution by a dilution factor of 1,000–10,000. Preliminary tests showed that the carryover of growth media posed negligible influence on the UV-based ADP performance. For each sample, a ten-fold serial dilution was performed up to 1/10,000 dilution ratio using 30 mM PBS at pH 7.1. Three replicates of 0.3-mL aliquot of each diluted solution was mixed with 0.1 mL host *E. coli* suspension and 4.5 mL soft agar liquid (at 50°C). The mixture was then transferred onto a 47-mm sterile Petri dish containing bottom agar. Plaque forming units (PFU) were counted after incubation at 37 °C for 12 h.

Stocks of *Bacillus subtilis* spores were prepared from a freeze-dried pellet of *B. subtilis* (ATCC

6633), which was rehydrated aseptically using a nutrient broth and incubated at 37 °C for 18 h. Bacterial cells were then harvested in similar fashion as *E. coli*. Several 47-mm sterile Petri dishes containing 1/10 diluted nutrient agar (0.8 g/L nutrient broth + 15 g/L agar,) were subsequently inoculated and incubated at 37 °C for 5-6 days to induce sporulation. After incubation, *B. subtilis* spores were collected into 50-mL conical tubes by rinsing the agar with PBS. The spores were cleaned by repeated centrifugation at 3,500 g for 10 min and resuspended in PBS three times. In order to inactivate any remaining vegetative cells, the stock solution was heat treated at 80 °C for over 20 min before each experiment. To achieve an initial density of *B. subtilis* spores around 4×10^6 CFU/mL for each disinfection experiment, the stock suspension of *B. subtilis* spores was spiked in reaction solution by a dilution factor of 1,000–10,000. For each sample, a ten-fold serial dilution was performed up to 1/10,000 dilution ratio using 30 mM PBS at pH 7.1. Three replicates of 0.1-mL aliquot of each diluted solution was inoculated onto three replicate 47-mm sterile Petri dishes containing nutrient agar (8 g/L nutrient broth + 15 g/L agar,). Colony forming units (CFU) were counted after incubation at 37 °C for 24 h.

Text S3. Conversion between UV fluence and area-metric light intensity

UV fluence (I_λ , in Einstein·L⁻¹) and area-metric light intensity (I_λ' , in J·cm⁻²) can be converted using the equation below:

$$I_\lambda = \frac{I_\lambda' \cdot 0.25\pi D^2}{V} \cdot \frac{1}{N_A \cdot \frac{h \cdot c}{\lambda}} \quad (\text{Einstein} \cdot \text{L}^{-1}) \quad (\text{S1})$$

I_λ' = area-metric light intensity, J·cm⁻²;

D = reactor diameter, cm;

V = the volume of reaction solution, L;

N_A = Avogadro's number, 6.022×10^{23} ;

h = Planck's constant, $6.626 \times 10^{-34} \text{ m}^2 \cdot \text{kg} \cdot \text{s}^{-1}$;

c = the speed of light, $3 \times 10^8 \text{ m} \cdot \text{s}^{-1}$;

λ = wavelength, m.

Text S4. Model validation

The concentrations of hydroxyl radical, sulfate radical and carbonate radical were measured in systems with UV/H₂O₂, UV/PDS and UV/H₂O₂/NaHCO₃, respectively. The degradation of nitrobenzene, anisole and *para*-nitroaniline, respectively, was monitored to calculate radical concentrations. The calculation method was detailed in Zhang et al. (2015).¹ The results (Table S3) showed that the model used in this study could successfully predict radical concentrations.

Text S5. Estimation of diffusion-controlled limits

The commonly referred “diffusion-controlled limits”, which is around 10^9 – $10^{10} \text{ M}^{-1}\text{s}^{-1}$ is derived based on the assumption that the reactants are approximately equal in size in the bimolecular association reaction. For a reaction $A + B \rightarrow \text{product}$, the reaction rate, k , can be expressed as:²

$$k = (2k_B T) / (3\eta) * ((r_A / r_B) + (r_B / r_A) + 2)$$

where $k_B T$ is the product of the Boltzmann constant and the absolute temperature; η is the solvent viscosity; r_A and r_B are the radii of molecules A and B, respectively. Therefore, when A and B are approximately equal in size, one finds $k = 8k_B T / 3\eta$, which corresponds to $k = 6.6 \times 10^9 \text{ M}^{-1}\text{s}^{-1}$ at

20°C. However, in the case of radicals (R) inactivating microbial surrogates (MS), r_{MS}/r_R is higher than 100 (e.g., the size of MS2 is about 27 nm,³ and the bond length of hydroxyl radical is around 0.1 nm.⁴). Therefore, it is possible that $k > 6.6 \times 10^{11} \text{ M}^{-1}\text{s}^{-1}$ (i.e., $\sim 4 \times 10^{13} \text{ M}^{-1}\text{min}^{-1}$). Considering the values in Table 2 are all based on \log_{10} of inactivation (instead of natural log), the upper limit of slope values should be $1.74 \times 10^{13} \text{ M}^{-1}\text{min}^{-1}$, which is higher than all the slope values obtained in this study.

Text S6. Unit conversion of H₂O₂ and PDS

The price of H₂O₂ (50% by weight) on Alibaba.com was \$400 per ton (April, 2015). Considering the average electricity cost is around 12 cent/kWh in the U.S., one milligram of H₂O₂ can be converted to 6.67×10^{-6} kWh. As for PDS, the price of sodium persulfate on Alibaba.com was \$1130 per ton (April, 2015). Therefore, with the same electricity cost, one milligram of PDS can be converted to 9.42×10^{-6} kWh.

Text S7. Demonstration of EE/O calculation

Example conditions: surface water matrix, H₂O₂ is at 0.19 mM, photo fluence is at 1.0×10^{-7} Einstein · L⁻¹ · s⁻¹, reaction time (t) is 4 min.

Calculation of -log (N/N₀): Applying 0.19 mM of H₂O₂ and 1.0×10^{-7} Einstein · L⁻¹ · s⁻¹ into the Matlab Simbiology program, the hydroxyl radical concentration ([·OH]), sulfate radical concentration ([SO₄^{·-}]) and carbonate radical concentration ([CO₃^{·-}]) were calculated to be

5.35×10^{-14} M, 4.54×10^{-22} M and 2.07×10^{-12} M, respectively. The photo fluence, $[\cdot\text{OH}]$, $[\text{SO}_4^{\cdot-}]$ and $[\text{CO}_3^{\cdot-}]$ were then used in Eqn. 10 in the main text with the reaction time of 4 min to calculate the overall reduction of bacteriophage MS2 ($-\log (N/N_0)_t = 2.42$).

Calculation of energy input over volume P/V : The photo fluence rate is at 1.0×10^{-7} Einstein $\cdot \text{L}^{-1} \cdot \text{s}^{-1}$. Since one mole of photons (1 Einstein) at 254 nm is equivalent to 0.1308 kWh of energy,⁵ the energy received by the system was 1.31×10^{-8} kWh $\cdot \text{L}^{-1} \cdot \text{s}^{-1}$. It is also assumed that energy efficiency of UV lamps was about 25%,⁵ and energy input was 5.23×10^{-8} kWh $\cdot \text{L}^{-1} \cdot \text{s}^{-1}$. With the exposure time of 4 min, the energy input P/V is equal to 1.26×10^{-5} kWh $\cdot \text{L}^{-1}$.

Substituting $-\log (N/N_0)_t = 2.42$, $P/V = 1.26 \times 10^{-5}$ kWh $\cdot \text{L}^{-1}$ and $[\text{H}_2\text{O}_2] = 0.19$ mM in Eqn. 11 in the main text, EE/O was calculated to be 2.29×10^{-5} kWh $\cdot \text{L}^{-1}$.

Table S1. Characteristics of the Water Samples.

Water	pH	A ₂₅₄ (cm ⁻¹)	DOC (mg C·L ⁻¹)	TIC (mg C·L ⁻¹)	Nitrate (mM)	Sulfate (mM)	Chloride (mM)
Surface water	7.4	0.069	3.07	5.63	0.017	0.022	0.092
Wastewater	7.6	0.085	7.33	11.76	1.07	0.46	1.64

DOC= dissolved organic carbon; TIC = total inorganic carbon.

Table S2. Elementary reactions

No.	Reaction	Rate Constant	Reference
1	$\text{H}_2\text{O}_2/\text{HO}_2^- \xrightarrow{h\nu} 2 \cdot \text{OH}$ $\text{S}_2\text{O}_8^{2-} \xrightarrow{h\nu} 2 \cdot \text{SO}_4^{\bullet -}$ $\text{NO}_3^- \xrightarrow{h\nu} \text{NO}_2^{\bullet} + \cdot \text{OH}$	$r_{\text{UV,oxidant}} = \frac{\Phi I_0 f_{\text{oxidant}} F_s}{[\text{oxidant}]}$ <p> Φ = quantum yield of H_2O_2/PDS/nitrate; I_0 = light intensity; f_{oxidant} = fraction of light absorbed by oxidant = $\frac{\varepsilon_{\text{oxidant}}[\text{oxidant}]l}{A_{\text{solution}}}$; F_s = fraction of light absorbed by the system = $1 - e^{-A_{\text{solution}}}$; $[\text{oxidant}]$ = concentration of H_2O_2, PDS or nitrate </p>	a
2	$\text{H}^+ + \text{OH}^- \rightarrow \text{H}_2\text{O}$	$1.0 \times 10^{11} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
3	$\text{H}_2\text{O} \rightarrow \text{H}^+ + \text{OH}^-$	$1.0 \times 10^{-3} \text{ s}^{-1}$	a
4	$\text{H}^+ + \text{HO}_2^- \rightarrow \text{H}_2\text{O}_2$	$5.0 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
5	$\text{H}_2\text{O}_2 \rightarrow \text{H}^+ + \text{HO}_2^-$	$1.3 \times 10^{-1} \text{ s}^{-1}$	a
6	$\text{H}^+ + \text{SO}_5^{2-} \rightarrow \text{HSO}_5^-$	$5.0 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
7	$\text{HSO}_5^- \rightarrow \text{H}^+ + \text{SO}_5^{2-}$	19.9 s^{-1}	a
8	$\text{H}^+ + \text{O}_2^{\bullet -} \rightarrow \text{HO}_2^{\bullet}$	$5 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
9	$\text{HO}_2^{\bullet} \rightarrow \text{H}^+ + \text{O}_2^{\bullet -}$	$7.9 \times 10^5 \text{ s}^{-1}$	a
10	$\text{HCO}_3^- + \text{H}^+ \rightarrow \text{H}_2\text{CO}_3$	$5.0 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
11	$\text{H}_2\text{CO}_3 \rightarrow \text{HCO}_3^- + \text{H}^+$	$2.5 \times 10^4 \text{ s}^{-1}$	a
12	$\text{CO}_3^{2-} + \text{H}^+ \rightarrow \text{HCO}_3^-$	$5 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
13	$\text{HCO}_3^- \rightarrow \text{CO}_3^{2-} + \text{H}^+$	2.5 s^{-1}	a
14	$\text{H}_2\text{PO}_4^- + \text{H}^+ \rightarrow \text{H}_3\text{PO}_4$	$5 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a

15	$\text{H}_3\text{PO}_4 \rightarrow \text{H}_2\text{PO}_4^- + \text{H}^+$	$3.97 \times 10^8 \text{ s}^{-1}$	a
16	$\text{HPO}_4^{2-} + \text{H}^+ \rightarrow \text{H}_2\text{PO}_4^-$	$5 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
17	$\text{H}_2\text{PO}_4^- \rightarrow \text{HPO}_4^{2-} + \text{H}^+$	$3.2 \times 10^3 \text{ s}^{-1}$	a
18	$\text{PO}_4^{3-} + \text{H}^+ \rightarrow \text{HPO}_4^{2-}$	$5 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
19	$\text{HPO}_4^{2-} \rightarrow \text{PO}_4^{3-} + \text{H}^+$	$2.5 \times 10^{-2} \text{ s}^{-1}$	a
20	$\cdot\text{OH} + \cdot\text{OH} \rightarrow \text{H}_2\text{O}_2$	$5.5 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
21	$\cdot\text{OH} + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2\cdot + \text{H}_2\text{O}$	$2.7 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
22	$\cdot\text{OH} + \text{HO}_2^- \rightarrow \text{HO}_2\cdot + \text{OH}^-$	$7.5 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
23	$\cdot\text{OH} + \text{S}_2\text{O}_8^{2-} \rightarrow \text{S}_2\text{O}_8^{\cdot-} + \text{OH}^-$	$1.4 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
24	$\cdot\text{OH} + \text{HO}_2\cdot \rightarrow \text{O}_2 + \text{H}_2\text{O}$	$6.6 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
25	$\cdot\text{OH} + \text{O}_2^{\cdot-} \rightarrow \text{O}_2 + \text{OH}^-$	$7.0 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
26	$\text{HO}_2\cdot + \text{HO}_2\cdot \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	$8.3 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
27	$\text{HO}_2\cdot + \text{O}_2^{\cdot-} \rightarrow \text{HO}_2^- + \text{O}_2$	$9.7 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
28	$\text{HO}_2\cdot + \text{H}_2\text{O}_2 \rightarrow \text{O}_2 + \cdot\text{OH} + \text{H}_2\text{O}$	$3.0 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
29	$\text{O}_2^{\cdot-} + \text{H}_2\text{O}_2 \rightarrow \text{O}_2 + \cdot\text{OH} + \text{OH}^-$	$0.13 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
30	$\cdot\text{OH} + \text{CO}_3^{2-} \rightarrow \text{CO}_3^{\cdot-} + \text{OH}^-$	$3.9 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
31	$\cdot\text{OH} + \text{HCO}_3^- \rightarrow \text{CO}_3^{\cdot-} + \text{H}_2\text{O}$	$8.6 \times 10^6 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
32	$\text{H}_2\text{O}_2 + \text{CO}_3^{\cdot-} \rightarrow \text{HCO}_3^- + \text{HO}_2\cdot$	$4.3 \times 10^5 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
33	$\text{HO}_2^- + \text{CO}_3^{\cdot-} \rightarrow \text{CO}_3^{2-} + \text{HO}_2\cdot$	$3.0 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
34	$\cdot\text{OH} + \text{CO}_3^{\cdot-} \rightarrow \text{product}$	$3.0 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
35	$\text{O}_2^{\cdot-} + \text{CO}_3^{\cdot-} \rightarrow \text{CO}_3^{2-} + \text{O}_2$	$6.0 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
36	$\text{CO}_3^{\cdot-} + \text{CO}_3^{\cdot-} \rightarrow \text{product}$	$3.0 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
37	$\cdot\text{OH} + \text{HPO}_4^{2-} \rightarrow \text{HPO}_4\cdot^- + \text{OH}^-$	$1.5 \times 10^5 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
38	$\cdot\text{OH} + \text{H}_2\text{PO}_4^- \rightarrow \text{HPO}_4\cdot^- + \text{H}_2\text{O}$	$2.0 \times 10^4 \text{ M}^{-1} \cdot \text{s}^{-1}$	a

39	$\text{H}_2\text{O}_2 + \text{HPO}_4^{\cdot-} \rightarrow \text{H}_2\text{PO}_4^- + \text{HO}_2^{\cdot}$	$2.7 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
40	$\text{SO}_4^{\cdot-} + \text{OH}^- \rightarrow \text{SO}_4^{2-} + \cdot\text{OH}$	$7 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
41	$\text{SO}_4^{\cdot-} + \text{H}_2\text{O} \rightarrow \text{HSO}_4^- + \cdot\text{OH}$	660 s^{-1}	a
42	$\text{SO}_4^{\cdot-} + \cdot\text{OH} \rightarrow \text{HSO}_5^-$	$1.0 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
43	$\text{SO}_4^{\cdot-} + \text{HSO}_5^- \rightarrow \text{SO}_5^{\cdot-} + \text{HSO}_4^-$	$1.0 \times 10^6 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
44	$\text{SO}_4^{\cdot-} + \text{SO}_5^{2-} \rightarrow \text{SO}_5^{\cdot-} + \text{SO}_4^{2-}$	$1.0 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
45	$\text{SO}_5^{\cdot-} + \text{SO}_5^{\cdot-} \rightarrow \text{SO}_4^{\cdot-} + \text{SO}_4^{\cdot-} + \text{O}_2$	$2.1 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
46	$\text{SO}_5^{\cdot-} + \text{SO}_5^{\cdot-} \rightarrow \text{S}_2\text{O}_8^{2-} + \text{O}_2$	$2.2 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
47	$\text{SO}_4^{\cdot-} + \text{SO}_4^{\cdot-} \rightarrow \text{S}_2\text{O}_8^{2-}$	$7.0 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
48	$\text{SO}_4^{\cdot-} + \text{S}_2\text{O}_8^{2-} \rightarrow \text{S}_2\text{O}_8^{\cdot-} + \text{SO}_4^{2-}$	$6.5 \times 10^5 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
49	$\text{S}_2\text{O}_8^{2-} + \text{CO}_3^{\cdot-} \rightarrow \text{CO}_3^{2-} + \text{S}_2\text{O}_8^{\cdot-}$	$3.0 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
50	$\text{SO}_4^{\cdot-} + \text{HPO}_4^{2-} \rightarrow \text{HPO}_4^{\cdot-} + \text{SO}_4^{2-}$	$1.2 \times 10^6 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
51	$\text{SO}_4^{\cdot-} + \text{H}_2\text{PO}_4^- \rightarrow \text{HPO}_4^{\cdot-} + \text{HSO}_4^-$	$5.0 \times 10^4 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
52	$\text{SO}_4^{\cdot-} + \text{HCO}_3^- \rightarrow \text{CO}_3^{\cdot-} + \text{HSO}_4^-$	$2.8 \times 10^6 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
53	$\text{SO}_4^{\cdot-} + \text{CO}_3^{2-} \rightarrow \text{CO}_3^{\cdot-} + \text{SO}_4^{2-}$	$6.1 \times 10^6 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
54	$\cdot\text{OH} + \text{Cl}^- \rightarrow \text{ClOH}^{\cdot-}$	$4.3 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
55	$\text{ClOH}^{\cdot-} \rightarrow \cdot\text{OH} + \text{Cl}^-$	$6.1 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
56	$\text{SO}_4^{\cdot-} + \text{Cl}^- \rightarrow \text{SO}_4^{2-} + \text{Cl}^{\cdot}$	$3.0 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
57	$\text{SO}_4^{2-} + \text{Cl}^{\cdot} \rightarrow \text{SO}_4^{\cdot-} + \text{Cl}^-$	$2.5 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
58	$\text{ClOH}^{\cdot-} + \text{H}^+ \rightarrow \text{Cl}^{\cdot} + \text{H}_2\text{O}$	$2.1 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
59	$\text{ClOH}^{\cdot-} + \text{Cl}^- \rightarrow \text{Cl}_2^{\cdot-} + \text{OH}^-$	$1.0 \times 10^4 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
60	$\text{Cl}^{\cdot} + \text{H}_2\text{O} \rightarrow \text{ClOH}^{\cdot-} + \text{H}^+$	$4.5 \times 10^3 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
61	$\text{Cl}^{\cdot} + \text{OH}^- \rightarrow \text{ClOH}^{\cdot-}$	$1.8 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
62	$\text{Cl}^{\cdot} + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2^{\cdot} + \text{Cl}^- + \text{H}^+$	$2.0 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a

63	$\text{Cl}^\cdot + \text{Cl}^\cdot \rightarrow \text{Cl}_2^\cdot$	$8.5 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
64	$\text{Cl}^\cdot + \text{Cl}^\cdot \rightarrow \text{Cl}_2$	$8.8 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
65	$\text{Cl}^\cdot + \text{HOCl} \rightarrow \text{ClO}^\cdot + \text{H}^+ + \text{Cl}^-$	$3.0 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
66	$\text{Cl}^\cdot + \text{OCl}^- \rightarrow \text{ClO}^\cdot + \text{Cl}^-$	$8.3 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
67	$\text{Cl}_2^\cdot \rightarrow \text{Cl}^\cdot + \text{Cl}^\cdot$	$6.0 \times 10^4 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
68	$\text{Cl}_2 + \text{OH}^\cdot \rightarrow \text{HOCl} + \text{Cl}^\cdot$	$1.0 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
69	$\text{Cl}_2^\cdot + \text{Cl}_2^\cdot \rightarrow \text{Cl}_2 + 2\text{Cl}^\cdot$	$9.0 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
70	$\text{Cl}_2^\cdot + \text{Cl}^\cdot \rightarrow \text{Cl}_2 + \text{Cl}^\cdot$	$2.1 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
71	$\text{Cl}_2^\cdot + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2^\cdot + 2\text{Cl}^\cdot + \text{H}^+$	$1.4 \times 10^5 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
72	$\text{Cl}_2^\cdot + \text{HO}_2^\cdot \rightarrow \text{O}_2 + 2\text{Cl}^\cdot + \text{H}^+$	$3.0 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
73	$\text{Cl}_2^\cdot + \text{O}_2^\cdot \rightarrow \text{O}_2 + 2\text{Cl}^\cdot$	$2.0 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
74	$\text{Cl}_2^\cdot + \text{H}_2\text{O} \rightarrow \text{Cl}^\cdot + \text{HClOH}$	$23.38 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
75	$\text{Cl}_2^\cdot + \text{OH}^- \rightarrow \text{Cl}^\cdot + \text{ClOH}^\cdot$	$4.5 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
76	$\text{HClOH} \rightarrow \text{ClOH}^\cdot + \text{H}^+$	$1.0 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
77	$\text{HClOH} \rightarrow \text{Cl}^\cdot + \text{H}_2\text{O}$	$1.0 \times 10^2 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
78	$\text{HClOH} + \text{Cl}^\cdot \rightarrow \text{Cl}_2^\cdot + \text{H}_2\text{O}$	$5.0 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
79	$\text{Cl}_2 + \text{Cl}^\cdot \rightarrow \text{Cl}_3^\cdot$	$2.0 \times 10^4 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
80	$\text{Cl}_3^\cdot \rightarrow \text{Cl}_2 + \text{Cl}^\cdot$	$1.1 \times 10^5 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
81	$\text{Cl}_3^\cdot + \text{HO}_2^\cdot \rightarrow \text{Cl}_2^\cdot + \text{HCl} + \text{O}_2$	$1.0 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
82	$\text{Cl}_3^\cdot + \text{O}_2^\cdot \rightarrow \text{Cl}_2^\cdot + \text{Cl}^\cdot + \text{O}_2$	$3.8 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
83	$\text{Cl}_2 + \text{H}_2\text{O} \rightarrow \text{Cl}^\cdot + \text{HOCl} + \text{H}^+$	$0.27 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
84	$\text{Cl}^\cdot + \text{HOCl} + \text{H}^+ \rightarrow \text{Cl}_2 + \text{H}_2\text{O}$	$18.2 \text{ M}^{-2} \cdot \text{s}^{-1}$	a
85	$\text{Cl}_2 + \text{H}_2\text{O}_2 \rightarrow \text{O}_2 + 2\text{HCl}$	$1.3 \times 10^4 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
86	$\text{Cl}_2 + \text{O}_2^\cdot \rightarrow \text{O}_2 + \text{Cl}_2^\cdot$	$1.0 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a

87	$\text{Cl}_2 + \text{HO}_2^\cdot \rightarrow \text{H}^+ + \text{O}_2 + \text{Cl}_2^{\cdot-}$	$1.0 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
88	$\text{H}^+ + \text{OCl}^- \rightarrow \text{HOCl}$	$5.0 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
89	$\text{HOCl} \rightarrow \text{H}^+ + \text{OCl}^-$	$1.4 \times 10^3 \text{ s}^{-1}$	a
90	$\text{HOCl} + \text{H}_2\text{O}_2 \rightarrow \text{HCl} + \text{H}_2\text{O} + \text{O}_2$	$1.1 \times 10^4 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
91	$\text{OCl}^- + \text{H}_2\text{O}_2 \rightarrow \text{Cl}^- + \text{H}_2\text{O} + \text{O}_2$	$1.7 \times 10^5 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
92	$\text{HOCl} + \cdot\text{OH} \rightarrow \text{ClO}^\cdot + \text{H}_2\text{O}$	$2.0 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
93	$\text{HOCl} + \text{O}_2^{\cdot-} \rightarrow \text{Cl}^- + \text{OH}^- + \text{O}_2$	$7.5 \times 10^6 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
94	$\text{HOCl} + \text{HO}_2^\cdot \rightarrow \text{Cl}^\cdot + \text{OH}^- + \text{O}_2$	$7.5 \times 10^6 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
95	$\text{OCl}^- + \cdot\text{OH} \rightarrow \text{ClO}^\cdot + \text{OH}^-$	$8.8 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
96	$\text{OCl}^- + \text{O}_2^{\cdot-} + \text{H}_2\text{O} \rightarrow \text{Cl}^- + 2\text{OH}^- + \text{O}_2$	$2 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
97	$\text{OCl}^- + \text{CO}_3^{\cdot-} \rightarrow \text{OCl}^\cdot + \text{CO}_3^{2-}$	$5.7 \times 10^5 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
98	$\text{Cl}^\cdot + \text{CO}_3^{2-} \rightarrow \text{Cl}^- + \text{CO}_3^{\cdot-}$	$5.0 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
99	$\text{Cl}^\cdot + \text{HCO}_3^- \rightarrow \text{Cl}^- + \text{CO}_3^{\cdot-} + \text{H}^+$	$2.2 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
100	$\text{Cl}_2^{\cdot-} + \text{CO}_3^{2-} \rightarrow 2\text{Cl}^- + \text{CO}_3^{\cdot-}$	$1.6 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
101	$\text{Cl}_2^{\cdot-} + \text{HCO}_3^- \rightarrow 2\text{Cl}^- + \text{CO}_3^{\cdot-} + \text{H}^+$	$8.0 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
102	$\text{H}^+ + \text{Cl}^- \rightarrow \text{HCl}$	$5.0 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	a
103	$\text{HCl} \rightarrow \text{H}^+ + \text{Cl}^-$	$8.6 \times 10^{16} \text{ s}^{-1}$	a
104	$\cdot\text{OH} + \text{NH}_3 \rightarrow \cdot\text{NH}_2 + \text{H}_2\text{O}$	$9.0 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
105	$\text{SO}_4^{\cdot-} + \text{NH}_3 \rightarrow \cdot\text{NH}_2 + \text{SO}_4^{2-} + \text{H}^+$	$1.4 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
106	$\cdot\text{NH}_2 + \text{O}_2 \rightarrow \text{NH}_2\text{O}_2^\cdot$	$10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
107	$\text{NH}_2\text{O}_2^\cdot \rightarrow \cdot\text{NO} + \text{H}_2\text{O}$	$\sim 7 \times 10^5 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
108	$\cdot\text{NO} + \text{O}_2^{\cdot-} \rightarrow \text{ONOO}^-$	$6.7 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
109	$\text{ONOO}^- \rightarrow \cdot\text{NO} + \text{O}_2^{\cdot-}$	$2.0 \times 10^{-2} \text{ s}^{-1}$	a
110	$\text{ONOO}^- + \text{CO}_2 \rightarrow \cdot\text{NO}_2 + \text{CO}_3^{\cdot-}$	$2.9 \times 10^4 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
111	$\text{ONOO}^- \rightarrow \text{NO}_3^-$	$\sim 8 \times 10^{-6} \text{ s}^{-1}$	a

112	$\text{ONOO}^- \rightarrow \cdot\text{NO}_2 + \text{O}^{\cdot-}$	$\sim 10^{-6} \text{ s}^{-1}$	a
113	$\cdot\text{NO}_2 + \text{O}^{\cdot-} \rightarrow \text{ONOO}^-$	$3.5 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
114	$\text{ONOO}^- + \cdot\text{OH} \rightarrow \cdot\text{NO} + \text{O}_2 + \text{OH}^-$	$4.8 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
115	$\text{ONOO}^- + \text{CO}_3^{\cdot-} \rightarrow \cdot\text{NO} + \text{O}_2 + \text{CO}_3^{2-}$	$3.7 \times 10^6 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
116	$\cdot\text{NO}_2 + \cdot\text{OH} \rightarrow \text{ONOOH}$	$4.5 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
117	$\text{ONOOH} \rightarrow \cdot\text{NO}_2 + \cdot\text{OH}$	$3.5 \times 10^{-1} \text{ s}^{-1}$	a
118	$\cdot\text{NO} + \text{HO}_2^{\cdot} \rightarrow \text{ONOOH}$	$3.2 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
119	$\text{ONOOH} \rightarrow \text{NO}_3^- + \text{H}^+$	$9.0 \times 10^{-1} \text{ s}^{-1}$	a
120	$\text{ONOOH} + \text{H}^+ \rightarrow \text{NO}_3^- + 2\text{H}^+$	$4.3 \text{ M}^{-1} \text{ s}^{-1}$	a
121	$\text{ONOOH} + \text{H}_2\text{O} + \text{H}^+ \rightarrow \text{HNO}_2 + \text{H}_2\text{O}_2 + \text{H}^+$	$1.1 \times 10^{-1} \text{ M}^{-2} \cdot \text{s}^{-1}$	a
122	$\text{HNO}_2 + \text{H}_2\text{O}_2 + \text{H}^+ \rightarrow \text{ONOOH} + \text{H}_2\text{O} + \text{H}^+$	$9.6 \times 10^3 \text{ M}^{-2} \cdot \text{s}^{-1}$	a
123	$\cdot\text{NO}_2 + \text{O}_2^{\cdot-} \rightarrow \text{O}_2\text{NOO}^-$	$4.5 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
124	$\text{O}_2\text{NOO}^- \rightarrow \cdot\text{NO}_2 + \text{O}_2^{\cdot-}$	1.0	a
125	$\text{O}_2\text{NOO}^- \rightarrow \text{NO}_2^- + \text{O}_2$	1.4	a
126	$\cdot\text{NO}_2 + \text{HO}_2^{\cdot} \rightarrow \text{O}_2\text{NOOH}$	$1.8 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
127	$\text{O}_2\text{NOOH} \rightarrow \cdot\text{NO}_2 + \text{HO}_2$	$2.6 \times 10^{-2} \text{ s}^{-1}$	a
128	$\text{H}^+ + \text{ONOO}^- \rightarrow \text{ONOOH}$	$5 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	assumed
129	$\text{ONOOH} \rightarrow \text{H}^+ + \text{ONOO}^-$	$1.25 \times 10^4 \text{ s}^{-1}$	calculated
130	$\text{H}^+ + \text{O}_2\text{NOO}^- \rightarrow \text{O}_2\text{NOOH}$	$5 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	assumed
131	$\text{O}_2\text{NOOH} \rightarrow \text{H}^+ + \text{O}_2\text{NOO}^-$	$6.9 \times 10^4 \text{ s}^{-1}$	calculated
132	$\text{H}^+ + \text{NO}_2^- \rightarrow \text{HNO}_2$	$5 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	assumed
133	$\text{HNO}_2 \rightarrow \text{H}^+ + \text{NO}_2^-$	$2.51 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	calculated
134	$\text{CO}_3^{\cdot-} + \text{NH}_3 \rightarrow \cdot\text{NH}_2 + \text{HCO}_3^-$	$\sim 3 \times 10^4 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
135	$\text{CO}_3^{\cdot-} + \cdot\text{NH}_2 \rightarrow \text{NH}_2\text{O}^- + \text{CO}_2$	$7.5 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
136	$\cdot\text{NO}_2 + \cdot\text{NO}_2 \rightarrow \text{N}_2\text{O}_4$	$4.5 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	a

137	$\text{N}_2\text{O}_4 \rightarrow \cdot\text{NO}_2 + \cdot\text{NO}_2$	$6.9 \times 10^3 \text{ s}^{-1}$	a
138	$\text{N}_2\text{O}_4 \rightarrow \text{NO}_2^- + \text{NO}_3^- + 2\text{H}^+$	$1 \times 10^3 \text{ s}^{-1}$	a
139	$\cdot\text{NO}_2 + \cdot\text{NO} \rightarrow \text{N}_2\text{O}_3$	$1.1 \times 10^9 \text{ M}^{-1} \cdot \text{s}^{-1}$	a
140	$\text{N}_2\text{O}_3 \rightarrow \text{NO}_2^- + \text{NO}_2^- + 2\text{H}^+$	530 s^{-1}	a
141	$\text{O}^- + \text{H}_2\text{O} \rightarrow \cdot\text{OH} + \text{OH}^-$	$9.4 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	b
142	$\cdot\text{OH} + \text{OH}^- \rightarrow \text{O}^- + \text{H}_2\text{O} \rightarrow$	$1.3 \times 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$	b
143	$\text{DOM} + \cdot\text{OH} \rightarrow \text{product}$	$3.9 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	c
144	$\text{DOM} + \text{CO}_3^{\cdot-} \rightarrow \text{product}$	$2.3 \times 10^4 \text{ M}^{-1} \cdot \text{s}^{-1}$	d
145	$\text{DOM} + \text{SO}_4^{\cdot-} \rightarrow \text{product}$	$1.0 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	estimated
146	$\text{TBA} + \cdot\text{OH} \rightarrow \text{product}$	$7.6 \times 10^8 \text{ M}^{-1} \cdot \text{s}^{-1}$	b
147	$\text{TBA} + \text{SO}_4^{\cdot-} \rightarrow \text{product}$	$9.1 \times 10^5 \text{ M}^{-1} \cdot \text{s}^{-1}$	b
148	$\text{H}_2\text{O}_2 + \text{SO}_4^{\cdot-} \rightarrow \text{HO}_2^- + \text{SO}_4^{2-} + \text{H}^+$	$1.2 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$	b

a Zhang et al. (2015)¹

b NIST⁶

c Brezonik et al. (1998)⁷

d Canonica et al. (2005)⁸

Table S3. Radical concentrations determined by experiments and by kinetic modeling.

System	Radical probe	Radical species	Measured by exp. (M)	Predicted by model (M)
UV/H ₂ O ₂	Nitrobenzene	Hydroxyl radical	4.2×10^{-15}	4.4×10^{-15}
UV/PDS	Nitrobenzene, Anisole	Sulfate radical	1.7×10^{-15}	1.4×10^{-15}
UV/H ₂ O ₂ /NaHCO ₃	Nitrobenzene, <i>para</i> -nitroaniline	Carbonate radical	1.1×10^{-12}	9.8×10^{-13}

Table S4. UV fluence (Einstein·L⁻¹) for experiments in Figure 2.

System	<i>E. coli</i>	MS2	<i>Bacillus</i> spores
7*/7	8.9×10^{-7}	2.2×10^{-6}	1.6×10^{-6}
6*/6	8.9×10^{-7}	4.4×10^{-6}	1.6×10^{-6}
5*/5	1.1×10^{-6}	4.4×10^{-6}	1.6×10^{-6}

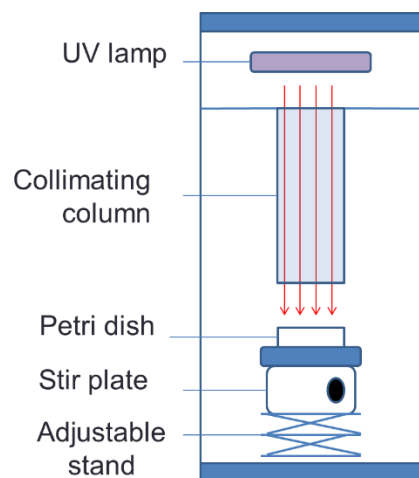


Figure S1. Illustration of collimated beam photoreactor.

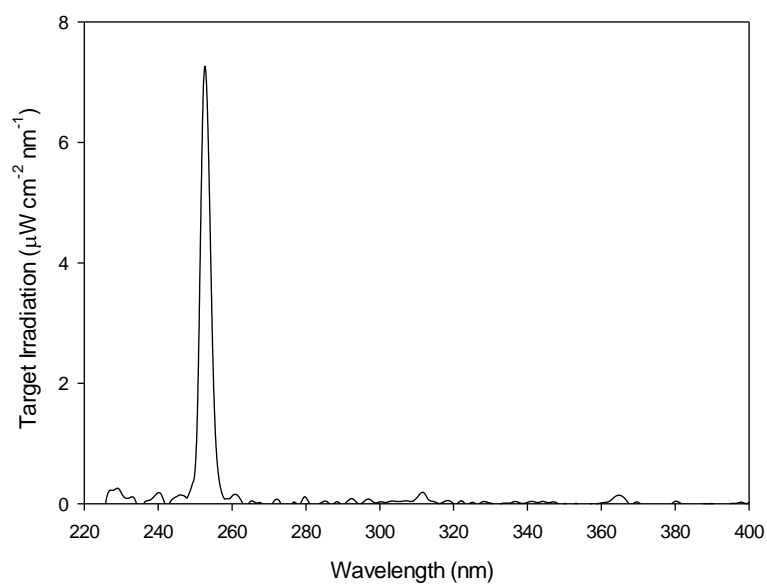


Figure S2. Light spectra of low pressure UV lamp.

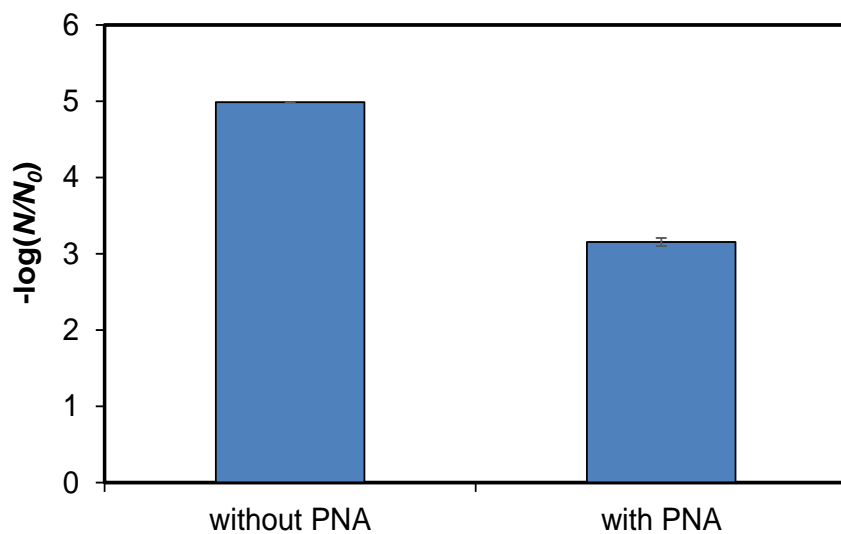


Figure S3. Inactivation of MS2 in the UV/H₂O₂/NaHCO₃ system with or without 0.01 mM *para*-nitroaniline (PNA). Conditions: UV irradiation at 2.2×10^{-7} Einstein·L⁻¹·s⁻¹ with 0.3 mM H₂O₂ and 0.1 M NaHCO₃ in PBS. The irradiation time = 20 min. Error bars represent one standard deviation of the means (n = 2).

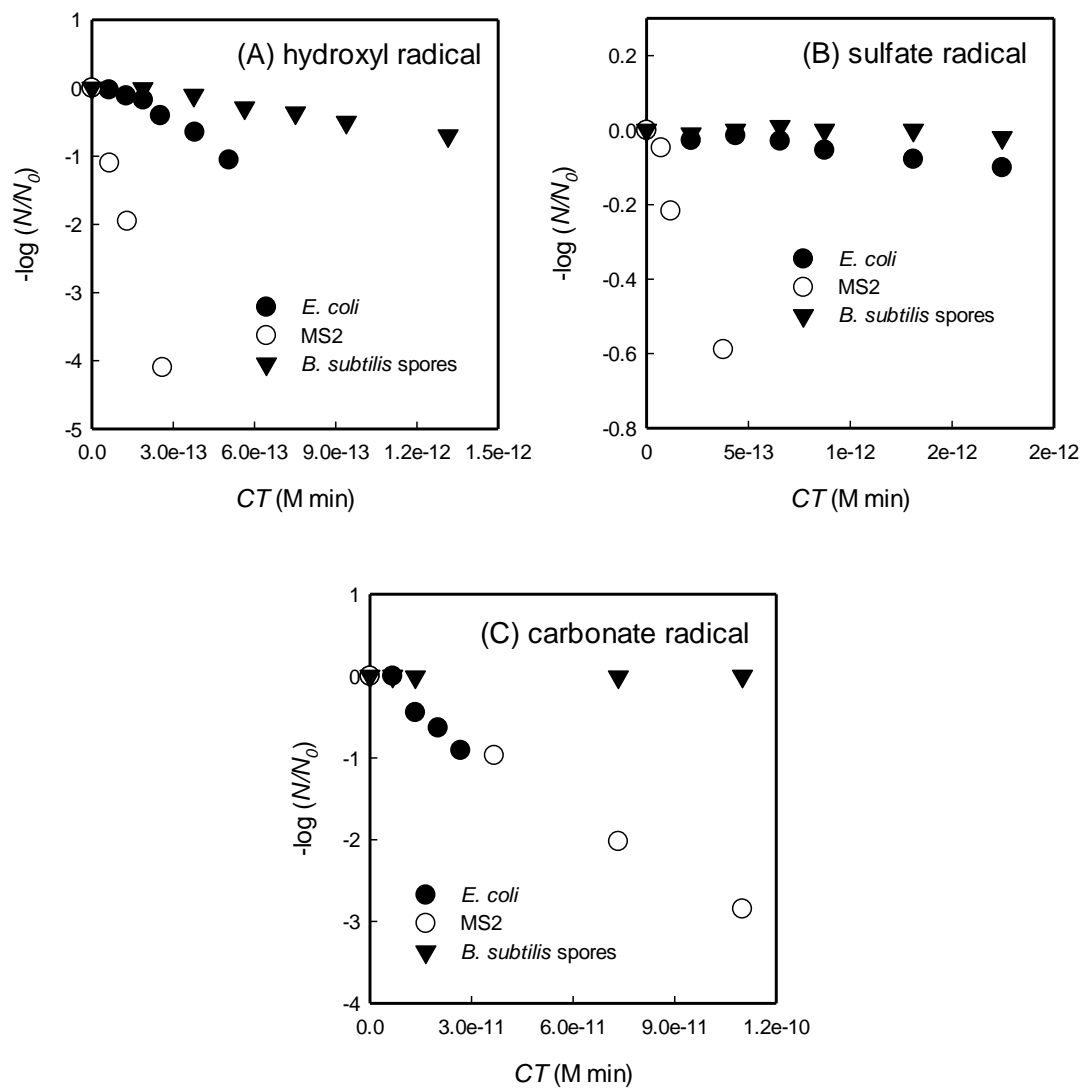


Figure S4. Inactivation of *E. coli*, bacteriophage MS2 and *Bacillus subtilis* spores versus CT values of (A) hydroxyl radical, (B) sulfate radical, and (C) carbonate radical.

REFERENCES

- (1) Zhang, R.; Sun, P.; Boyer, T. H.; Zhao, L.; Huang, C.-H. Degradation of pharmaceuticals and metabolite in synthetic human urine by UV, UV/H₂O₂, and UV/PDS. *Environ. Sci. Technol.* **2015**, *49* (5), 3056-3066.
- (2) Berg, O. G.; von Hippel, P. H. Diffusion-controlled macromolecular interactions. *Annu. Rev. Biophys. Biophys. Chem.* **1985**, *14* (1), 131-158.
- (3) Strauss, J. H.; Sinsheimer, R. L. Purification and properties of bacteriophage MS2 and of its ribonucleic acid. *J. Mol. Biol.* **1963**, *7* (1), 43-54.
- (4) Zhou, Z.; Qu, Y.; Fu, A.; Du, B.; He, F.; Gao, H. Density functional complete study of hydrogen bonding between the water molecule and the hydroxyl radical (H₂O· HO). *Int. J. Quantum. Chem.* **2002**, *89* (6), 550-558.
- (5) Bolton, J. R.; Bircher, K. G.; Tumas, W.; Tolman, C. A. Figures-of-merit for the technical development and application of advanced oxidation technologies for both electric- and solar-driven systems - (IUPAC Technical Report). *Pure Appl. Chem.* **2001**, *73* (4), 627-637.
- (6) NIST, NDRL/NIST Solution Kinetics Database on the Web (<http://kinetics.nist.gov/solution/>).
- (7) Brezonik, P. L.; Fulkerson-Brekken, J. Nitrate-induced photolysis in natural waters: controls on concentrations of hydroxyl radical photo-intermediates by natural scavenging agents. *Environ. Sci. Technol.* **1998**, *32* (19), 3004-3010.
- (8) Canonica, S.; Kohn, T.; Mac, M.; Real, F. J.; Wirz, J.; von Gunten, U. Photosensitizer method to determine rate constants for the reaction of carbonate radical with organic compounds. *Environ. Sci. Technol.* **2005**, *39* (23), 9182-9188.