Supplementary Materials

Multiphysics simulation details including initial conditions, boundary conditions, and simulation parameters are arranged in this supplementary data. **Table S1** summarizes the initial and boundary conditions applied in UV/H_2O_2 simulation. Parameters used in this simulation are listed in **Table S2**. To improve understanding, visualized simulation domains and boundaries of the UV/H_2O_2 reactor are shown in **Fig. S1**.

Table S1. Initial and boundary conditions for multiphysics simulations

Initial conditions	
Equations	**Location**
$\mathbf{u}_x = 0, \mathbf{u}_y = 0, \mathbf{u}_z = 0, p = 0$	at Ω_{fp}
$\mathrm{c} = \mathrm{c}_{0,i}$	at Ω_{fp}
GG_{i} (The blackbody radiative intensity at initial temperature)	at Ω_{pm}
Boundary conditions	
Equations	**Location**
$\mathbf{u} \cdot \mathbf{n} = 0$ (No slip)	at Ω_{pw}
$\mathbf{u} = -U_0\mathbf{n}$ (Normal inflow velocity), $\mathbf{n} \cdot (\mathbf{J}_i + \mathbf{u}\mathrm{c}_i) = \mathbf{n} \cdot (\mathbf{u}\mathrm{c}_{\mathrm{in},i})$	at Ω_{i1} and Ω_{i2}
$[-p\boldsymbol{I} + \boldsymbol{K}]\boldsymbol{n} = -\boldsymbol{p}_0^{\wedge}\boldsymbol{n}$, $\boldsymbol{p}_0^{\wedge} \leq \boldsymbol{p}_0, \nabla k \cdot \boldsymbol{n} = 0$, $\nabla\epsilon \cdot n = 0, \mathbf{n} \cdot D_i\nabla\mathrm{c}_i = 0$	at Ω_{o}
$-\mathbf{n} \cdot (-D_{\mathrm{p1}}\nabla G) = -\mathrm{q}_{\mathrm{r,net}}$, $\mathrm{q}_{\mathrm{r,net}} = \frac{1}{2}(4\pi I_{\mathrm{b,w}} - G)$ (black wall)	at Ω_{os}
$I_i = I_{\mathrm{wall}}$	at Ω_{l1} and Ω_{l2}

Table S2. Simulation parameters for multiphysics simulations (a: assumed, c: controlled, m: measured)

Description	Symbol	Value	Ref.
Temperature [K]	T	298.15	a
Fully developed inflow flow rate [L/min]	U_0	7	c
Density of liquid water [kg/m^3]	p	1000	a
Viscosity of liquid water [Pa·s]	μ	0.001	a
Absorption coefficient [1/cm]	κ	0.05	a
Scattering coefficient [1/cm]	σ_s	0.003	a
Boundary radiation intensity [W/(cm^2×sr)]	I_{wall}	1500	a
Initial concentration of H_2O_2 [mg/L]	$c_{0,H2O2}$	15, 10, 7.5, 5, 2.5	c
Initial concentration of $CO_3^{\bullet-}$ [mol/L]	$c_{0,CO3\cdot-}$	1×10^{-16}	a
Initial concentration of CO_3^{2-} [mol/L]	$c_{0,CO32-}$	2.91×10^{-7}	a
Initial concentration of caffeine [mol/L]	$c_{0,caffeine}$	1×10^{-5}	c
Initial concentration of DOC [mg/L]	$c_{0,DOC}$	4.5	m
Initial concentration of H^+ [mol/L]	$c_{0,H}$	1×10^{-7}	m
Initial concentration of H_2CO_3 [mol/L]	$c_{0,H2CO3}$	1.119×10^{-4}	m
Initial concentration of HCO_3^- [mol/L]	$c_{0,HCO3-}$	5.81×10^{-4}	a
Initial concentration of O_2 [mol/L]	$c_{0,O2}$	2.656×10^{-4}	m
Initial concentration of OH^- [mol/L]	$c_{0,OH-}$	1×10^{-7}	m
Initial concentration of *p*CBA [mol/L]	$c_{0,pCBA}$	1×10^{-5}	c
Inlet concentration of H_2O_2 [mg/L]	$c_{\text{in},H2O2}$	15, 10, 7.5, 5, 2.5	c
Inlet concentration of $CO_3^{\bullet-}$ [mol/L]	$c_{\text{in}CO3\cdot-}$	1×10^{-16}	a
Inlet concentration of CO_3^{2-} [mol/L]	$c_{\text{in}CO32-}$	2.91×10^{-7}	a
Inlet concentration of caffeine [mol/L]	$c_{\text{in},caffeine}$	1×10^{-5}	c
Inlet concentration of DOC [mg/L]	$c_{\text{in},DOC}$	4.5	m
Inlet concentration of H^+ [mol/L]	$c_{\text{in},H}$	1×10^{-7}	m
Inlet concentration of H_2CO_3 [mol/L]	$c_{\text{in},H2CO3}$	1.119×10^{-4}	m
Inlet concentration of HCO_3^- [mol/L]	$c_{\text{in},HCO3-}$	5.81×10^{-4}	a
Inlet concentration of O_2 [mol/L]	$c_{\text{in},O2}$	2.656×10^{-4}	m
Inlet concentration of OH^- [mol/L]	$c_{\text{in},OH-}$	1×10^{-7}	m
Inlet concentration of *p*CBA [mol/L]	$c_{\text{in},pCBA}$	1×10^{-5}	c
Diffusivity of all chemical species [m^2/s]	D	1×10^{-9}	a

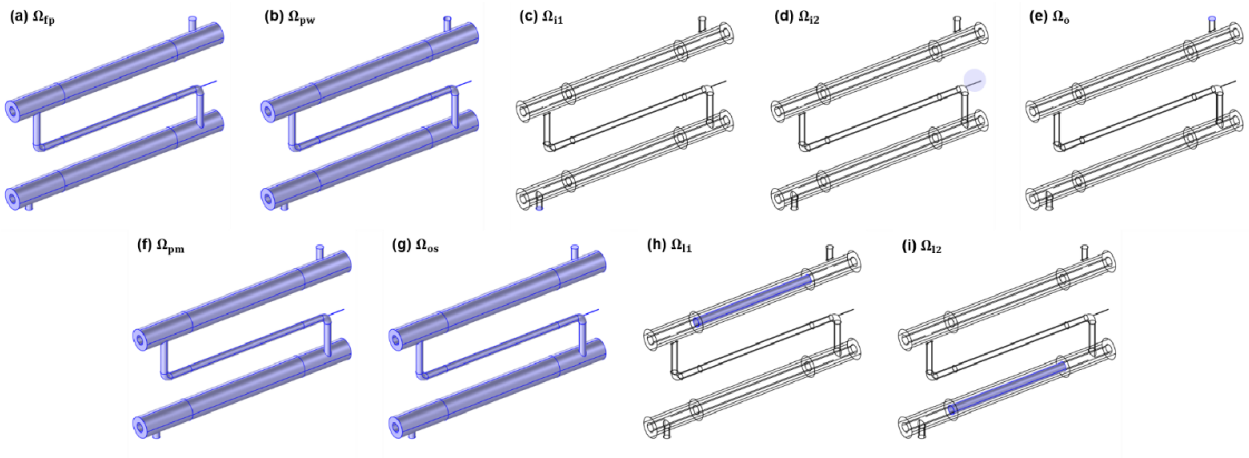

Fig. S1. Visualization of simulation domain and boundary of the UV/H_2O_2 reactor. The corresponding part is shown in purple: (a) flow path domain (Ω_{fp}) is the domain for the CFD and transport simulation. (b) pipe wall (Ω_{pw}), (c) inlet 1 (Ω_{I1}), (d) inlet 2 (Ω_{I2}), and (e) outlet (Ω_{o}) are the boundaries for the CFD and transport simulation. (f) participating medium (Ω_{pm}) is the domain for the radiation simulation. (g) opaque surface (Ω_{os}), (h) lamp 1 (Ω_{l1}), and (i) lamp 2 (Ω_{l2}) are the boundaries for the radiation simulation.

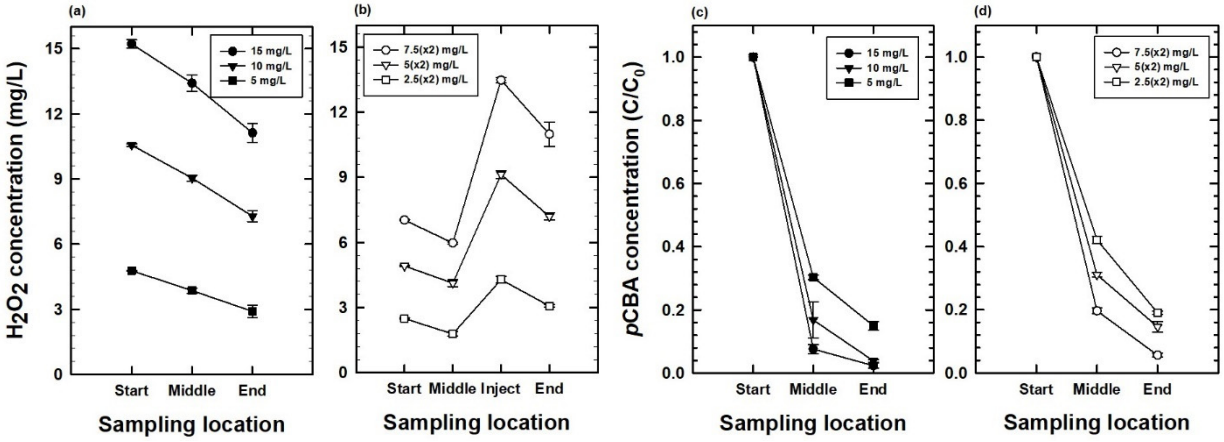

Fig. S2. H_2O_2 concentration change for (a) single injection and (b) two-step injection UV/H_2O_2 experiments. *p*CBA concentration change for (c) single injection and (d) two-step injection UV/H_2O_2 experiments ($[pCBA]_0$ = 10 uM).

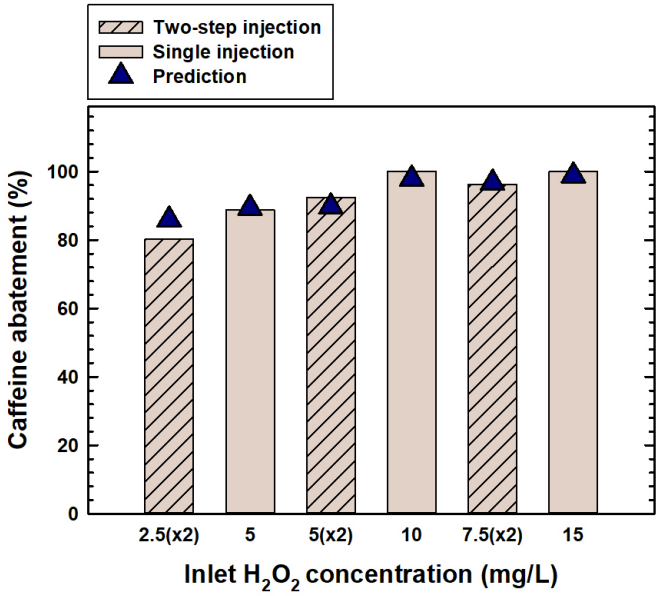

Fig. S3. Experimental results vs. prediction values of caffeine abatement using *p*CBA degradation results and subsequent $^{\bullet}OH$ exposure calculations ($[caffeine]_0$ = 10 μM).