Electronic supplementary information:

Ion-Concentration-Polarization-Assisted Photocatalytic Reactor for Highly Efficient Water Purification[†]

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Fig. S1. (a) Quantitative comparison of the photocatalytic activities of TiO_2 with rutile-toanatase ratio of 85:15 (RA81), 40:60 (RA46), 15:85 (RA18), and control (without TiO_2) by evaluating the MB decomposition efficiency in bulk container. After UV irradiation, the dispersed TiO_2 nanoparticles (1 mg/mL) in the MB solution were removed by centrifugation and the absorption spectra of the MB solution were measured using a UV-vis spectrophotometer. (b) Durability of TiO_2 nanoparticle coating on various fabrics: cotton, carbon cloth, and carbon cloth with microporous layer (MPL) after thermal treatment at 80 and 220 °C.



Fig. S2. Photos of the purified water using (a) various TiO_2 nanoparticles (The control samples were the MB solution under UV irradiation without TiO_2 nanoparticles) and (b) TiO_2 -nanoparticle-coated fabrics with different carbon contents (*i.e.*, cotton and carbon fabrics).



Fig. S3. (a) Schematic illustration of the proposed photocatalytic microfluidic reactor and its cross sectional view. (b) The photocatalytic reactor consists of Nafion-coated ITO glass, silicon spacer, TiO₂ nanoparticle-coated carbon fabrics, and PMMA plate. (c) The experimental setup for quantitative evaluation of Methylene blue (MB) degradation and (d) the fabricated photocatalytic reactor connected with a voltage source.

Model Calculation

In this study, we present a 2D numerical model to calculate the ion concentration distribution and electric potential in the microfluidic channel by using COMSOL Multiphysics 6.0 with built-in equations. The model was solved by using the "Tertiary Current Distribution, Nernst-Planck" interface which contains equations such as Nernst-Planck equation, mass balance, electroneutrality, current density, and current density balance. The variation of the ion concentration distribution and electric potential distribution in the electrolyte with and without ion-selective membrane domain (*i.e.*, Nafion membrane) was investigated here.



Fig. S4. (a) The geometry of the model with free electrolyte and ion-selective membrane domains. (b) ion concentration distribution and (c) electric potential drop in the microchannels by using numerical simulation for explaining the effective potential drop across the photocatalyst film. When the same potential bias was applied in the reactors with and without Nafion membrane, linear and non-linear potential drop was observed, respectively.

Parameter	Value	Description
Vtot	3 V	Total potential drop over unit cell
Dmb	2.032e-9 m ² /s	Diffusion coefficient in bulk solution, anion (Cl ⁻)
Dpb	1.957e-9 m ² /s	Diffusion coefficient in bulk solution, cation (K ⁺)
Dmm	2.032e-10 m ² /s	Diffusion coefficient in ion-selective membrane, anion (Cl ⁻) ^{1, 2}
Dpm	1.957e-10 m ² /s	Diffusion coefficient in ion-selective membrane, cation $(K^+)^{1, 2}$
СО	0.1 mol/m ³	Ion concentration in the electrolyte
v_avg	0.1 mm/s	Flow velocity in the microchannel
Sigma	5000 C/m ³	Fixed space charge density of ion-selective membrane

 Table S1. Parameters used in the model.

Fig. S5. Schematic illustration of the ICP-assisted photocatalytic reactor with different configuration: (a) C-Ti/Naf-ITO, and (b) C-Ti-Naf/ITO (in the case of C-Naf-Ti/ITO, TiO2 nanoparticles were coated on the top of Nafion, but the mechanism is similar). (c) Comparison of the MB degradation in different 600-µm reactors. C-Ti-Naf/ITO, C-Naf-Ti/ITO, and C-Ti/Naf-ITO represent the order of TiO2 nanoparticle and Nafion coating. C (*i.e.*, carbon fabrics) and ITO (*i.e.*, ITO glass) are cathode and anode, respectively.

References:

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