Regenerable Photovoltaic Devices with a Hydrogel-Embedded Microvascular Network

Hyung-Jun Koo^{1,2} and Orlin D. Velev¹

¹ Department of Chemical & Biomolecular Engineering, North Carolina State University, Raleigh, NC 27695-7905, USA.

² Present address: Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801-2325, USA.

Simulation of the reagent transport in the hydrogel medium with microfluidic channels.

The time-dependent profiles of reagent concentration in the microfluidic hydrogel based photovoltaics were calculated by using the common convection/diffusion equation.

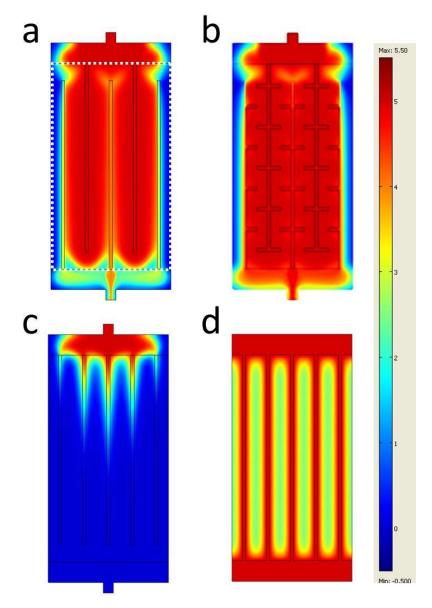
$$\frac{\delta c}{\delta t} = -v\nabla c + D\nabla \bullet \nabla c$$

where *c* is the concentration of reagent, *D* is the diffusion coefficient of the reagent $(3 \times 10^{-10} \text{ m}^2/\text{s} \text{ for this study})$ and *v* is the velocity of fluid. The velocity of fluid through the porous media and in the microfluidic channels was calculated numerically from the preceding equation by using the Brinkman equation and the Navier-Stokes equations for incompressible fluid

$$\frac{\eta}{k}\vec{v} = \nabla \cdot \left\{ -\vec{p} + \frac{\eta}{\varepsilon_p} (\nabla \vec{v} + (\nabla \vec{v})^T) \right\} \text{ (in porous media)}$$
$$\rho \vec{v} \cdot \nabla \vec{v} = \nabla \cdot \left\{ -\vec{p} + \eta (\nabla \vec{v} + (\nabla \vec{v})^T) \right\} \text{ (in nonporous media)}$$
$$\nabla \cdot \vec{v} = 0 \text{ (in all media)}$$

where η is the viscosity of the solutions (1 × 10⁻³ Pa s), ρ is the density of the solvent (1 × 10³ kg/m³ for water), *k* is the permeability of the agarose gel (5.4 × 10⁻¹⁶ m²)¹ and ε_p is the porosity

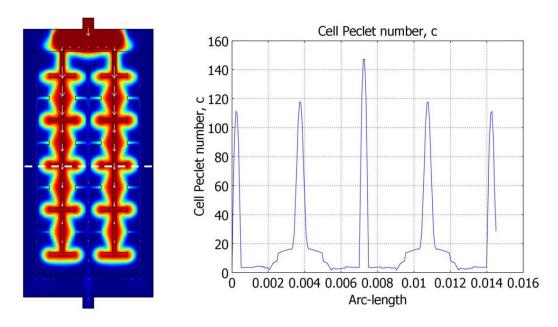
of the gel (0.98). The volume fraction of the agarose in the hydrated gel is almost the same as its mass fraction². The inlet boundary conditions are a constant pressure of 7×10^3 Pa and a concentration of 5 mol/L. The outlet boundary conditions are zero pressure and conserved convective flux.



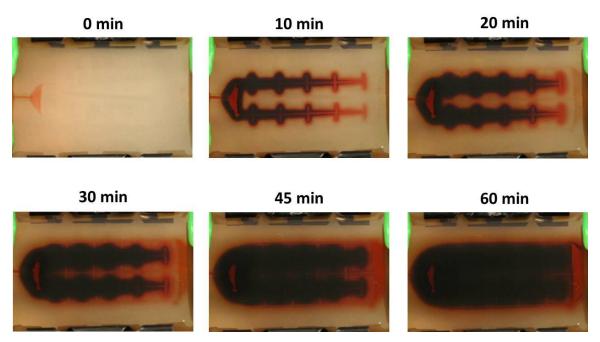
Supplementary Figure S1 | Effect of the channel geometry on the reagent supply. Simulation results for reagent distribution at 3600 s after injection in different channel designs. In design (d), it was assumed that the dye was filled in the channels at 0 s and was transported only by diffusion. For comparison of uniformity of the reagent supply, the percentage of the dye coverage was calculated by the equation below.

The dye coverage percentage =
$$\frac{Area where the concentration is higher than 4 mol/L}{Total area of the microfluidic hydrogel}$$

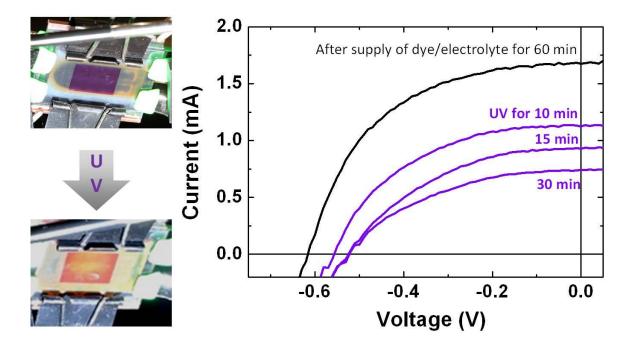
The rectangle enclosed by the white dotted lines in (a) indicates the total area of the microfluidic hydrogel, which is the denominator of the equation. The dye coverage percentages calculated by the above definition are 68% in (a), 78% in (b), 0.8% in (c) and 42% in (d), respectively. We chose the channel geometry (b), which achieved highest dye coverage.



Supplementary Figure S2 I The distribution of Peclet number in the μ -FGPVs. The graph on the right shows the Peclet numbers along the dotted line on the left figure.



Supplementary Figure S3 l Experimental images of the infusion and transport of the injected dye/electrolyte solution in the μ -FGPVs (compare with simulation in Figure S2).



Supplementary Figure S4 I Deterioration of photovoltaic performance of the μ -FGPVs caused by illumination of intense UV light. (Left) TiO₂ films before and after the intense UV illumination. The photographs were taken under illumination. (Right) The decrease of photocurrent of the μ -FGPVs as a function of UV illumination time.

References

- 1. Johnson, E. M. & Deen, W. M. Hydraulic permeability of agarose gels. *AIChE J.* **42**, 1220-1224 (1996).
- 2. Johnson, E. M., Berk, D. A., Jain, R. K. & Deen, W. M. Diffusion and partitioning of proteins in charged agarose gels. *Biophys. J.* 68, 1561-1568 (1995).