Supplementary Information

Fluorescent Liquid-Core/Air-Cladding Waveguides Towards Integrated Optofluidic Light Sources

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Monte Carlo simulation of the captured fraction, η

A fraction of the emitted light will be captured by the waveguide wall according to well-known '*Snell's law*'. If one can reduce somehow the size of the pumping spot close to the diffraction limit, then a single point-like source positioned at the waveguide axis will describe the situation. For such a point light source lying in the center of circular waveguide, one can obtain the exact form of an analytic solution for the captured fraction, η, which is given by $\eta = (n_{core} - n_{clad})/(2n_{core})$.[1] However, when the source is randomly distributed over the entire cross-section, calculation of η is nontrivial, and it becomes even worse if the cross-section does not have a simple geometry as in the case of our LA waveguide. Since a typical width of the LA waveguide (~100 μm) is much smaller than the size of the pumping beam (from a UV lamp), one can safely assume that all dye molecules uniformly are distributed over the entire cross-section of the waveguide and emit light randomly in all directions.

Let us consider the following general optical waveguide of which the cross-section is represented by its contour function, $C(x, y) = 0$ (See Figure S1). A single point source positioned at a point $(X, Y, Z = 0)$ emits light in the direction specified by the azimuthal and polar angles (θ, ϕ), and eventually arriving a point (X', Y', Z') on the wall of the waveguide. The wave is either 100% reflected or refracted (i.e., partially transmitted and partially reflected) at that point. The surface normal vector $\vec{n}$ is given by taking gradient of the contour function such as $\vec{n} = \nabla C(x, y)|_{x=X', y=Y'}$. Then, the Snell's law states that the light undergoes the '*total internal reflection*' (TIR) only when the following condition is satisfied.

$$\sin\varphi = \left|\frac{\vec{n}\times\vec{l}}{|\vec{n}||\vec{l}|}\right| \geq \left(\frac{n_{clad}}{n_{core}}\right) \qquad \text{(S1)}$$

Here, φ is an angle between $\vec{n}$ and $\vec{l}$, where $\vec{l}$ is a vector connecting from the source $(X, Y, Z = 0)$ to a point (X', Y', Z').

With all these backgrounds, one can obtain the captured fraction using numerical simulation which is in the spirit of the '*Monte Carlo* method'. Here, we give brief explanation on the algorithm, step by step.

(1) Generate random variables (X, Y) and (θ, ϕ), which will be used as a source point and a direction of emission, respectively. Note that we take the origin of Z axis as in the source plane.

(2) Calculate an intersection point (X',Y',Z') between $\vec{l}$ and the wall of the waveguide. First, one can solve the following equations to get $r = |\vec{l}|$.

$$\begin{aligned} X' &= X + r\sin\theta\cos\phi \\ Y' &= Y + r\sin\theta\sin\phi \end{aligned} \qquad \text{(S2)}$$

$$C(X',Y') = 0 \qquad \text{(S3)}$$

Then, insert the result into (S2) and $Z' = r\cos\theta$ to obtain (X',Y',Z').

(3) Check out the confinement condition (S1), which gives one outcome (‘confined’ or ‘leak’) of the deterministic calculation.

Then, one completes a single iterative calculation. After repeating the whole process, (1) to (3), and collecting the results, we can estimate the ‘captured fraction’, which is defined as

$$\eta = \frac{1}{2}\frac{\textbf{Number of captured events}}{\textbf{Total number of events}} \qquad \text{(S4)}$$

Note that a factor (1/2) is included since either one of the propagation directions (forward or backward) should be considered.

In order to confirm validity of our method, the above mentioned simple situation (a point source in the circular waveguide) were taken as a test example. The waveguide is assumed to consist of an EG core and air cladding (n_{core} = 1.432 and n_{clad} = 1.000). Then, the analytic solution of captured fraction is given as $\eta = (n_{core} - n_{clad})/(2n_{core})$ = 0.1508. Figure S2 shows the Monte Carlo estimation as a function of the number of iterations, demonstrating that the result obviously approaches to the analytical solution within 1% error.

The result of the fluorescent waveguide in which light sources are uniformly distributed over the circular cross-section is shown in Figure S3. As the number of iterations increases, the estimated captured fraction is shown to be saturated to 0.2693, which is almost twice as large as the previous result. This increase can be understood by the following physics: Consider a special situation in which a point source located at the center of the circular cross-section, emitting light in the radial direction ($\theta = 0$). Then, no light can be captured since all the emitted light will be normally incident on the wall. On the other hand, in an extreme case where a point source is located on the wall and emits radially ($\theta = 0$), considerable amount of light can be guided along the wall by TIR. Therefore, it is very straightforward that the effect of moving a point source away from the axis of the waveguide would allow more light to be captured by TIR, even for more general cases ($\theta \neq 0$).

The cross-sectional shape of our LA waveguide is shown in Figure S4. In our system, the air-liquid meniscus is convex in shape due to the large contact angle of ethylene glycol on the FDTS treated PDMS (θ_{cont} = 104°). The meniscus is a part of a circle and the radius of curvature is affected by the contact angle of the core fluid because the gravitational effect is negligible for small Bond numbers. The height of the waveguide is fixed by 140 μm and *w* can vary by changing the flow rate of the core liquid or the air suction pressure. The point light sources are assumed to be distributed over the cross-section. The results of the Monte Carlo simulations for the LA and L^2 waveguides are summarized in Table S1.

References

1. D. V. Vezenov, B. T. Mayers, D. B. Wolfe and G. M. Whitesides, *Appl. Phys. Lett.*, 2005, **86**, 041104.

Figure S1. The schematic of general optical waveguide, of which the cross-section is represented by its contour function, $C(x, y) = 0$

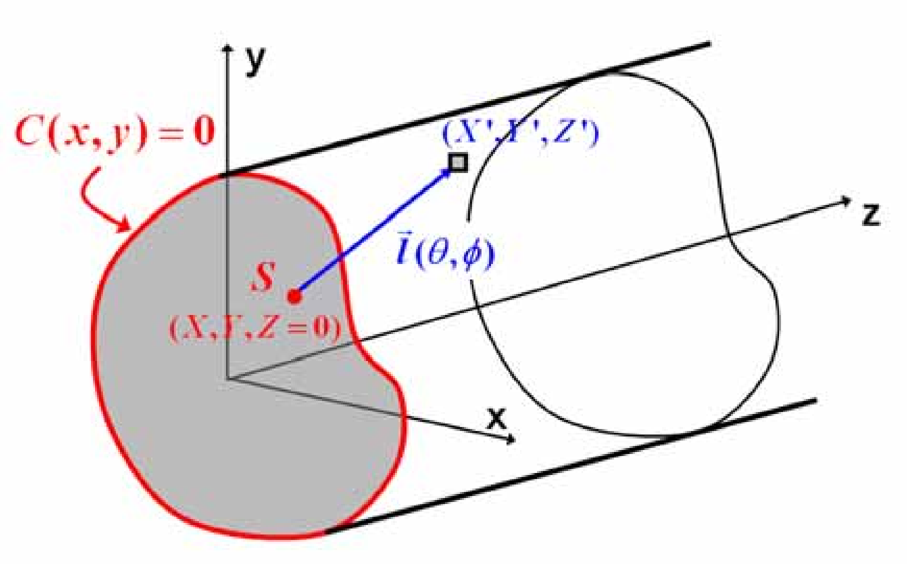


Figure S2. Monte Carlo simulation of the captured fraction and relative error compared to analytical solution as a function of the number of iterations, when the point source exists in the center of circular waveguide. The waveguide is assumed to consist of ethylene glycol core and air cladding (n_{core} = 1.432 and n_{clad} = 1.000).

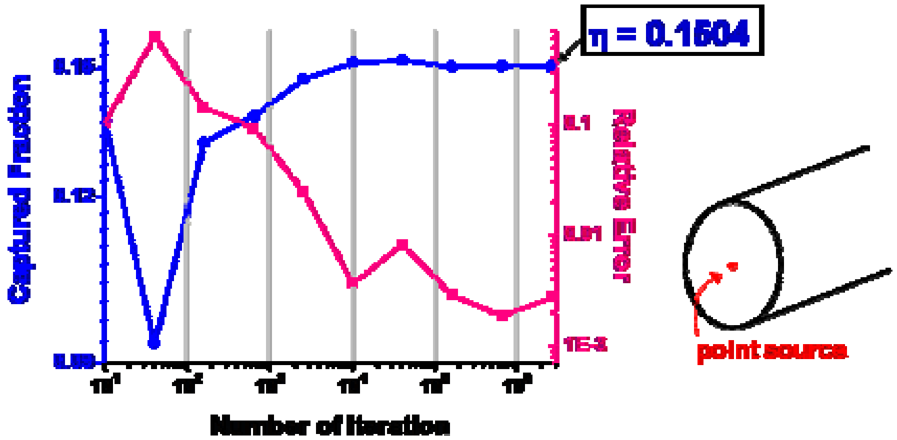


Figure S3. Monte Carlo simulation of the captured fraction as a function of the number of iterations, when the light sources are uniformly distributed over the circular cross-section. The waveguide is assumed to consist of ethylene glycol core and air cladding (n_{core} = 1.432 and n_{clad} = 1.000).

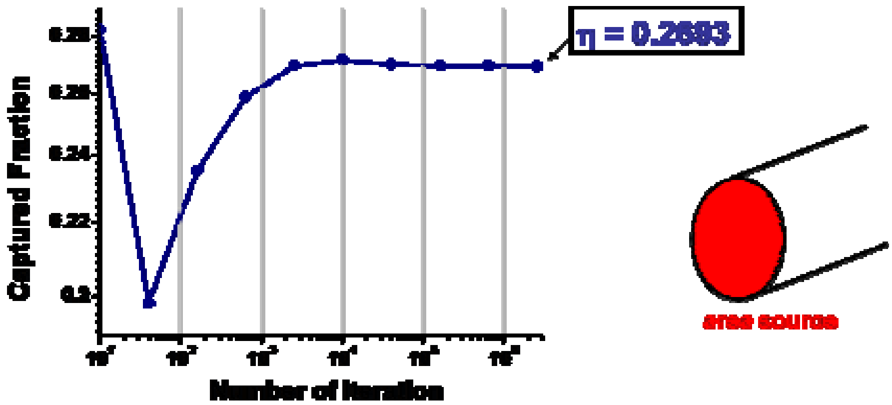
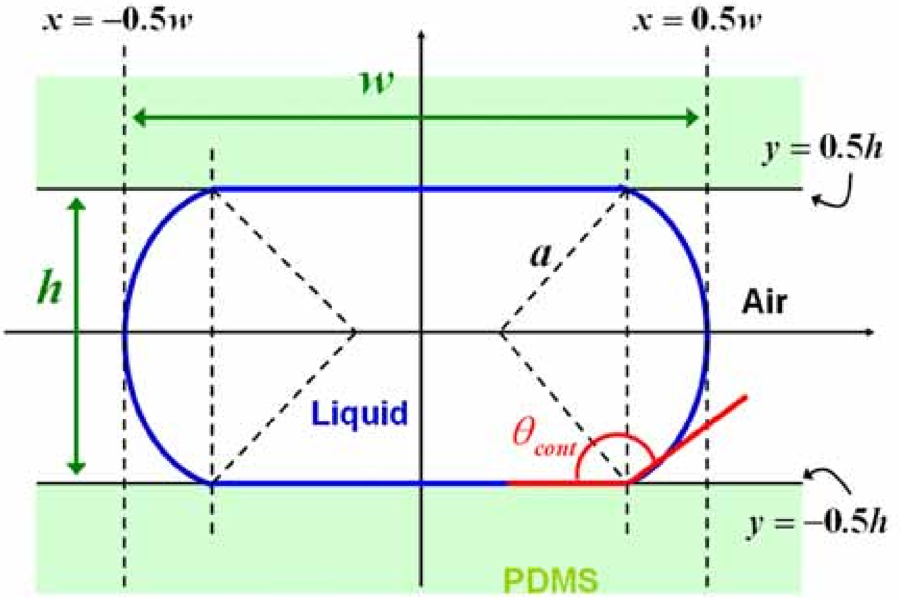


Figure S4. The schematic cross-sectional shape of the LA waveguide.



$$a = \frac{h}{2\sin(\theta_{cont} - \pi/2)}$$

Table S1. Captured fraction (η) of LA and L^2 waveguide by changing the maximum width of the core stream (w).

w **(μm)**	**η of LA waveguide**	**η of L^2 waveguide**
65	0.2283	0.0799
200	0.1260	0.0475
330	0.0990	0.0444