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Molecular Concentration Field Design using Closed-Form Steady-State Solutions

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Section S1: Detailed Derivation of Closed-Form Analytical Solutions

S1.1 Assumptions

Diffusion is assumed to occur with the same effective diffusivity inside and outside the source, characterized by the diffusion coefficient D such as DNA-immobilized hydrogels.[1-3] The source is assumed to have a symmetric geometry in 1D, 2D, or 3D systems to allow the reduction of the spatial coordinate from the center of the source to a variable r. The 1D model—the system length is significantly longer than width and height of the system leading to negligible height and width—provides intuitive insights into gradient formation along a single spatial axis, suitable for narrow channels.[2] The 2D model—height negligible compared to length and width—extends this understanding to planar geometries relevant in thin films or surface patterning[1], while the 3D model encompasses volumetric systems with spherical sources, such as lipid vesicles, hydrogel

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microparticles, or polymer coacervates[4]. These model frameworks provide the capacity for the prediction and design of concentration fields across a spectrum of geometries in biological tissues, engineered DNA reaction-diffusion networks, and microfabricated devices.[5-8]

S1.2 One-Dimensional Configuration

For one-dimensional configurations, we consider systems where the length dimension significantly exceeds both width and height, creating effectively linear diffusion along the longitudinal coordinate. The governing steady-state reaction-diffusion equations reduce to ordinary differential equations in Cartesian coordinates (*x* (=*r*), *y*, *z*):

$$0 = D\frac{d^2C}{dr^2} - kC + r_p, \text{ where } r < \mathrm{R} \tag{S1}$$

$$0 = D\frac{d^2C}{dr^2} - kC, \text{ where } r > \mathrm{R} \ . \tag{S2}$$

The general solution approach involves assuming exponential forms consistent with the characteristic equation. For the homogeneous parts of both equations, the characteristic equation is $D\lambda^2 - k = 0$ yielding characteristic length ($\lambda = \sqrt{k/D}$). For **Eq. S1** (with source term), we seek solutions of the form: $C(r) = c_1 e^{\lambda r} + c_2 e^{-\lambda r} + r_p/k$. For **Eq. S2** (homogeneous), the solution takes the form: $C(r) = c_3 e^{\lambda r} + c_4 e^{-\lambda r}$ where λ represents the inverse decay length.

The physical constraints of our system translate into mathematically precise boundary conditions that capture realistic molecular behavior. At the system center, symmetry demands zero flux to prevent unphysical molecular accumulation:

$$\left.\frac{dC}{dr}\right|_{r=0} = 0 \ . \tag{S3}$$

At the source boundary ($r = R$), physical continuity requires that both concentration and flux remain constant as molecules transition from the production region to the decay-only region:

$$C_{\mathrm{in}}(R) = C_{\mathrm{out}}(R) \tag{S4}$$

$$\left.\frac{dC_{\mathrm{in}}}{dr}\right|_{r=\mathrm{R}} = \left.\frac{dC_{\mathrm{out}}}{dr}\right|_{r=\mathrm{R}} \ . \tag{S5}$$

Finally, the requirement that concentration vanishes at infinite distance ensures finite total molecular populations and reflects the dominance of degradation over production in extended systems:

$$\lim_{r\to\infty} C(r) = 0 \ . \tag{S6}$$

These boundary conditions with the steady-state condition that concentration fields reach temporal equilibrium ($\partial C/\partial t$=0) transform the piecewise differential equations into a well-defined boundary value problem with unique solutions. The detailed process to derive the analytical solutions is described in the SI.

Using the boundary conditions (**Eqs S3-S6**), the constants (c_1-c_4) can be derived. Using the symmetry condition at origin (**Eq. S3**), differentiating the inner solution: $dC/dr = c_1\lambda e^{\lambda r} - c_2\lambda e^{-\lambda r}$. At r = 0, $c_1 - c_2 = 0$. therefore $c_1 = c_2$. Also, using decay condition at infinity (**Eq. S6**): $\lim_{r\to\infty} C(r) = 0$, we require c_3 = 0. For continuity conditions at the boundary (**Eqs. S4** and **S5**), concentration continuity at $r = R$ requires c_2 and c_4:

$$c_1 = c_2 = \frac{r_p}{2k} e^{-\lambda R} \tag{S7}$$

$$c_4 = \frac{r_p}{k} \sinh(\lambda R) \ . \tag{S8}$$

The final analytical solution for 1D configuration is obtained as follows,

$$C(r) = \frac{r_p}{k}\left(1 - e^{-\lambda R}\cosh(\lambda r)\right), \text{ where } r < R \tag{S9}$$

$$C(r) = \frac{r_p}{k} \sinh(\lambda R) e^{-\lambda r}, \text{ where } r > R \ . \tag{S10}$$

S1.3 Two-Dimensional Configuration

Two-dimensional configurations represent planar systems where both length and width dimensions significantly exceed the height, creating effectively cylindrical diffusion patterns. This geometry is relevant for thin films, membranes, or confined planar reactor systems where out-of-plane diffusion is negligible.

In cylindrical coordinates with radial symmetry, the governing equations become:

$$0 = D\frac{1}{r}\frac{d}{dr}\left(r\frac{dC}{dr}\right) - kC + r_p, \text{ where } r < R \tag{S11}$$

$$0 = D\frac{1}{r}\frac{d}{dr}\left(r\frac{dC}{dr}\right) - kC, \text{ where } r > R \ . \tag{S12}$$

Let $x = \lambda r$ where $\lambda = \sqrt{k/D}$ and $y = C$. The equations transform to:

$$x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} - (x^2 + 0)y = -\frac{r_p}{k}x^2, \text{ where } r < R \tag{S13}$$

$$x^2 \frac{d^2 y}{dx^2} + x\frac{dy}{dx} - (x^2 + 0)y = 0, \text{ where } r < R \quad . \tag{S14}$$

These are modified Bessel equations of order zero. The homogeneous equation has general solution: $y(x) = c_1 K_0(x) + c_2 I_0(x)$ where I_0 and K_0 are modified Bessel functions of the first and second kind, respectively. $I_0(x)$ is an exponentially growing function for large x, finite at $x = 0$. $K_0(x)$ is an exponentially decaying function for large x, $K_0(0) = \infty$ at $x = 0$. For derivatives, $I_0'(x) = I_1(x)$, $K_0'(x) = -K_1(x)$.

For the inhomogeneous equation (inside region), the particular solution is r_p/k, giving $y(x) = C(r) = c_1 K_0(\lambda r) + c_2 I_0(\lambda r) + r_p/k$. For the homogeneous equation (outside region): $y(x) = C(r) = c_3 K_0(\lambda r) + c_4 I_0(\lambda r)$. Using the boundary conditions (**Eqs S3-S6**), the constants (c_1-c_4) can be derived. For the finite concentration at origin, we require $c_1 = 0$ since $K_0(0) = \infty$. For decay at infinity, we require $c_4 = 0$ since $I_0(x) \sim e^x/(2\pi x)^{0.5}$ as x goes to ∞. Using continuity conditions at $r = R$, c_2 and c_3 can be obtained:

$$c_2 = -\frac{r_p}{k} \frac{K_0'(\lambda R)}{I_0(\lambda R) K_0'(\lambda R) - I_0'(\lambda R) K_0(\lambda R)} \tag{S15}$$

$$c_3 = -\frac{r_p}{k} \frac{I_1(\lambda R)}{I_0(\lambda R) K_0'(\lambda R) - I_0'(\lambda R) K_0(\lambda R)} \quad . \tag{S16}$$

This can be simplified with $I_0'(x) = I_1(x)$ and $K_0'(x) = -K_1(x)$ and Wronskian relationship, $I_0(x)K_1(x) + I_1(x)K_0(x) = 1/x$:

$$c_2 = -\frac{r_p}{k} \lambda R K_1(\lambda R) \tag{S17}$$

$$c_3 = \frac{r_p}{k} \lambda R I_1(\lambda R) \quad . \tag{S18}$$

The final analytical solution for 2D configuration is derived as follows,

$$C(r) = \frac{r_p}{k}\left(1 - \lambda R K_1(\lambda R) I_0(\lambda r)\right), \text{ where } r < R \tag{S19}$$

$$C(r) = \frac{r_p}{k} \lambda R I_1(\lambda R) K_0(\lambda r), \text{ where } r > R \quad . \tag{S20}$$

S1.4 Three-Dimensional Configuration

Three-dimensional configurations represent fully volumetric systems where all spatial dimensions are comparable. This geometry applies to spherical reactors, droplets, or bulk phase systems where diffusion occurs isotropically in all directions. In spherical coordinates with radial symmetry, the governing equations are:

$$0 = D\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dC}{dr}\right) - kC + r_p,\ \text{where } r < R \tag{S21}$$

$$0 = D\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dC}{dr}\right) - kC,\ \text{where } r > R\ . \tag{S22}$$

Let $y = rC$ to simplify the spherical Laplacian. The equations become:

$$\frac{d^2y}{dr^2} - \lambda^2 y = -\frac{r_p}{D}r,\ \text{where } r < R \tag{S23}$$

$$\frac{d^2y}{dr^2} - \lambda^2 y = 0,\ \text{where } r > R\ . \tag{S24}$$

These are linear second-order ODEs with constant coefficients. For **Eq. S23**, the homogeneous solution is $y_h = c_1e^{\lambda r} + c_2e^{-\lambda r}$. The particular solution for the inhomogeneous term is $y_p = (r_p/k)r$. Therefore, the complete solution is: $y = Cr = c_1e^{\lambda r} + c_2e^{-\lambda r} + (r_p/k)r$. For **Eq. S24**, and $y = Cr = c_3e^{\lambda r} + c_4e^{-\lambda r}$.

Using the boundary conditions (**Eqs S3-S6**), the constants (c_1-c_4) can be derived. Using the finite concentration at origin (**Eq. S3**), we need $c_1 = -c_2$, and the condition of the decay at infinity (**Eq. 6**) gives $c_3 = 0$. For the continuity at $r = R$ (**Eqs S4** and **S5**), we require c_1 and c_4:

$$c_1 = -\frac{r_p}{k}\frac{\lambda R + 1}{2\lambda e^{\lambda R}} \tag{S25}$$

$$c_4 = \frac{r_p}{k}\left(\lambda R\cosh(\lambda R) - \sinh(\lambda R)\right)\frac{1}{\lambda}\ . \tag{S26}$$

The final analytical solution for 3D configuration is derived as follows,

$$C(r) = \frac{r_p}{k}\left(1 - (\lambda R + 1)e^{-\lambda R}\frac{\sinh(\lambda r)}{\lambda r}\right),\ \text{where } r < R \tag{S27}$$

$$C(r) = \frac{r_p}{k}\left(\lambda R\cosh(\lambda R) - \sinh(\lambda R)\right)\frac{e^{-\lambda r}}{\lambda r},\ \text{where } r > R\ . \tag{S28}$$

The derived solutions are summarized in **Table S1**.

Table S1. **A summary of the analytical solutions for 1-3D configurations**. C is the concentration, R is the radius of the generator, r is a spatial coordinate from the center of the generator, λ is decay length calculated by $(k/D)^{0.5}$, D is diffusion constant, r_p is production rate, k

is degradation rate constant, I_0, I_1, K_0, and K_1 are the solution of the modified Bessel functions.

Dimension	$r < R$	$r > R$
1D	$C(r)=\frac{r_p}{k}\left(1-e^{-\lambda R}\cosh(\lambda r)\right)$	$C(r)=\frac{r_p}{k}\sinh(\lambda R)e^{-\lambda r}$
2D	$C(r)=\frac{r_p}{k}\left(1-\lambda R K_1(\lambda R) I_0(\lambda r)\right)$	$C(r)=\frac{r_p}{k}\lambda R I_1(\lambda R) K_0(\lambda r)$
3D	$C(r)=\frac{r_p}{k_c}\left(1-\left(\lambda R+1\right)e^{-\lambda R}\frac{\sinh(\lambda r)}{\lambda r}\right)$	$C(r)=\frac{r_p}{k_c}\left(\lambda R\cosh(\lambda R)-\sinh(\lambda R)\right)\frac{e^{-\lambda r}}{\lambda r}$

Section S2: Gradient Characteristic Parameters

S2.1 Surface Concentration Analysis

The surface concentration occurs at the surface of the source region ($r = R$) for all dimensional configurations. This represents the point of the highest concentration outside the source. The surface concentrations for each dimension are summarized in **Table S2**.

Table S2. **Surface concentration**. The surface concentration (C'_{surface}) can be calculated at the center concentration ($C'(r/R{=}1)$). $C' = C(r/R)/(r_p/k)$, $\Phi = R(k/D)^{0.5}$. R is the radius of the generator, r is a spatial coordinate from the center of the generator, D is diffusion constant, r_p is production rate, k is degradation rate constant.

Dimension	C'_{surface}
1D	$1-e^{-\Phi}\cosh(\Phi)$
2D	$1-\Phi K_1(\Phi) I_0(\Phi)$
3D	$1-\left(1+1/\Phi\right)e^{-\Phi}\sinh(\Phi)$

S2.2 Half-Width at Half-Maximum (HWHM) Analysis

The *HWHM* represents the distance from the center where the concentration drops to half surface concentration. This parameter quantifies the spatial extent of the concentration field and is crucial for applications requiring specific gradient steepness. The *HWHM* is determined by solving: $C'(r'_{HWHM})=C'_{\text{surface}}/2$. The *HWHM* for each dimension is summarized in **Table S3**.

Table S3. **Half-width at half-maximum (*HWHM*).** The $HWHM$ / R ($=r'_{HWHM}$) can be calculated by solving the equation the position where the concentration is half of the surface concentration: $C'(r'_{HWHM})=C'_{\text{surface}}/2$. $C' = C(r)/(r_p/k)$, $\Phi = R(k/D)^{0.5}$. R is the radius of the generator, r is a spatial coordinate from the center of the generator, D is diffusion constant, r_p is production rate, k is degradation rate constant.

Dimension	Half-width at half-maximum (HWHM)
1D	$\sinh(\Phi)e^{-\Phi r'_{HWHM}} - (1-e^{-\Phi}\cosh(\Phi))/2 = 0$
2D	$\Phi I_1(\Phi)K_0(\Phi r'_{HWHM}) - (1-\Phi K_1(\Phi)I_0(\Phi))/2 = 0$
3D	$\left(\Phi\cosh(\Phi)-\sinh(\Phi)\right)\dfrac{e^{-\Phi r'_{HWHM}}}{\Phi r'_{HWHM}} - \left(1-\left(1+1/\Phi\right)e^{-\Phi}\sinh(\Phi)\right)/2 = 0$

Table S4. **Experimental data for Figure 3b.** Zadorin et al.[9] used morphogen gradients in 1D microfluidic devices to direct particle organization. The others (Kim et al.[1], Gines et al.[10], Karzbrun et al.[11]) built concentration fields in 2D microfluidic devices. Thiele modulus (Φ) is $R(k/D)^{0.5}$, λ is $(k/D)^{0.5}$, R is the radius of the source, D is diffusion constant, and k is degradation rate constant.

Ref.	System chamber	Chamber thickness	k (s^{-1})	D ($\mu m^2/s$)	R (μm)	$1/\lambda$ (μm)	Φ	*HWHM* (μm)	*HWHM*/*R*
Kim et al.	2D microfluidic device	100 μm	7.5×10^{-5}	150	50	1400	0.036	300	6
			1.5×10^{-4}			1000	0.05	250	5
			3×10^{-4}			700	0.07	200	4
Gines et al.		130 μm	1.2×10^{-3}	300	17[a]	500	0.02	125	7.3
Karzbrun et al.		100 μm	-	33	50[b]	380	0.13	200	4
Zadorin et al.	1D microfluidic device	200 μm	-	-	2×10^3 [c]	16.7×10^3	0.12	12×10^3	6

a. microbead size; b. radius of chamber ends; c. chip width

Section S3: Nomenclature and Physical Parameters

Symbol	Definition	Units
C	Concentration	mol/m^3
C'	Dimensionless concentration, C/(r$_p$/k)	-
D	Diffusion coefficient	m^2/s
k	Degradation rate constant	1/s
R	Source radius	m
Φ	Dimensionless source radius, λR	-
r	Radial coordinate	m
r'	Dimensionless radial coordinate, r/R	-
r_p	Production rate	mol/(m^3·s)
λ	Inverse decay length, $\sqrt{(k/D)}$	1/m
I_0, I_1	Modified Bessel functions of the first kind	-
K_0, K_1	Modified Bessel functions of the second kind	-

References

1. D. W. Kim, M. Rubanov, A. Grinthal, P. Moerman and R. Schulman, *Matter*, 2025.
2. P. J. Dorsey, M. Rubanov, W. Wang and R. Schulman, *ACS Macro Letters*, 2019, **8**, 1133-1140.
3. K. Abe, I. Kawamata, M. N. Shin-ichiro and S. Murata, *Molecular Systems Design & Engineering*, 2019, **4**, 639-643.
4. E. Kengmana, E. Ornelas-Gatdula, K.-L. Chen and R. Schulman, *Journal of the American Chemical Society*, 2024, **146**, 32942-32952.
5. J. Zenk, D. Scalise, K. Wang, P. Dorsey, J. Fern, A. Cruz and R. Schulman, *RSC advances*, 2017, **7**, 18032-18040.

6. P. J. Dorsey, D. Scalise and R. Schulman, *Angewandte Chemie*, 2021, **133**, 342-348.

7. S. Kondo and T. Miura, *science*, 2010, **329**, 1616-1620.

8. A. N. Landge, B. M. Jordan, X. Diego and P. Müller, *Developmental biology*, 2020, **460**, 2-11.

9. A. S. Zadorin, Y. Rondelez, G. Gines, V. Dilhas, G. Urtel, A. Zambrano, J.-C. Galas and A. Estevez-Torres, *Nature chemistry*, 2017, **9**, 990-996.

10. G. Gines, A. Zadorin, J.-C. Galas, T. Fujii, A. Estevez-Torres and Y. Rondelez, *Nature nanotechnology*, 2017, **12**, 351-359.

11. E. Karzbrun, A. M. Tayar, V. Noireaux and R. H. Bar-Ziv, *science*, 2014, **345**, 829-832.