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Size of quorum sensing communities

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Cylindrical colony, reflective boundary

In this supplementary we will derive the steady state concentration of a circular colony with radius $r_0 = \mathcal{R}$ and height $z_0 = \mathcal{H}$ growing on a signal-reflecting surface. The signal concentration is denoted s, D its diffusion constant, and κ_s the intracellular signal production rate per volume. When ρ_v is the (v/v) cell density the volume normalized production is $k(r,z) = \rho_v(r,z)\kappa_s(r,z)$.

The steady state diffusion equation in cylindrical coordinates (assuming rotational symmetry) reads

$$\frac{\partial^2 s}{\partial r^2} + \frac{1}{r}\frac{\partial s}{\partial r} + \frac{\partial^2 s}{\partial z^2} = -\frac{k(r,z)}{D} \qquad (27)$$

where $k(r,z)$ is the source term, which is assumed to be homogeneous in the colony, $k(r,z) = k\theta(z_0 - z)\theta(r_0 - r)$ and $\theta(x)$ is the Heaviside unit step function. Eq. (27) is most easily solved by using the Hankel transformation (of order zero)[33].

$$\tilde{f}(q) = \mathcal{F}(f)(q) = \int_0^\infty f(r)J_0(qr)r\,dr$$

where $J_0(x)$ is the Bessel function of order 0. A useful property of the Hankel transformation is

$$\mathcal{F}(f'' + r^{-1}f')(q) = -q^2\mathcal{F}(f)(q) = -q^2\tilde{f}(q)$$

Applying the Hankel transformation to (27) therefore gives

$$-q^2\tilde{s}(q,z) + \frac{d^2\tilde{s}(q,z)}{dz^2} = -\tilde{k}(q,z) \qquad (28)$$

where

$$\tilde{k}(q,z) = \frac{k}{D}\theta(z_0 - z)\int_0^{r_0} J_0(qr)rdr = \frac{k}{D}\theta(z_0 - z)q^{-2}\int_0^{qr_0} J_0(x)xdx$$

Set $A(qr_0) = \int_0^{qr_0} J_0(x)xdx$, so

$$-q^2\tilde{s}(q,z) + \frac{d^2\tilde{s}(q,z)}{dz^2} = -\frac{k\theta(z_0 - z)A(qr_0)}{Dq^2} \qquad (29)$$

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The solution to the $h$omogeneous part of (29) is

$$\tilde{s}_h(q,z) = a(q)\mathrm{e}^{-qz} + b(q)\mathrm{e}^{qz}$$

where a and b are integration constants. The $p$articular solution can be chosen as

$$\tilde{s}_p(q,z) = \frac{k\theta(z_0 - z)A(qr_0)}{Dq^4}$$

The full solution therefore becomes

$$\tilde{s}(q,z) = \begin{cases} a_-(q)\mathrm{e}^{-qz} + b_-(q)\mathrm{e}^{qz} + \frac{kA(qr_0)}{Dq^4} & , z < z_0 \\ a_+(q)\mathrm{e}^{-qz} + b_+(q)\mathrm{e}^{qz} & , z > z_0 \end{cases} \qquad (30)$$

The integration constants are determined from the boundary conditions. Since $\tilde{s} \to 0$ for $z \to \infty$, we have $b_+(q) = 0$. The reflective boundary condition gives

$$\frac{\partial \tilde{s}(0)}{\partial z} = 0 \quad \Rightarrow \quad a_-(q) = b_-(q)$$

The two pieces of the solution has to be continuous with continuous derivative at $z = z_0$. This second condition implies

$$a_-(q)(\mathrm{e}^{qz_0} - \mathrm{e}^{-qz_0}) = -a_+(q)\mathrm{e}^{-qz_0} \quad \Rightarrow \quad a_+(q) = a_-(q)(1 - \mathrm{e}^{2qz_0})$$

The first condition gives

$$a_-(q)(\mathrm{e}^{-qz_0} - \mathrm{e}^{qz_0}) = a_-(q)(\mathrm{e}^{-qz_0} + \mathrm{e}^{qz_0}) + \frac{kA(qr_0)}{Dq^4} \quad \Rightarrow \quad a_-(q) = -\frac{kA(qr_0)\mathrm{e}^{-qz_0}}{2Dq^4}$$

Inserting into (30) we obtain

$$\tilde{s}(q,z) = \frac{kA(qr_0)}{2Dq^4}\begin{cases} 2 - \mathrm{e}^{-q(z+z_0)} - \mathrm{e}^{q(z-z_0)} & , z < z_0 \\ \mathrm{e}^{-q(z-z_0)} - \mathrm{e}^{-q(z+z_0)} & , z > z_0 \end{cases}$$

For convenience we define

$$I_-(q,z) = 2 - \mathrm{e}^{-q(z+z_0)} - \mathrm{e}^{q(z-z_0)}$$
$$I_+(q,z) = \mathrm{e}^{-q(z-z_0)} - \mathrm{e}^{-q(z+z_0)}$$

To obtain

$$s(r,z) = \begin{cases} s_-(r,z) & \text{for } 0 \le z \le z_0 \\ s_+(r,z) & \text{for } z > z_0 \end{cases}$$

we need to apply the inverse Hankel transformation again.

$$s_{\pm}(r,z) = \frac{k}{2D}\int_0^{\infty}\frac{A(qr_0)}{q^4}I_{\pm}(q,z)J_0(qr)qdq$$

Using that $A(qr_0) = qr_0J_1(qr_0)$, we finally get

$$s_{\pm}(r,z) = \frac{kr_0}{2D}\int_0^{\infty}\frac{I_{\pm}(q,z)}{q^2}J_0(qr)J_1(qr_0)dq \qquad (31)$$

Note that $I_{\pm}(q,z) > 0$ and $I_{\pm}(q,z) = 2qz_0 + \mathcal{O}(q^2)$. This ensures that s is well-defined ($J_1(x) = \mathcal{O}(x)$) and positive. To make the dimensionality of (31) clearer, set $x = qr_0$, $r' = r/r_0$, $z' = z/r_0$ and $z'_0 = z_0/r_0$ (aspect ratio) to obtain

$$s_{\pm}(r',z') = \frac{kr_0^2}{2D}\int_0^{\infty}\frac{I_{\pm}(x,z')}{x^2}J_0(xr')J_1(x)dx \qquad (32)$$

where

$$\begin{aligned} I_-(x,z') &= 2 - \mathrm{e}^{-x(z'+z'_0)} - \mathrm{e}^{x(z'-z'_0)} \\ &= 2\big(1 - \mathrm{e}^{-xz'_0}\cosh(xz')\big) \\ I_+(x,z') &= \mathrm{e}^{-x(z'-z'_0)} - \mathrm{e}^{-x(z'+z'_0)} \\ &= 2\mathrm{e}^{-xz'}\sinh(xz'_0) \end{aligned}$$

The integral in (32) can be evaluated in specific points. At the top, $r' = 0, z' = z'_0$ we have

$$\begin{aligned} s_-(0,z'_0) &= \frac{kr_0^2}{D}\int_0^{\infty}\frac{1 - \mathrm{e}^{-xz'_0}\cosh(xz'_0)}{x^2}J_1(x)dx \\ &= \frac{kr_0^2}{2D}\left(2z'_0(-2z'_0 + \sqrt{4z'^2_0 + 1}) + \sinh^{-1}(2z'_0)\right) \\ &\approx \frac{kr_0^2}{2D}\left(2z'_0 - 2z'^2_0 + \frac{4}{3}z'^3_0 + \mathcal{O}(z'^4_0)\right) \\ s_-(0,z'_0) &= 0.958\frac{kr_0^2}{2D} \quad , z'_0 = 1 \\ s_-(0,z'_0) &= 2\frac{kr_0z_0}{2D} \quad , z'_0 \ll 1 \end{aligned}$$

At the border of the supporting surface, $r' = 1, z' = 0$, we get

$$\begin{aligned} s_-(1,0) &= \frac{kr_0^2}{D}\int_0^{\infty}\frac{1 - \mathrm{e}^{-xz'_0}}{x^2}J_0(x)J_1(x)dx \\ &\approx \frac{kr_0^2}{2D}\left(1.273z'_0 - 0.5z'^2_0 + \mathcal{O}(z'^3_0)\right) \\ s_-(1,0) &= 0.926\frac{kr_0^2}{2D} \quad , z'_0 = 1 \\ s_-(1,0) &= 1.273\frac{kr_0z_0}{2D} \quad , z'_0 \ll 1 \end{aligned}$$

Finally, in the center, we have

$$\begin{aligned} s_-(0,0) &= \frac{kr_0^2}{D}\int_0^{\infty}\frac{1 - \mathrm{e}^{-xz'_0}}{x^2}J_1(x)dx \\ &= \frac{kr_0^2}{2D}\left(z'_0(-z'_0 + \sqrt{z'^2_0 + 1}) + \sinh^{-1}(z'_0)\right) \\ &\approx \frac{kr_0^2}{2D}\left(2z'_0 - z'^2_0 + \frac{z'^3_0}{3} + \mathcal{O}(z'^5_0)\right) \\ s_-(0,0) &= 1.296\frac{kr_0^2}{2D} \quad , z'_0 = 1 \\ s_-(0,0) &= 2\frac{kr_0z_0}{2D} \quad , z'_0 \ll 1 \end{aligned}$$

Note that in all points the algebraic prefactor is of order unity. In order to get the expression needed for a thin biofilm in the main text, recall that $z_0 = \mathcal{H}$, $r_0 = \mathcal{R}$, and $k = \rho_v\kappa_s$. Specifically the last equation reads

$$s(0,0) = 2\frac{\kappa_s\mathcal{R}\mathcal{H}\rho_v}{2D} \quad , \mathcal{H} \ll \mathcal{R} \qquad (33)$$