Supplementary Information: A generalized model for predicting different morphologies of bacterial swarming on a porous solid surface

Uttam Kumar¹, Subramaniam Pushpavanam^{2, *}

^{1,2} Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, Tamil Nadu 600036, India

¹ORCID ID: 0000-0002-0751-9388. ²ORCID ID: 0000-0002-5782-0670.

* To whom correspondence should be addressed. Email: spush@iitm.ac.in



Fig. S1. Surfactant concentration contour corresponding to Fig. 3(a) and 3(b) for the parameters: (a) w = 0.01, $\Gamma_m = 0.1$ at $t = 8 \times 10^6$, and (b) w = 0.05, $\Gamma_m = 0.05$ at $t = 10^7$. The remaining parameters are taken from Table 2. The length of the black arrow signifies the magnitude of Marangoni stress. The color bar indicates the non-dimensionalized surfactant concentration.



Fig. S2. Surfactant concentration contour corresponding to Fig. 4(a) and 4(b) for the parameters: w = 0.01, (a) $\Gamma_m = 0.4$, and (b) $\Gamma_m = 0.5$. The remaining parameters are taken from Table 2. The length of the black arrow signifies the magnitude of Marangoni stress. The numerical solution profiles are plotted at $t = 5 \times 10^6$. The color bar indicates the non-dimensionalized surfactant concentration.

II. NUMERICAL VALIDATION

To validate our COMSOL code, we simulated the thin film model from Trinschek *et al.*¹ and Kotian *et al.*² as discussed below.

А.

The Trinschek *et al.*¹ model has two equation one for the height of the swarm and another for the surfactant mass balance, given by:

$$\frac{\partial h}{\partial t} - \nabla \cdot \left(\frac{h^3}{3} \nabla p + \frac{h^2}{2} \nabla \Gamma\right) = \eta_c h \left(1 - \frac{h}{h_{1s}}\right) f_{mod}(h), \tag{S1a}$$

$$\frac{\partial\Gamma}{\partial t} - \boldsymbol{\nabla} \cdot \left[\Gamma \left(\frac{h^2}{2} \boldsymbol{\nabla} p + h \boldsymbol{\nabla} \Gamma \right) \right] = D \boldsymbol{\nabla}^2 \Gamma + \eta_\Gamma h (\Gamma_m - \Gamma) \Theta (h - h_u) \Theta (\Gamma_m - \Gamma), \quad (S1b)$$

where,

$$p = -\nabla^2 h + w \left(\frac{1}{h^3} - \frac{1}{h^6}\right), \quad f_{mod}(h) = \left(1 - \frac{h_u}{h}\right) \left[1 - \exp\left(1 - \frac{h}{h_a}\right)\right]$$

In this model, h(x, y, t) represents the shape of the biofilm as a function of both space and time, while $\Gamma(x, y, t)$ denotes the surfactant concentration. The parameters are consistent with those described in detail in the main text. The value of parameters used for simulation is given in Table S1.

The initial conditions on h and Γ are set to h_0 and Γ_m in a circular region of radius 200, situated concentrically with the simulation domain of radius 5000. Additionally, h and Γ are set to h_a and $0.05\Gamma_m$ in the annular domain, respectively. The system is simulated with no flux boundary conditions on the outer domain.

The simulated profile by using our COMSOL code, shown in Fig. S3(b) closely resembles the profile from Trinschek *et al.*¹ as depicted in Fig. S3(a).

Parameter	Value	Parameter	Value	Parameter	Value
η_c	10^{-5}	Γ_m	0.5	h_{1s}	20
$\eta_{arGamma}$	10 ⁻⁶	W	0.03	h_0	4
D	0.01	h_a	1	h_u	2

Table S1 Parameters and their base numerical value



Fig. S3. (a) Numerically simulated swarm height profile using our COMSOL code based on the model from Trinschek *et al.*¹ and (b) swarm height profile from Trinschek *et al.*¹ paper. The corresponding parameter values are provided in Table S1. The color bar represents the non-dimensionalized height of the swarm.

В.

The Kotian et al.² model without the chemotaxis term is given below

$$\frac{\partial h}{\partial t} - \nabla \cdot \left(\frac{h^3}{3} \nabla p + \frac{h^2}{2} \nabla \Gamma\right) = f(h, \rho_B), \qquad (S2a)$$

$$\frac{\partial\Gamma}{\partial t} - \boldsymbol{\nabla} \cdot \left[\Gamma \left(\frac{h^2}{2} \boldsymbol{\nabla} p + h \boldsymbol{\nabla} \Gamma \right) \right] = D \boldsymbol{\nabla}^2 \Gamma + p_{\Gamma}(\rho_B, \Gamma), \tag{S2b}$$

$$\frac{\partial \rho_B}{\partial t} - \boldsymbol{\nabla} \cdot \left[\Gamma \left(\frac{\chi \rho_B h^2}{3} \boldsymbol{\nabla} p + \frac{\chi \rho_B h}{2} \boldsymbol{\nabla} \Gamma \right) \right] = G(\rho_B), \tag{S2c}$$

where,

$$p = -\nabla^2 h + w \left(\frac{1}{h^3} - \frac{1}{h^6} \right), \quad f(h, \rho_B) = f_w(h_{mx}\rho_B - h)\Theta(h - h_a),$$

$$p_{\Gamma}(\rho_B,\Gamma) = p_s \rho_B(\Gamma_{mx} - \Gamma)\Theta(\Gamma_{mx} - \Gamma), \qquad G(\rho_B) = g\rho_B(1 - \rho_B)\Theta(\rho_B - \rho_{mn}),$$

In this model, h(x, y, t) represents the shape of the biofilm as a function of both space and time, while $\Gamma(x, y, t)$ denotes the surfactant concentration. The bacteria concentration is represented by $\rho_B(x, y, t)$ as the number density. The active behaviour of the bacteria is defined by the term motility parameter χ . Θ represents a Heaviside function, which is defined in the main text.

Bacteria and surfactant production are given by $G(\rho_B)$ and $p_{\Gamma}(\rho_B, \Gamma)$, respectively. Bacteria growth followed a logistic equation with g as the doubling rate of the bacteria and ρ_{mn} , the minimum bacterial density, ensuring at least one bacterium is present for population growth. In the surfactant production equation, Γ_{mx} limits the surfactant production and p_s is the surfactant production rate constant. The osmosis of water is included by $f(\rho_B, h)$ where, f_w is equal to the growth rate of bacteria. Other parameters are consistent with those described in detail in the main text. The values used in the simulation are provided in Table S2.

For the initial conditions, the height was set to h_a (height of adsorption water film), and surfactant concentration was initialized to 0 in the whole domain. At the start of the simulation, bacteria density was set to 1 within a circular region (radius = 300) concentric with the simulation domain of radius 4000. The system was simulated with no flux boundary conditions on the outer domain.

The simulated profile using our COMSOL code, shown in Fig. S4(b) closely matches the profile from Kotian *et al.*² paper as depicted in Fig. S4(a).

Parameter	Value	Parameter	Value	Parameter	Value
g	10 ⁻⁵	Γ_{mx}	0.5	h_{mx}	10
p_s	10 ⁻⁵	W	0.07	$ ho_{mn}$	0.5
X	1	D	0.1	h_a	1

Table S1 Parameters and their base numerical value



Fig. S4. (a) Numerically simulated swarm height profile using our COMSOL code based on the model from Kotian *et al.*² and (b) swarm height profile from Kotian *et al.*² paper. The corresponding parameter values are provided in Table S2. The color bar represents the non-dimensionalized height of the swarm.

References

- 1 S. Trinschek, K. John and U. Thiele, *Soft Matter*, 2018, **14**, 4464–4476.
- 2 H. S. Kotian, A. Z. Abdulla, K. N. Hithysini, S. Harkar, S. Joge, A. Mishra, V. Singh and M. M. Varma, *Phys. Rev. E*, 2020, **101**, 012407.