

S1 Appendix: Additional Simulation Results.

1 We present here the details of additional simulation results, the implications of which are
2 discussed in the main text. We refer the reader to the main text for model description,
3 definition of output parameters, and simulation parameter values.

4 **Biofilm growth and dispersal**

5 We conducted more simulation experiments to investigate how quorum sensing induced
6 dispersal affects the biofilm growth and dispersal events when the maximum dispersal
7 rate η_1 is varied. We considered a situation where the nutrient concentration has no
8 influence on the quorum sensing signal production, i.e. $\gamma(C) = 1$. The parameters used
9 are listed in Table 1 in the main text, except for the dispersal rate η_1 , which was varied as
10 0.6, 1.2, 1.8, 2.4, 3.0, 3.6, $4.2d^{-1}$ and the dispersal threshold concentration $\tau = 10nM$. For
11 low values of η_1 , we observe a continuous biomass loss and that the amount of biomass in
12 the biofilm, as well as the autoinducer concentration levels off, as shown in Figs.1a and
13 1c. The smaller the maximum erosion rates η_1 , the higher the plateau will be. Smaller
14 maximum erosion rates lead to larger biofilms, cf Fig.1d.

15 The lower the dispersal rate is, the more continuous is cell dispersal, even for small
16 value of τ . For higher values of η_1 , the dispersal events are rapid and discrete as we have
17 seen before for small induction thresholds (see main text). Again, after each dispersal
18 event, too few bacterial cells are left behind to produce enough autoinducers to maintain
19 dispersal; the signal concentration falls back below threshold, cf Fig.1c and the biofilm
20 starts growing again. When the amount of biomass becomes strong enough for the con-
21 centration of the quorum sensing signal molecule to reach threshold, the next dispersal
22 event is triggered, etc. The frequency of the dispersal events changes as η_1 changes, but
23 the amplitude appears to be insensitive to this parameter. In all cases the vast majority
24 of biomass produced in the biofilm is lost, cf Fig.1b.

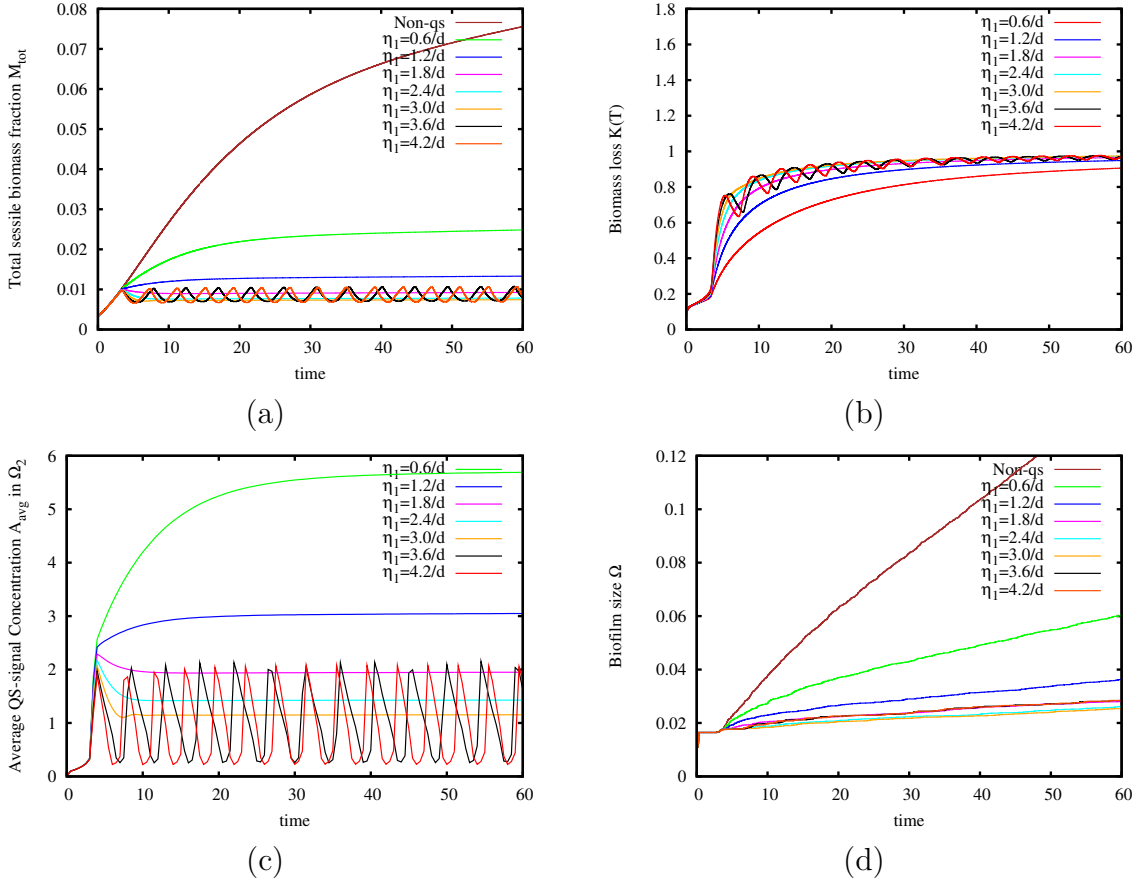
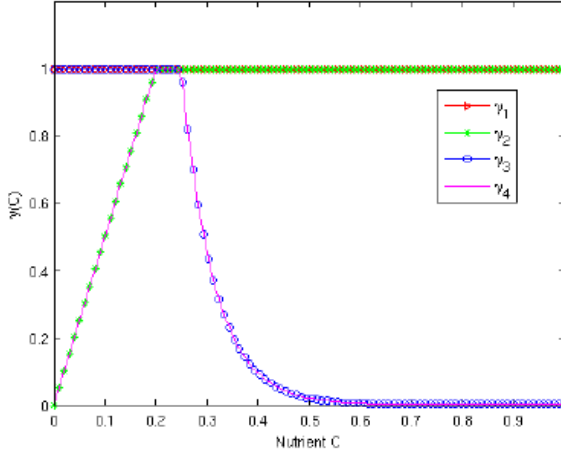


Fig. 1: **Temporal plots of simulations of a non-quorum sensing biofilm (Non-QS) and a quorum sensing biofilm.** Here we used seven different dispersal rates $\eta_1 = \{0.6, 1.2, 1.8, 2.4, 3.0, 3.6, 4.2d^{-1}\}$ and fixed quorum sensing threshold $\tau = 10nM$. Shown are (a) the total amount of sessile biomass in the biofilm, $M_{tot}(t)$, (b) biomass loss $K(T)$ indicating the amount of biomass that actually dispersed, (c) the average autoinducer concentration $A_{avg}(t)$ in Ω_2 , (d) the biofilm size $\Omega(t)$.

25 Nutrient induced autoinducer production

26 The dependence of the quorum sensing signal production is controlled by the function
 27 $\gamma(C)$ which is defined in such a way that $0 < \gamma(C) \leq 1$ where the nutrient concentration
 28 C lies between zero and unity. The $\gamma(C)$ is so defined to help capture the effect of
 29 nutrient availability on the production of quorum sensing when the nutrient is limited
 30 and when it is in abundance respectively. We test for different choices of $\gamma(C)$, depicted
 31 in Fig.2. $\gamma_1(C) \equiv 1$ reflects the scenario where signal production does not depend on
 32 nutrient availability. This is our baseline scenario. Function $\gamma_2(C)$ describes the scenario



$$\begin{aligned} \gamma_1(C; k_2, k_3) &= 1 \\ \gamma_2(C; k_2, k_3) &= \begin{cases} \frac{C}{k_2}, & \text{if } C \leq k_2 \\ 1, & \text{otherwise} \end{cases} \\ \gamma_3(C; k_2, k_3) &= \begin{cases} 1, & \text{if } C \leq k_3 \\ -e^{-(C-k_3)\log(\frac{eps}{2-k_3})}, & \text{otherwise} \end{cases} \\ \gamma_4(C; k_2, k_3) &= \begin{cases} \frac{C}{k_2}, & \text{if } C \leq k_2 \\ 1, & k_2 < C \leq k_3 \\ -e^{-(C-k_3)\log(\frac{eps}{2-k_3})}, & \text{otherwise} \end{cases} \end{aligned}$$

Fig. 2: **The nutrient dependent functions** $\gamma_i(C)$, $i = 1, 2, 3, 4$. This function controls the production of quorum sensing molecule in the biofilm

33 where for low nutrient concentrations the signal production rate is proportional to the
 34 nutrient concentration whereas for larger nutrient concentrations the signal production
 35 rate is independent of the nutrient concentration, cf [2]. This reflects the argument that
 36 signal production is expensive and not affordable under unfavourable conditions. The
 37 opposite is the scenario described by $\gamma_3(C)$, where the signal production rate is highest
 38 during periods of low substrate availability, but it decreases if the substrate concentration
 39 increases. In this scenario signal production is a stress response. In $\gamma_4(C)$ these both
 40 effects are accounted for: the signal production rate is proportional to the substrate
 41 concentrations under conditions of low availability, it attains its maximum at intermediate
 42 substrate concentrations and declines as substrate becomes more and more plentiful, cf
 43 also [1].

44 For the simulation results shown in Fig.3, we fix $\tau = 120nM$ and $\eta_1 = 0.6d^{-1}$ while
 45 every other parameter used is listed on Table 1 in the main text. The choice of parameters
 46 in this simulation enables the investigation under limited substrate concentration for a
 47 biofilm with all the boundary conditions defined and described in the previous sections.

48 Note that the value of τ is chosen here higher than in our other simulations, in order
49 to delay induction to allow the biofilm to grow bigger before dispersal starts and thus
50 to enforce a lower nutrient concentration. A similar effect could have been achieved by
51 reducing α and β .

52 On the other hand to enable the investigation under increased availability of nutrients
53 we have considered also a microfloc, i.e. a biofilm without substratum. We prescribe a
54 non-homogeneous Dirichlet boundary condition for the substrate on all the boundaries
55 to ensure a constant supply of nutrients to the flocs across all domain boundaries i.e.
56 $C = C_\infty$, where C_∞ is the bulk concentration value. Moreover, we pose a homogeneous
57 Neumann boundary condition for the autoinducers on all the boundaries of the microfloc
58 system to ensure that the signal molecules does not leave the system and is not diluted, i.e.
59 $\partial_n A = 0$. For the biomass, we pose a homogeneous Dirichlet boundary condition on all
60 the boundaries for the biomass i.e. $M = N = 0$, which allows the bacterial cells to leave
61 from any of the boundaries. For the microfloc, we fix the signal threshold concentration
62 $\tau = 50nM$ and the maximum dispersal rate $3.6d^{-1}$ while every other parameter used is
63 as listed in Table 1 in the main text. Lumped output parameters for these simulations
64 are presented in Figs.3 and 4.

65 We first focus on the biofilm (Fig.3). High nutrient concentrations are observed only
66 initially and decline quickly as the biofilm grows. The concentration of the nutrient
67 in the biofilm is not affected by the production of the quorum sensing signal molecule
68 production rate which depends on the nutrient. Once the nutrient concentration drops
69 below the concentration value k_2 we see a clear separation of curves for the total biomass
70 density, biofilm size, fraction of dispersed cells and total amount of dispersed cells. The
71 curves obtained for $\gamma_2(C)$ and $\gamma_4(C)$, which are sensitive to low concentration values are
72 grouped together, as well as the curves for $\gamma_1(C)$ and $\gamma_3(C)$ which are not sensitive to
73 low substrate concentrations. As long as the substrate concentration is above k_2 we do
74 not detect a notable difference between the four curves.

75 In contrast to the biofilm, the autoinducer concentration level in the microfloc is sen-
76 sitive to high nutrient concentration as shown in Fig.4. There is an increased autoinducer
77 concentration level in the case of γ_3 and γ_4 when the nutrient concentration is above the
78 concentration value k_2 and below k_3 ; these results are grouped together and are sensitive to
79 high nutrient concentration. On the other hand, the autoinducer concentration is low for
80 γ_1 and γ_2 which are grouped together and are insensitive to high nutrient concentration.

81 In general, we observe that the different concentration levels of the quorum sensing
82 signal does not translate to cell dispersal.

83 References

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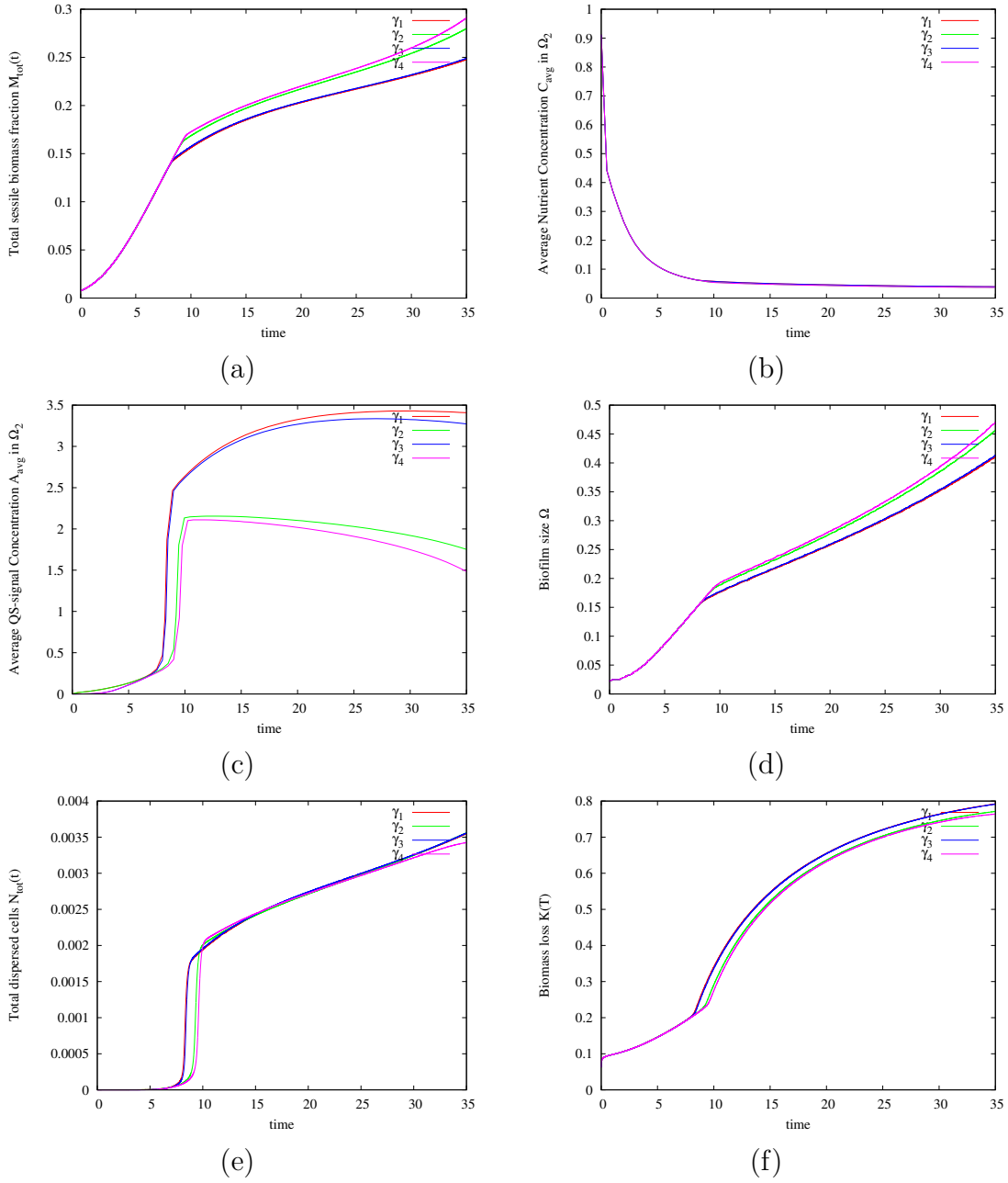


Fig. 3: **Temporal plots of simulations of a biofilm using different $\gamma_i(C)$.** Here we used $\tau = 120nM$, $\eta_1 = 0.6d^{-1}$. Shown are (a) total sessile biomass fraction M_{tot} in the biofilm, (b) average concentration of the nutrients C_{avg} in Ω_2 , (c) average autoinducer concentration A_{avg} in Ω_2 , (d) biofilm size ω , (e) total dispersed cells N_{tot} , (f) biomass loss $K(T)$ indicating the fraction of the produced biomass that are actually dispersed from the biofilm.

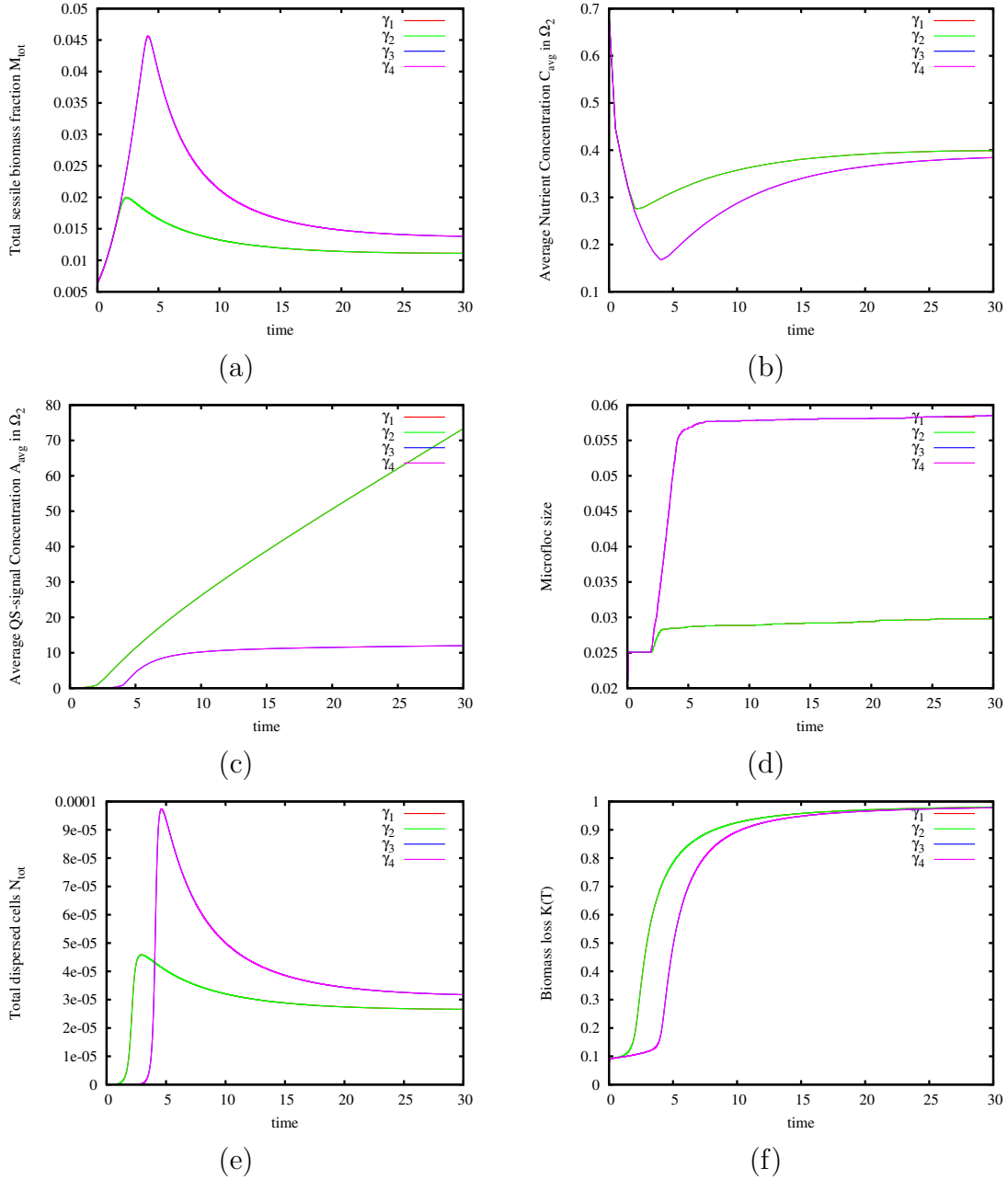


Fig. 4: **Temporal plots of simulations of a microfloc using different $\gamma_i(C)$.** Here we used $\tau = 50nM$, $\eta_1 = 3.6d^{-1}$. Shown are (a) total sessile biomass fraction M_{tot} in the microfloc, (b) average concentration of the nutrients C_{avg} in Ω_2 , (c) average autoinducer concentration A_{avg} in Ω_2 , (d) microfloc size Ω , (e) total dispersed cells N_{tot} , (f) biomass loss $K(T)$ indicating the fraction of the produced biomass that are actually dispersed from the microfloc. The curves of γ_1 and γ_2 (insensitive to high nutrient concentrations) are grouped together and appear as one curve; and so are those of γ_3 and γ_4 (sensitive to high nutrient concentrations).