Supplementary material for "A novel model for biofilm initiation in porous media flow"

Christoph Lohrmann and Christian Holm

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1 Surface attachment in flow with increased attachment time

Complementary to fig. 1 of the main text, fig. 1 shows the histogram of attachment angles on a cylindrical obstacle for motile bacteria, but with an increased average time-to-attachment $\langle t_{\mathrm{attach}} \rangle = 10\,\mathrm{s}$. This time is much larger than the time $2R_{\mathrm{cyl}}/v_{\mathrm{swim}} = 1.6\,\mathrm{s}$ it takes a bacterium to travel the diameter of a cylinder. Many encounters are therfore needed until a bacterium attaches to a surface. This constitutes the opposite limit compared to the instantaneous attachment discussed in the main text. Yet, the qualitative features of the histogram are the same, with a large probability of downstream attachment ($\Theta < \pi/2$) and a peak at $\Theta = 0$. This shows that the exact value of $\langle t_{\mathrm{attach}} \rangle$ does not influence the qualitative phenomenon of preferential attachment on the downstream end of obstacles.

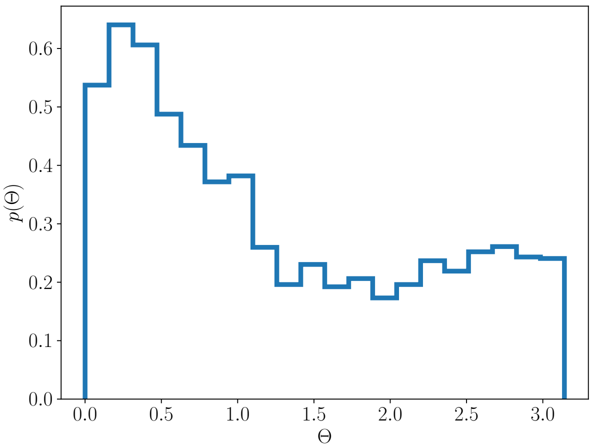

Figure 1: Normalized histogram of the angular position of attachment for $\langle t_{\mathrm{attach}} \rangle = 10\,\mathrm{s}$.

2 Parameters for simulations

In the following sections we list the parameters needed to reproduce all simulations we performed. The section headings correspond to the respective sections in the main text. The symbols used here are introduced in the main text.

2.1 Qualitative biofilm morphologies

Table 1 lists the parameters that are common to all simulations that show the qualitative biofilm morphologies. Table 2 lists the parameters that differ between the four simulations. $\dot{\gamma}_{\text{wall}}$ denotes the shear rate at the planar walls, the force applied to the fluid to achieve this shear rate is calculated from the Poiseuille flow profile as

$$\mathbf{F}_{\text{fluid}} = \frac{2\dot{\gamma}_{\text{wall}}\mu}{h}\mathbf{e}_x. \tag{1}$$

The simulations are meant as a showcase of model capabilities and not to model a specific system. We use units of $c_{\text{length}} = 1\,\mu\text{m}$, $c_{\text{time}} = 1\,\text{s}$, $c_{\text{density}} = \rho_{\text{water}} = 1000\,\text{kg/m}^3$.

Table 1: Common parameters for qualitative biofilm morphology simulations

Symbol	δt	Δt	δt_{LB}	a_{grid}	ρ	μ	h	γ_0	r_{growth}	r_{bact}	$l_{\text{bact, max}}$
Value	0.05	3.45	0.2	1	1	0.1	20	1.5	0.002	0.5	3
Symbol	t_{attach}	r_{attach}	r_{bond}	r_{detach}	N_{anchor}						
Value	0.01	0.55	0.55	0.65	2						

Table 2: Parameters for the individual biofilm morphology simulations

	ϵ^{LJ}	k	$\dot{\gamma}_{\text{wall}}$
Sphere	0.05	15	0
Flat	0.00005	15	0.05
Rolling	0.005	0.00001	0.05
Intermediate	0.02	15	0.05

2.2 Determination of model parameters

We choose units of $c_{\text{energy}} = \epsilon^{\text{LJ}}$, $c_{\text{length}} = 1\,\mu\text{m}$, $c_{\text{time}} = 1\,\text{s}$ Dynamic parameters (such as the friction coefficient γ_0) have no influence on the determination of all static properties like the biofilm tensile strength. They only affect the speed of convergence. Since we report tensile strength as a dimensionless quantity by dividing out the energy scale ϵ^{LJ}, we are free to set that value to 1.

Table 3: Parameters for determination of biofilm tensile strength

Symbol	δt	Δt	ϵ^{LJ}	γ_0	r_{growth}	r_{bact}	$l_{\text{bact, max}}$	cylinder radius	initial cylinder height
Value	0.035	2.765	1	0.4	0.0025	0.5	3	4.5	7.5
Symbol	t_{attach}	r_{attach}	r_{bond}	k	r_{detach}	N_{anchor}			
Value	0.01	0.75	0.6	15	0.8	2			

2.3 Simulation of biofilm formation in porous media

Table 4: Simulation parameters for biofilm formation simulation

Symbol	δt	Δt	δt_{LB}	a_{grid}	ρ	μ	h	τ_2	$\lvert\mathbf{F}_{\text{fluid}}\rvert$
Value	$0.006\,\text{s}$	$12\,\text{s}$	$0.03\,\text{s}$	$1\,\mu\text{m}$	$1000\,\text{kg}\,\text{m}^{-3}$	$1\times10^{-3}\,\text{Pa}\,\text{s}$	$10\,\mu\text{m}$	$1\,\text{h}$	$40\,\text{N}\,\text{m}^{-3}$
Symbol	r_{bact}	$l_{\text{bact, max}}$	t_{attach}	r_{attach}	k	r_{detach}	N_{anchor}	f	
Value	$0.5\,\mu\text{m}$	$3\,\mu\text{m}$	$0.001\,\text{s}$	$0.75\,\mu\text{m}$	$8\times10^{-2}\,\text{kg}\,\text{s}^{-2}$	$1\,\mu\text{m}$	2	2×10^{-6}	

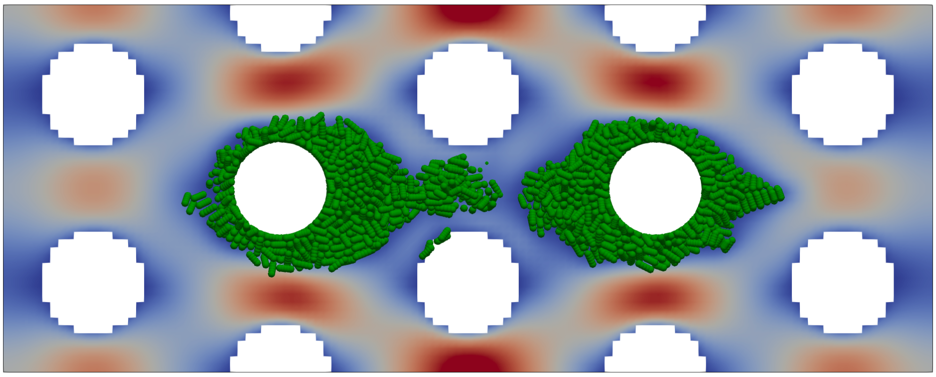

Figure 2: Snapshot of biofilm formation for soft ($\sigma_{\text{yield}} = 500\,\text{Pa}$) biofilm. Inbetween the central cylinders a section of biofilm is being advected to the right.

3 Soft biofilm in porous medium

Figure 2 shows an event where a piece of biofilm originally grown on the left cylinder gets detached by the flow and transported downstream to the next cylinder, where there is already a sizeable colony formed by previous biofilm transport events.

4 Description of SI movies

Movies S1-S3 show examples of biofilm formation corresponding to the simulations of section 3.4 of the manuscript. The simulation parameters are given in table 4, the value for the yield stress $\sigma_{\text{yield}} \in \{500, 1875, 6000\}$Pa for the individual movies is given in the file name.