Supplementary Material S1 to Mass Transfer Enhancement in Moving Biofilm Structures

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Model equations, dimensionless numbers and notations

The dimensionless model equations result by scaling each dimensional quantity with some characteristic value:

- space can be scaled with a characteristic length L_0 (for example, the biofilm head diameter d or an equivalent hydraulic diameter $4A_B/P_B$) and time with a conveniently chosen characteristic time t_0 (for example, the inverse of a streamer characteristic vibration frequency)
  $x^* = \frac{x}{L_0} \qquad y^* = \frac{y}{L_0} \qquad t^* = \frac{t}{t_0}$
- velocities, displacement, stresses and concentrations are scaled with the inlet flow velocity, characteristic length, Young modulus and inlet solute concentration, respectively. The pressure is made dimensionless on the viscous scale:
  $\mathbf{u}^* = \frac{\mathbf{u}}{u_0} \qquad p^* = \frac{L_0 p}{\mu_F u_0} \qquad \mathbf{d}^* = \frac{\mathbf{d}}{L_0} \qquad \mathbf{S}^* = \frac{\mathbf{S}}{E} \qquad c_F^* = \frac{c_F}{c_0} \qquad c_B^* = \frac{c_B}{c_0}$

In tables S1.1, S1.2, S1.3 and S1.4 the complete formulation of fluid-structure interaction and substrate transport and uptake in biofilm streamers are introduced in both dimensional and also non-dimensional forms. As a result of scaling the model equations, a few dimensionless numbers appear which are lissted in Table S1.5.

Table S1.1: Dimensional and non-dimensional forms of fluid dynamics equations solved on the moving mesh frame with spatial coordinates $\boldsymbol{\chi}$.

Scope	Dimensional equations	Dimensionless equations
Ω_F	Incompressible unsteady laminar flow.	
	$\rho_F \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} - \mathbf{u}_G) \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu_F \nabla^2 \mathbf{u}$	$St\, Re\, \frac{\partial \mathbf{u}^*}{\partial t^*} + Re\, (\mathbf{u}^* - \mathbf{u}_G^*) \cdot \nabla \mathbf{u}^* = -\nabla p^* + \nabla^2 \mathbf{u}^*$
	$\nabla \cdot \mathbf{u} = 0$	$\nabla \cdot \mathbf{u}^* = 0$
	Initial condition: the steady-state solution $\mathbf{u} = \mathbf{u}_{st}$	$\mathbf{u}^* = \mathbf{u}_{st}^*$
Γ_I	Uniform inlet velocity $u_x = u_0, \quad u_y = 0$	$u_x^* = 1, \quad u_y^* = 0$
Γ_U, Γ_L	Slip condition $\partial u_x / \partial y = 0, \quad u_y = 0$	$\partial u_x^* / \partial y^* = 0, \quad u_y^* = 0$
Γ_O	No viscous forces and fixed zero pressure $\partial u_x / \partial y + \partial u_y / \partial x = 0, \quad p = 0$	$\partial u_x^* / \partial y^* + \partial u_y^* / \partial x^* = 0, \quad p^* = 0$
Γ_H	Non-slip condition $\mathbf{u} = 0$	$\mathbf{u}^* = 0$
Γ_{FSI}	Fluid velocity equals the biofilm deformation rate	
	$\mathbf{u} = \frac{d\mathbf{d}}{dt}$	$\mathbf{u}^* = St\, \frac{d\mathbf{d}^*}{dt^*}$

Table S1.2: Dimensional and non-dimensional forms of biofilm elastodynamics equations solved on the Lagrangian coordinate system $\mathbf{X}$ associated with the material points.

Scope	Dimensional equations	Dimensionless equations
Ω_B	Geometrically nonlinear isotropically elastic material	
	$\rho_B \frac{d^2\mathbf{d}}{dt^2} = \nabla \cdot (\mathbf{S} \cdot \mathbf{F})$	$St^2\, Re\, Q(\frac{\rho_F}{\rho_B})\frac{d^2\mathbf{d}^*}{dt^{*2}} = \nabla \cdot (\mathbf{S}^* \cdot \mathbf{F})$
	$\mathbf{S} = \frac{E\nu}{(1+\nu_B)(1-2\nu_B)}\operatorname{tr}\mathbf{E}\mathbf{I} + \frac{E}{(1+\nu_B)}\mathbf{E}$	$\mathbf{S}^* = \frac{\nu_B}{(1+\nu_B)(1-2\nu_B)}\operatorname{tr}\mathbf{E}\mathbf{I} + \frac{1}{(1+\nu_B)}\mathbf{E}$
	$\mathbf{E} = \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I}), \quad \mathbf{F} = \mathbf{I} + \nabla\mathbf{d}$	
	Initial condition: static system with no displacement and zero displacement rate	
	$\mathbf{d} = 0, \quad \frac{d\mathbf{d}}{dt} = 0$	$\mathbf{d}^* = 0, \quad \frac{d\mathbf{d}^*}{dt^*} = 0$
Ω_H, Γ_H	No displacement	
	$\mathbf{d} = 0$	$\mathbf{d}^* = 0$
Γ_{FSI}	Dynamic continuity of stresses in biofilm and fluid	
	$\mathbf{n} \cdot \sigma = \mathbf{n} \cdot \left[p\mathbf{I} + \mu_F \nabla\mathbf{u} + \mu_F (\nabla\mathbf{u})^T\right] \frac{dv}{dV}$	$\mathbf{n} \cdot \sigma^* = \mathbf{n} \cdot \left\{ Q\Big[p^*\mathbf{I} + \nabla\mathbf{u}^* + (\nabla\mathbf{u}^*)^T\Big] \right\} \frac{dv^*}{dV^*}$

Table S1.3: Dimensional and non-dimensional forms of solute transport in fluid equations solved on the moving mesh frame with spatial coordinates $\boldsymbol{\chi}$.

Scope	Dimensional equations	Dimensionless equations
Ω_F	Unsteady convection and diffusion of a dilute solute	
	$\frac{\partial c_F}{\partial t} = -(\mathbf{u} - \mathbf{u}_G) \cdot \nabla c_F + \nabla \cdot (D \nabla c_F)$	$St\, Pe \frac{\partial c_F^*}{\partial t^*} + Pe\, (\mathbf{u}^* - \mathbf{u}_G^*) \cdot \nabla c_F^* = \nabla^2 c_F^*$
	Initial condition: the steady-state solution	
	$c_F = c_{F,st}$	$c_F^* = c_{F,st}^*$
Γ_I	Constant concentration	
	$c_F = c_0$	$c_F^* = 1$
Γ_U, Γ_L	Insulation	
	$\partial c_F / \partial y = 0$	$\partial c_F^* / \partial y^* = 0$
Γ_O	No diffusion	
	$\partial c_F / \partial x = 0$	$\partial c_F^* / \partial x^* = 0$
Γ_H, Γ_{FSI}	Flux continuity	
	$\partial c_F / \partial n = \partial c_B / \partial n$	$\partial c_F^* / \partial n^* = \partial c_B^* / \partial n^*$

Table S1.4: Dimensional and non-dimensional forms of solute transport and reaction in biofilm equations solved on the Lagrangian coordinate system $\mathbf{X}$ associated with the material points.

Scope	Dimensional equations	Dimensionless equations
Ω_B	Unsteady diffusion and nonlinear (Monod) reaction for a dilute solute	
	$\frac{\partial c_B}{\partial t} = D\nabla^2 c_B + k\frac{c_B}{K + c_B}$	$St\,Pe\,\frac{\partial c_B^*}{\partial t^*} = \nabla^2 c_B^* + \Phi^2 \frac{c_B^*}{M + c_B^*}$
	Initial condition: the steady-state solution	
	$c_B = c_{B,st}$	$c_B^* = c_{B,st}^*$
Γ_H, Γ_{FSI}	Continuity of solute concentration	
	$c_B = c_F$	$c_B^* = c_F^*$

Table S1.5: Summary of dimensionless numbers

Dimensionless form	Name
1. *Fluid dynamics*	
$Re = \frac{L_0 u_0 \rho_F}{\mu_F}$	Reynolds number
$St = \frac{L_0}{t_0 u_0}$	Strouhal number
2. *Biofilm Elastodynamics*	
$Q = \frac{u_0 \mu_F}{E_B L_0}$	FSI number
$\tau_E^2 = \frac{\rho_B L_0^2}{E_B t_0^2} = \frac{t_{0,E}^2}{t_0^2} = St^2 Re \left(\frac{\rho_F}{\rho_B}\right) Q$	FSI time scale (squared)
3. *Solute mass transport in fluid and biofilm*	
$Pe = \frac{u_0 L_0}{D}$	Péclet number
$\Phi^2 = \frac{k L_0^2}{D c_0}$	Thiele number (squared)
$M = \frac{K}{c_0}$	Dimensionless Monod number
$\tau_D = \frac{L_0^2/D}{t_0} = \frac{t_{0,D}}{t_0} = St\, Pe$	Mass transport time scale
In addition, when considering the mass transfer in the liquid boundary layer adjacent to the biofilm, from $k_m(c - c_0) = D\, \partial c/\partial n\big\vert_\Gamma$ a Sherwood number can be defined as: $Sh = \frac{k_m L_0}{D} = \frac{L_0 \frac{\partial c}{\partial n}\big\vert_\Gamma}{c - c_0}$	Sherwood number
Usually, *Sh* is correlated with *Re* and *Sc* (Schmidt) numbers, where $Sc = \frac{\mu_F}{\rho_F D}$	Schmidt number

Nomenclature

Symbol	Description	Units
Subdomains and boundaries		
Ω_F	Fluid subdomain	
Ω_B	Biofilm subdomain	
Γ_I	Inlet boundary	
Γ_O	Outlet boundary	
Γ_U	Upper wall boundary	
Γ_L	Lower wall boundary	
Γ_H	Biofilm head boundary	
Γ_{FSI}	Biofilm tail boundary (Fluid-Structure Interaction boundary)	
Model variables and constants		
c_0	Solute concentration in inlet	$\text{mol} \cdot \text{m}^{-3}$
c_B	Solute concentration in biofilm	$\text{mol} \cdot \text{m}^{-3}$
c_F	Solute concentration in fluid	$\text{mol} \cdot \text{m}^{-3}$
$\mathbf{d}$	Biofilm displacement	m
D	Solute diffusion coefficient	$\text{m} \cdot \text{s}^{-2}$
E_B	Biofilm Young's modulus	$\text{kg} \cdot \text{m}^{-1} \cdot \text{s}^{-2}$
$\mathbf{E}$	Green-Lagrangian strains	-
$\mathbf{F}$	Deformation gradient	-
$\mathbf{I}$	Identity matrix	-
k	Reaction rate constant	$\text{mol} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$
k_m	Mass transfer coefficient	$\text{m} \cdot \text{s}^{-1}$
K	Monod saturation coefficient	$\text{mol} \cdot \text{m}^{-3}$
L_0	Characteristic length	m
n	Direction normal to boundary	m
$\mathbf{n}$	Vector normal to boundary	m
p	Fluid pressure	$\text{kg} \cdot \text{m}^{-1} \cdot \text{s}^{-2}$
$\mathbf{S}$	Second Piola-Kirchhoff stress tensor	$\text{kg} \cdot \text{m}^{-1} \cdot \text{s}^{-2}$
t	Time	s

Symbol	Description	Units
t_0	Characteristic time	s
$t_{0,D}$	Characteristic time for diffusion	s
u_x, u_y	Fluid velocity components	$m \cdot s^{-1}$
$\mathbf{u}$	Fluid velocity	$m \cdot s^{-1}$
$\mathbf{u}_G$	Mesh velocity	$m \cdot s^{-1}$
v	Volume in spatial frame	m^3
V	Volume in material frame	m^3
x, y	Spatial coordinates	m
$\mathbf{X}$	Material coordinates (Lagrangian frame, reference configuration)	m
μ_F	Fluid dynamic viscosity	$kg \cdot m^{-1} \cdot s^{-1}$
ν_B	Poisson's ratio biofilm material	-
ρ_F	Fluid density	$kg \cdot m^{-3}$
ρ_B	Biofilm density	$kg \cdot m^{-3}$
σ	Cauchy stress in the biofilm	$kg \cdot m^{-1} \cdot s^{-2}$
$\boldsymbol{\chi}$	Spatial coordinates (moving mesh frame)	m
Characteristic dimensionless numbers		
M	Dimensionless Monod number	-
Pe	Péclet number	-
Q	FSI number	-
Re	Reynolds number	-
Sh	Sherwood number	-
St	Strouhal number	-
Φ^2	Thiele number	-
τ_E	FSI time scale	-
τ_D	Solute diffusion time scale	-