Supplementary Material S3
to Mass Transfer Enhancement in Moving Biofilm Structures

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Mesh convergence studies

In order to obtain reliable and accurate results, we found that it is important to choose very carefully the size and distribution of finite element mesh, as well as the length and width of the computational domain. In the present study detailed mesh studies were carried out, where different mesh sizes for the domain Ω_F and biofilm-liquid boundary Γ_{CD} were investigated. The goal was to achieve mesh-size independence, while keeping some optimal simulation costs in terms of run times and memory requirements. Also, special care had to be taken with meshes around the moving parts because due to large structure deformations extremely small mesh sizes would lead to early mesh quality depreciation (and even to fatal mesh element inversions).

One additional difficulty is due to presence of very high Péclet numbers Pe (i.e., convection-dominated mass transport) in the current study, which require extremely dense meshes to be able to resolve the steep gradients of concentration. When courser meshes were used, local disturbances appeared around the boundaries, which quickly propagated into the domain and significantly reduced the solution accuracy and stability over time. The time step is also critical, and the solver was set up to avoid large time step jumps (the maximum time step was restricted to 5×10^{-4} s.

Because the scope of this work was to investigate the enhancement of mass transfer caused by biofilm movement, the overall Sherwood number $\overline{Sh}$ was chosen as the criterion for mesh convergence. Based on the results presented in Fig. S3.1a, we concluded that a maximum mesh size of 5×10^{-6} m on the biofilm-liquid boundary Γ_{CD} is sufficiently fine to resolve the flow and mass transfer fields. In addition, maximum mesh size of 6.67×10^{-5} m was selected for the rest of the domain following a similar analysis. These mesh sizes have been used in all computations reported in this work.

In order to optimize the minimum number of mesh elements that can produce a reliable result, we used a hybrid mesh (Fig. S3.1b). Boundary layer mesh elements, i.e., the highly anisotropic linear elements along the boundaries, were generated around the interface Γ_{CD}. A first order free triangular mesh constructed using advancing front technique is used for the rest of the subdomains.

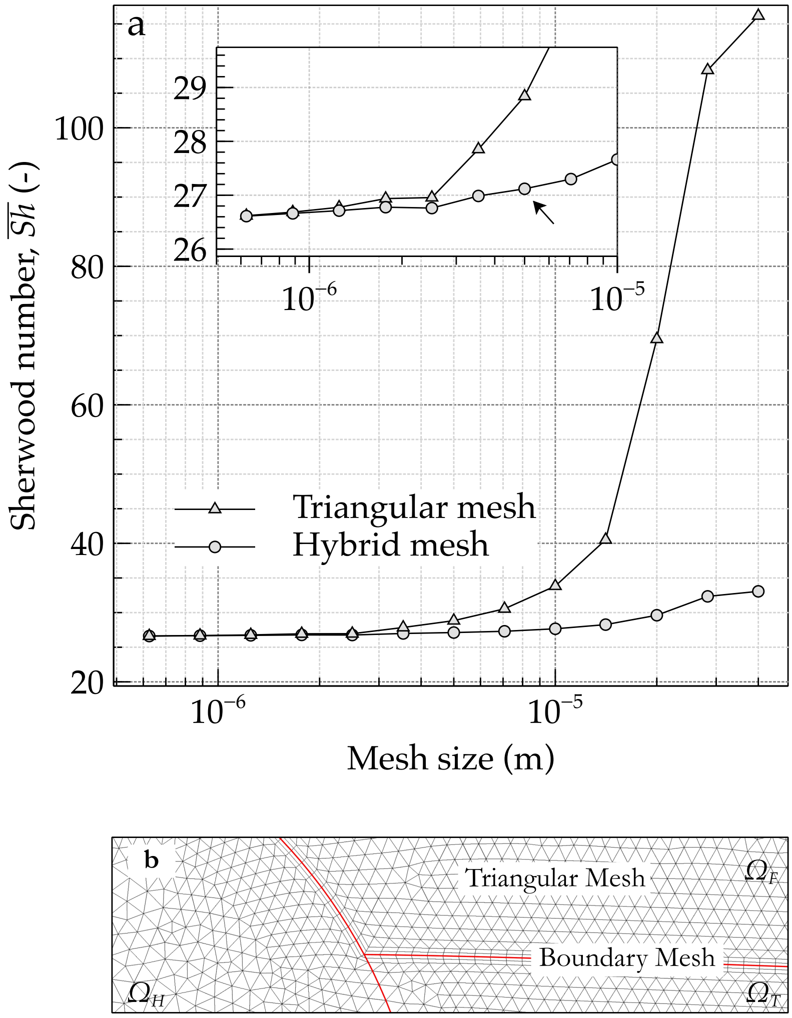
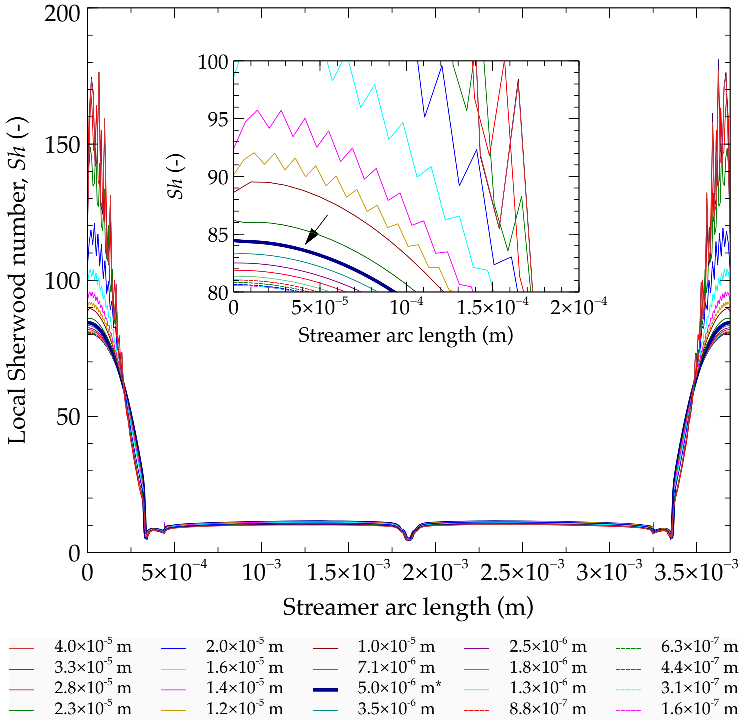
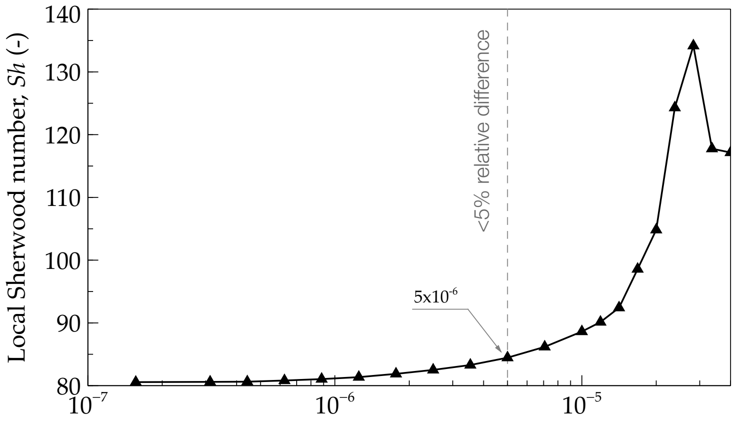


Figure S3.1: (a) Mesh size convergence studies for the boundary Γ_{CD} with respect to the *overall* mass transport number $\overline{Sh}$ along the biofilm perimeter. The arrow shows the maximum boundary mesh size selected throughout the simulations: 5×10^{-6} m. (b) Example of the hybrid mesh around the biofilm-liquid boundary Γ_{CD}.

The streamer lays in a non-homogenous field of concentration and flow velocity. Hence, it was needed to also perform a mesh convergence study based on the local Sherwood number, *Sh*. Fig. S3.2a demonstrates the magnitude of local Sherwood number *Sh* along the perimeter of the biofilm streamer using various mesh sizes. The highest variation of *Sh* appears to the left side of the circular streamer head (Ω_H), which frontally faces the flow and around which the thinnest boundary layer forms. Fig. S3.2b shows a close-up of this region, where the maximum mesh size selected also conforms to the selected mesh based on the overall Sherwood number $\overline{Sh}$.



(a) Local profile of *Sh* along the streamer arc length. The arrow shows the maximum boundary mesh size selected for the simulations.



(b) Close-up of the region with the highest variance of local Sherwood number, *Sh*, with respect to different mesh sizes. The dashed line highlights the maximum boundary mesh size selected for the simulations.

Figure S3.2: Mesh size convergence studies for the boundary Γ_{CD} with respect to the local mass transport number *Sh* along the biofilm perimeter.