

Modeling Biofilm Growth on a CO₂-Supplying, Membrane-Based Biofilm Photobioreactor (MB-PBR)

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Table S1. Main parameters used in the different simulations.

Simulation set	Main parameters values
Comparison MB-PBR vs conventional system (Fig. 4a-c)	$c_{i,NO_3} = 1.76 \text{ mol/m}^3$ $c_{i,P,Total} = 16.023 \text{ mol/m}^3$ $c_{i,CO_2,Total} = 0.035 \text{ mol/m}^3$ $pH_i = 7.5$ $I_0 = 18.5 \text{ W/m}^2$ $y_{CO_2} = 0.05 \text{ (5\% CO}_2\text{)}$
Effect of inorganic carbon in MB-PBR (Fig. 4d-f)	$c_{i,NO_3} = 1.76 \text{ mol/m}^3$ $c_{i,P,Total} = 16.023 \text{ mol/m}^3$ $c_{i,CO_2,T} = 0.035 \text{ mol/m}^3$ $pH_i = 7.5$ $I_0 = 18.5 \text{ W/m}^2$ $y_{CO_2} = 0.01, 0.05, 0.1, 0.2, 0.5, 0.99$
pH variability in MB-PBR (Fig. 5a-c)	$c_{i,NO_3} = 1.76 \text{ mol/m}^3$ $c_{i,P,Total} = 16.023, 0.023 \text{ mol/m}^3$ $c_{i,CO_2,Total} = 0.035 \text{ mol/m}^3$ $pH_i = 7.5$ $I_0 = 250 \text{ W/m}^2$ $y_{CO_2} = 0.05 \text{ (5\%)}$
Light inhibition in MB-PBR (Fig. 6a-c)	$c_{i,NO_3} = 1.76 \text{ mol/m}^3$ $c_{i,P,Total} = 16.023 \text{ mol/m}^3$ $c_{i,CO_2,Total} = 0.035 \text{ mol/m}^3$ $pH_i = 7.5$ $I_0 = 200 \text{ W/m}^2$ $y_{CO_2} = 0.05 \text{ (5\% CO}_2\text{)}$ $K_{LI} = 50 \text{ W/m}^2$
Oxygen stripping in MB-PBR (Fig. S5)	$c_{i,NO_3} = 1.76 \text{ mol/m}^3$ $c_{i,P,Total} = 16.023 \text{ mol/m}^3$ $c_{i,CO_2,Total} = 0.035 \text{ mol/m}^3$ $pH_i = 7.5$ $I_0 = 200 \text{ W/m}^2$ $y_{CO_2} = 0 \text{ (Only N}_2\text{ passing through membrane)}$

c_i =Initial concentrations in bulk liquid; pH_i =Initial pH in bulk liquid; ; I_0 =Light intensity;
 K_{LI} =Light inhibition coefficient; y_{CO_2} =CO₂ fraction in gas passing through membrane

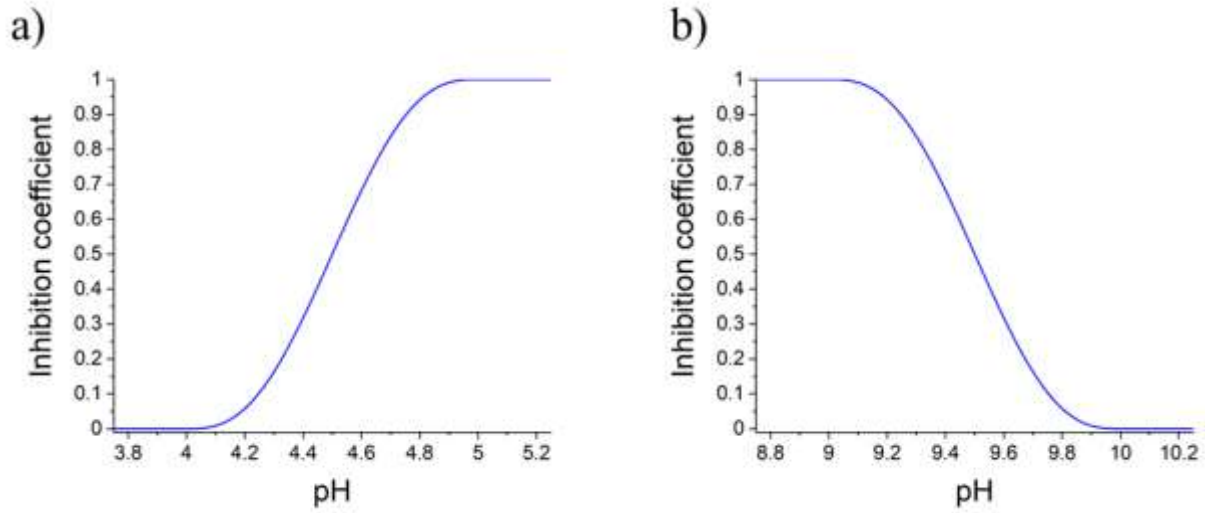


Figure S1. pH functions applied to growth (a) pH below 5.5 and b) pH above 8.5

Table S2. Acid-base reactions with equilibrium rate expressions and equilibrium constants. S are the solutes concentrations in (mol/m^3), the $\text{p}K_a$ are the acid dissociation constants, and $k_a=10^7/\text{s}$ is an arbitrarily large rate coefficient that ensures the reaction is close to equilibrium.

Rate name	Rate expression	Dissociation reaction	pKa
re_{CO_2}	$k_a \left(S_{\text{CO}_2} - \frac{S_H S_{\text{HCO}_3}}{K_{a,\text{CO}_2}} \right)$	$\text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{HCO}_3^- + \text{H}^+$	6.35
re_{HCO_3}	$k_a \left(S_{\text{HCO}_3} - \frac{S_H S_{\text{CO}_3}}{K_{a,\text{HCO}_3}} \right)$	$\text{HCO}_3^- \rightleftharpoons \text{CO}_3^{2-} + \text{H}^+$	10.33
$\text{re}_{\text{H}_3\text{PO}_4}$	$k_a \left(S_{\text{H}_3\text{PO}_4} - \frac{S_H S_{\text{H}_2\text{PO}_4}}{K_{a,\text{H}_3\text{PO}_4}} \right)$	$\text{H}_3\text{PO}_4 \rightleftharpoons \text{H}_2\text{PO}_4^- + \text{H}^+$	2.15
$\text{re}_{\text{H}_2\text{PO}_4}$	$k_a \left(S_{\text{H}_2\text{PO}_4} - \frac{S_H S_{\text{HPO}_4}}{K_{a,\text{H}_2\text{PO}_4}} \right)$	$\text{H}_2\text{PO}_4^- \rightleftharpoons \text{HPO}_4^{2-} + \text{H}^+$	7.21
re_{HPO_4}	$k_a \left(S_{\text{HPO}_4} - \frac{S_H S_{\text{PO}_4}}{K_{a,\text{HPO}_4}} \right)$	$\text{HPO}_4^{2-} \rightleftharpoons \text{PO}_4^{3-} + \text{H}^+$	12.35
$\text{re}_{\text{H}_2\text{O}}$	$k_a \left(1 - \frac{S_H S_{\text{OH}}}{K_{a,\text{H}_2\text{O}}} \right)$	$\text{H}_2\text{O} \rightleftharpoons \text{OH}^- + \text{H}^+$	14

Table S3. Acid-base equilibria stoichiometry.

Rate expression	$S_{H_2CO_3}$	S_{HCO_3}	S_{CO_3}	$S_{H_3PO_4}$	$S_{H_2PO_4}$	S_{HPO_4}	S_{PO_4}	S_{H_2O}	S_H	S_{OH}
$re_{H_2CO_3}$	-1	1							1	
re_{HCO_3}		-1	1						1	
$re_{H_3PO_4}$				-1	1				1	
$re_{H_2PO_4}$					-1	1			1	
re_{HPO_4}						-1	1		1	
re_{H_2O}								-1	1	1

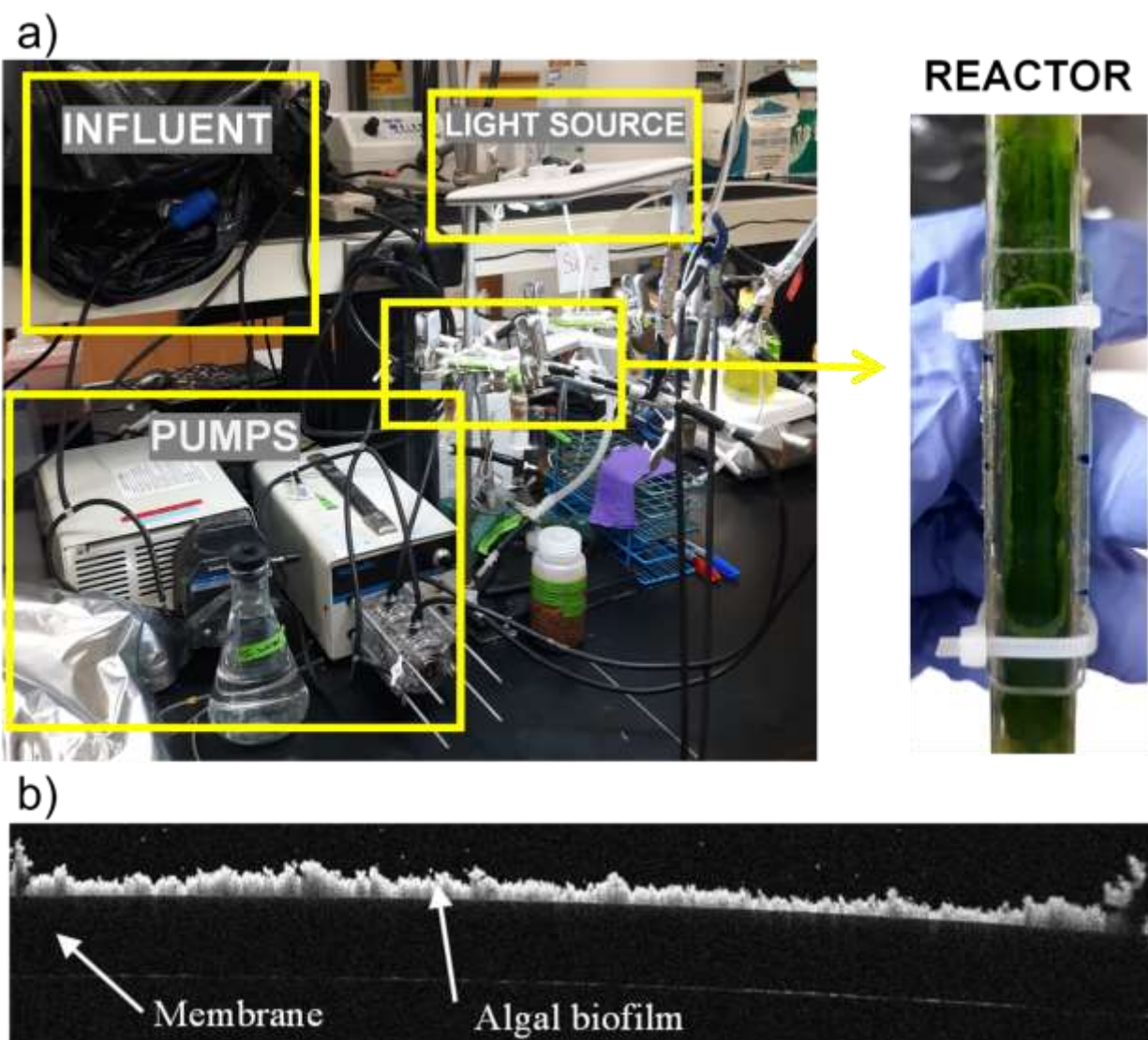


Figure S2. a) Experimental set-up. Influent media (10% BG-11) is pumped with a rate of 0.6 mL/min to the reactor. A recirculation pump provides mixing in the reactor. A panel white LED serves as light source. The membrane reactor is shown with algal biofilm. b) OCT image of algal biofilm growing on the membrane.

Table S4. Local sensitivity analysis of the light attenuation coefficient (k_e) and half-saturation coefficient of light irradiance (K_I) with a $\pm 5\%$ parameter variation in the MB-PBR model.

Case	K_I	k_e	L_F (μm)	ΔL_F (%)*	$ S = \Delta L_F(\%) / \Delta \text{Par}(\%)$
Reference	5	80,000	176.36	-	-
K_I (-5%)	4.75	80,000	91.86	2.48	0.50
K_I (+5%)	5.25	80,000	88.84	-2.32	0.46
k_e (-5%)	5	76,000	186.11	5.52	1.10
k_e (+5%)	5	84,000	167.63	-4.95	0.99

* ΔL_F (%) = $(L_{F_reference} - L_{F_new}) / L_{F_reference} \times 100$

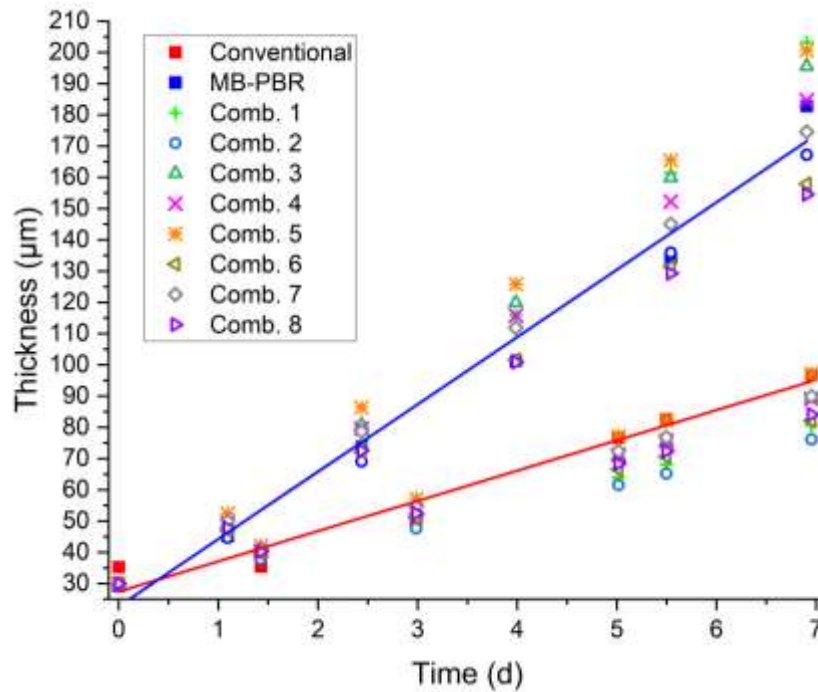


Figure S3. Data points used to estimate the light attenuation coefficient (k_e) and half-saturation coefficient of light irradiance (K_I) using a least square analysis. Solid squares represent experimental values and solid lines represent their linear fit. Eight different combinations of k_e and K_I (see **table S4**) were used for model simulations.

Table S5. Least squares analysis used to find the best fit of the parameters light attenuation coefficient (k_e) and half-saturation coefficient of light irradiance (K_I) in the model. Experimental values vs simulated values were used to calculate the least squares for each reactor.

K_I [W/m^2] $\rightarrow$	Comb. 1	Comb. 2	Comb. 3	Comb. 4	Comb. 5	Comb. 6	Comb. 7	Comb. 8
k_e [$1/m$] $\rightarrow$	20	18	10	8	5	8	5	5
	30,000	40,000	50,000	60,000	70,000	70,000	80,000	90,000
Σ LeastSq Control	665.81	990.31	198.14	204.40	128.80	507.69	183.11	392.83
Σ LeastSq MB-PBR	1373.64	271.05	1242.07	593.07	2107.48	636.64	348.15	833.45
Σ LeastSq Total	2039.45	1261.36	1440.21	797.46	2236.28	1144.33	531.26	1226.28

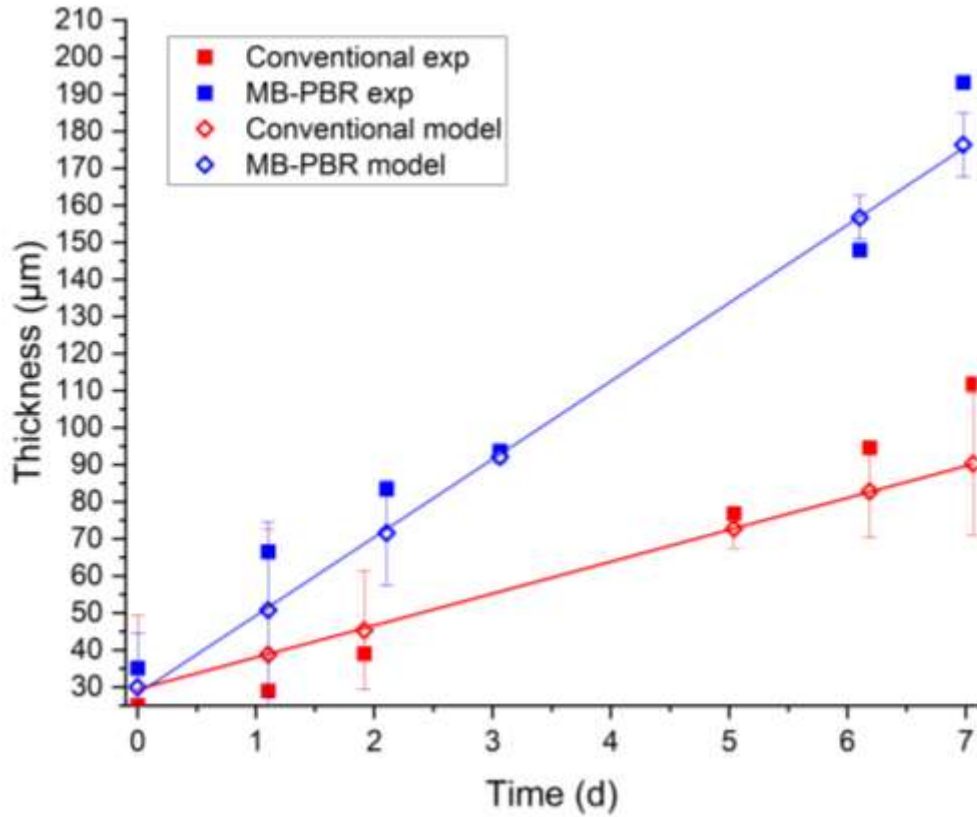


Figure S4. Validation for MB-PBR and Conventional models. Error bars in the figure represent the relative error (%) resulting from comparing the experimental results vs the model. The average error (%) for MB-PBR was calculated as 11.45% and for Conventional (control) as 17.70%. Hollow squares represent the models' outputs while the filled squares represent the experimental values.

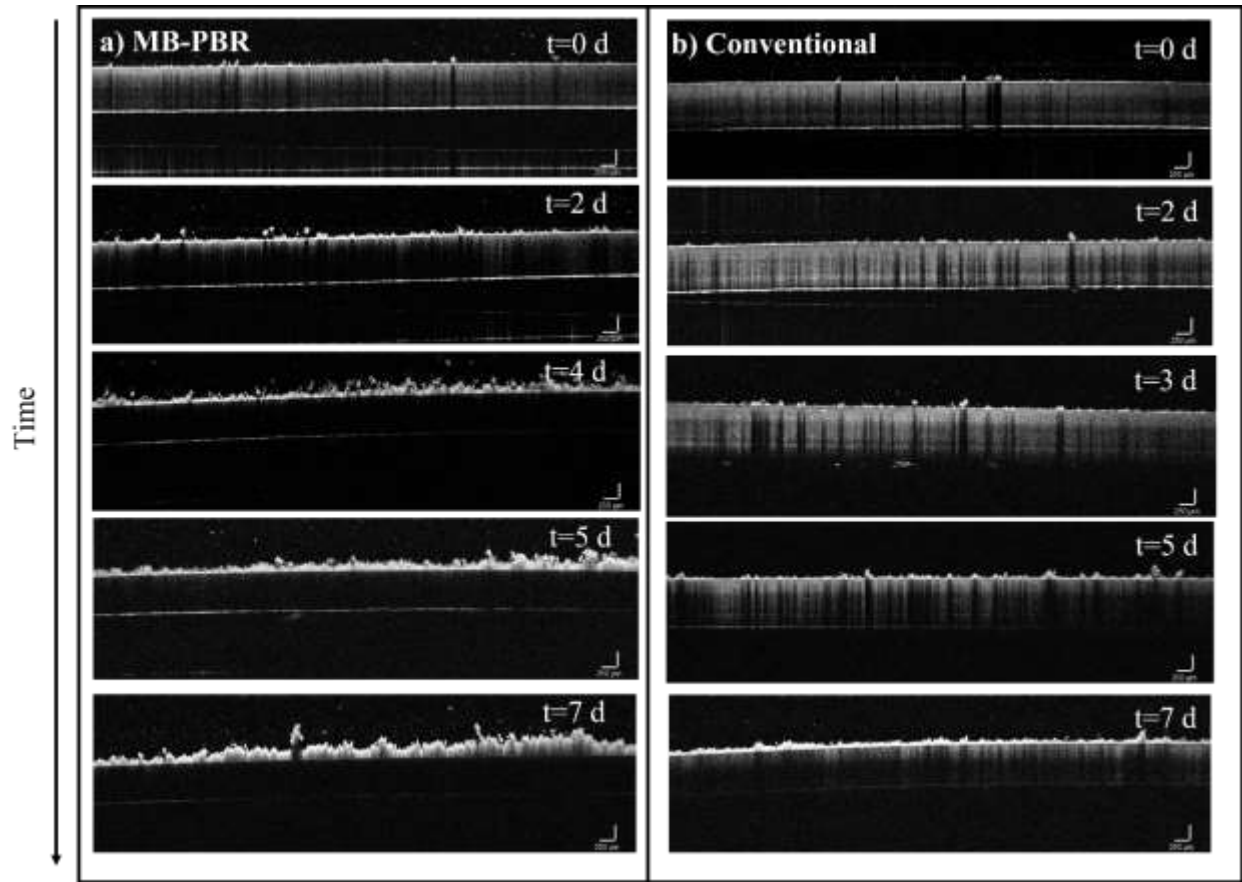


Fig S5. Biofilm progression. Longitudinal OCT images taken at different times for the MB-PBR and for the Conventional system (control). MB-PBR demonstrated to grow algal biofilm faster than the control. The scale bars on the bottom right of each figure is 250 μm .

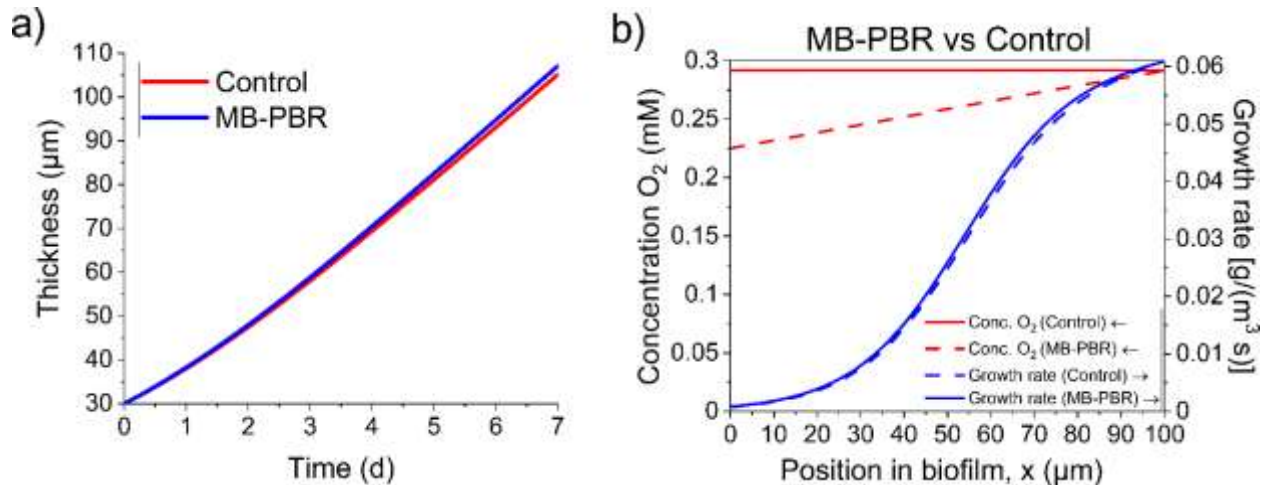


Figure S6. Assessment of O₂ stripping in the MB-PBR, via modeling. In the MB-PBR, the membrane supplies 100% nitrogen, i.e., no CO₂. Inorganic carbon is supplied from the bulk liquid. The MB-PBR and control are compared under the same conditions while including the oxygen inhibition term (S_{O_2}/K_{O_2}). Oxygen accumulation at the base of the biofilm in the control has a small negative effect on the growth rate, while the MB-PBR provides a stripping effect, avoiding oxygen accumulation. Simulation times for reaching 100 μm thickness: Control (t=6.6d); MB-PBR (t=6.45d).



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