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A novel mechanistic modelling approach for microbial selection dynamics: towards improved design and control of raceway reactors for purple bacteria – Supplementary material

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Abstract

This document contains supplementary material for the paper "A novel mechanistic modelling approach for microbial selection dynamics: Towards improved design and control of raceway reactors for purple bacteria" by A. Alloul, A. Moradvandi, D. Puyol, R. Molina, G. Gardella, S.E. Vlaeminck, B. De Schutter, E. Abraham, R.E.F. Lindeboom, and D.G. Weissbrodt, *Bioresource Technology*, vol. 390, p. 129844, Dec. 2023.

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Table S.1: Peterson matrix of the PBM.

State Variable (→) Process (↓)	S_{O2}	S_S	S_{VFA}	S_{IC}	S_{H2}	S_{IN}	S_{IP}	S_I	$X_{PB,ph}$	$X_{PB,aec}$	$X_{PB,anc}$	X_{AEB}	X_{ANB}	X_S		**Process rate (↓)**
Purple bacteria (X_{PB})																
Photoheterotrophic growth on S_S	0	$-1/Y_{PB,ph}$	0	$f_{IC,ph,SS}$	0	$-Y_{N,PB}$	$-Y_{P,PB}$	0	1	0	0	0	0	0	0	1
Photoheterotrophic growth on S_{VFA}	0	0	$-1/Y_{PB,ph}$	$f_{IC,ph,VFA}$	0	$-Y_{N,PB}$	$-Y_{P,PB}$	0	1	0	0	0	0	0	0	2
Aerobic chemoheterotrophic growth S_S	$-(1-Y_{PB,aec})/Y_{PB,aec}$	$-1/Y_{PB,aec}$	0	$f_{IC,aec,SS}$	0	$-Y_{N,PB}$	$-Y_{P,PB}$	0	0	1	0	0	0	0	0	3
Aerobic chemoheterotrophic growth S_{VFA}	$-(1-Y_{PB,aec})/Y_{PB,aec}$	0	$-1/Y_{PB,aec}$	$f_{IC,aec,VFA}$	0	$-Y_{N,PB}$	$-Y_{P,PB}$	0	0	1	0	0	0	0	0	4
Anaerobic chemoheterotrophic growth S_S	0	$-1/Y_{PB,anc}$	$f_{VFA,anc,SS}/Y_{PB,anc}$	$f_{IC,anc,SS}$	0	$-Y_{N,PB}$	$-Y_{P,PB}$	0	0	0	1	0	0	0	0	5
Decay of $X_{PB} = X_{PB,ph} + X_{PB,aec} + X_{PB,anc}$	0	0	0	$f_{IC,dec}$	0	$f_{IN,dec}$	$f_{IP,dec}$	0	-1	-1	-1	0	0	1	0	6
Aerobic bacteria (X_{AEB})																
Aerobic chemoheterotrophic growth on S_S	$-(1-Y_{AEB})/Y_{AEB}$	$-1/Y_{AEB}$	0	$f_{IC,AEB,SS}$	0	$Y_{N,AEB}$	$Y_{P,AEB}$	0	0	0	0	1	0	0	0	7
Aerobic chemoheterotrophic growth on S_{VFA}	$-(1-Y_{AEB})/Y_{AEB}$	0	$-1/Y_{AEB}$	$f_{IC,AEB,VFA}$	0	$Y_{N,AEB}$	$Y_{P,AEB}$	0	0	0	0	1	0	0	0	8
Decay of X_{AEB}	0	0	0	$f_{IC,dec}$	0	$f_{IN,dec}$	$f_{IP,dec}$	0	0	0	0	-1	0	1	0	9
Anaerobic bacteria (X_{ANB})																
Anaerobic chemoheterotrophic growth on S_S	0	$-1/Y_{ANB}$	$f_{VFA,ANB,SS}/Y_{ANB}$	$f_{IC,ANB,SS}$	$f_{VFA,ANB,H2}/Y_{ANB}$	$-Y_{N,ANB}$	$-Y_{P,ANB}$	0	0	0	0	0	1	0	0	10
Decay of X_{ANB}	0	0	0	$f_{IC,dec}$	0	$f_{IN,dec}$	$f_{IP,dec}$	0	0	0	0	0	-1	1	0	11
Hydrolysis																
Hydrolysis	0	$f_{SS,XS}$	$f_{VFA,XS}$	$f_{SIC,XS}$	$f_{SH2,XS}$	$f_{SIN,XS}$	$f_{SIP,XS}$	$f_{VFA,XS}$	0	0	0	0	0	-1		12
Physical processes																
Oxygen dissolution	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	13
Carbon dioxide stripping/dissolution	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	14
Hydrogen stripping	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	15
Nitrogen stripping	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	16

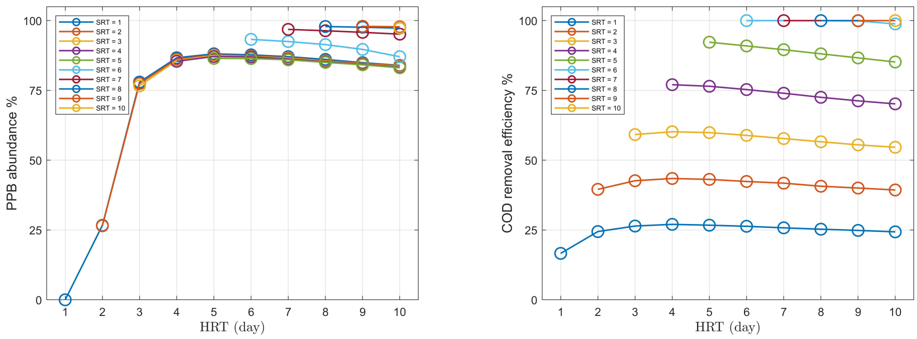

Figure S.1: Effects of HRT and SRT on PPB abundance and COD removal efficiency.

Table S.2: The PBM parameters required for simulation.

Symbol	Definition	Value	Unit
Kinetic parameters			
$\mu_{m,SS,PB,ph}$	Maximal specific phototrophic growth rate of PPB on soluble organics	0.0525	h^{-1}
$\mu_{m,VFA,PB,ph}$	Maximal specific phototrophic growth rate of PPB on volatile fatty acids	0.0783	h^{-1}
$\mu_{m,SS,PB,ch}$	Maximal specific aerobic chemotrophic growth rate of PPB on soluble organic	0.0500	h^{-1}
$\mu_{m,VFA,PB,ch}$	Maximal specific aerobic chemoheterotrophic growth rate of PPB on volatile fatty acids	0.0525	h^{-1}
$\mu_{m,SS,PB,an}$	Maximal specific anerobic chemoheterotrophic growth rate of PPB on soluble organic	0.0124	h^{-1}
$b_{m,PB,dec}$	Specific decay rate of PPB	0.0113	h^{-1}
$\mu_{m,SS,AHB}$	Maximal specific growth rate of AHB on soluble organics	0.0758	h^{-1}
$\mu_{m,VFA,AHB}$	Maximal specific growth rate of AHB on volatile fatty acids	0.0758	h^{-1}
$b_{m,AHB,dec}$	Specific decay rate of AHB	0.0156	h^{-1}
$\mu_{m,SS,AN}$	Maximal specific growth rate of AN on soluble organics	0.0238	h^{-1}
$b_{m,AN,dec}$	Specific decay rate of AN	0.00083	h^{-1}
μ_{hyd}	Hydrolysis rate of suspended solids	0.0035	h^{-1}
$K_{S,E}$	Light half-saturation constant of PPB	3	$W\,m^{-2}$
$K_{I,E}$	Light inhibitory constant for chemotrophic growth of PPB	100	$W\,m^{-2}$
$K_{I,O2,PB}$	Oxygen inhibitory constant for phototrophic growth of PPB	0.7	$mgCODL^{-1}$
$K_{S,O2,PB}$	Oxygen half-saturation constant for chemotrophic growth of PPB	0.05	$mgCODL^{-1}$
$K_{I,O2,AHB}$	Oxygen half-saturation constant for AHB	0.05	$mgCODL^{-1}$
$K_{I,O2,AN}$	Oxygen inhibitory constant for AN	0.05	$mgCODL^{-1}$
$K_{S,SS,ph}$	Soluble organic half-saturation constant for phototrophic growth of PPB	5	$mgCODL^{-1}$
$K_{S,VFA,ph}$	Volatile fatty acid half-saturation constant for phototrophic growth of PPB	20	$mgCODL^{-1}$
$K_{S,SS,ch}$	Soluble organic half-saturation constant for chemotrophic growth of PPB	0.4	$mgCODL^{-1}$
$K_{S,VFA,ch}$	Volatile fatty acid half-saturation constant for chemotrophic growth of PPB	0.4	$mgCODL^{-1}$
$K_{S,SS,an}$	Soluble organic half-saturation constant for anaerobic chemotrophic growth of PPB	5	$mgCODL^{-1}$
$K_{S,SS,AHB}$	Soluble organic half-saturation constant for AHB	5	$mgCODL^{-1}$
$K_{S,VFA,AHB}$	Volatile fatty acid half-saturation constant for AHB	5	$mgCODL^{-1}$
$K_{S,SS,AN}$	Soluble organic half-saturation constant for AN	5	$mgCODL^{-1}$
$K_{S,IN}$	Inorganic nitrogen half-saturation constant	0.005	$mgCODL^{-1}$
$K_{S,IP}$	Inorganic phosphorus half-saturation constant	0.001	$mgCODL^{-1}$
M_S	Metabolic switch	0.28	
Stoichiometric parameters			
$Y_{PB,ph}$	Biomass yield for phototrophic growth of PPB	1.00	$mgCODmgCOD^{-1}$
$Y_{PB,ch}$	Biomass yield for aerobic chemotrophic growth of PPB	0.52	$mgCODmgCOD^{-1}$
$Y_{PB,an}$	Biomass yield for anaerobic chemotrophic growth of PPB	0.197	$mgCODmgCOD^{-1}$
Y_{AHB}	Biomass yield for AHB	0.67	$mgCODmgCOD^{-1}$
Y_{AN}	Biomass yield for AN	0.197	$mgCODmgCOD^{-1}$

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Symbol	Definition	Value	Unit
$f_{IC,ph,SS}$	Stoichiometry of inorganic carbon produced for phototrophic growth of PPB on soluble organics	3.897702e-3	$\mathrm{mgCODmgCOD^{-1}}$
$f_{IC,ph,VFA}$	Stoichiometry of inorganic carbon produced for phototrophic growth of PPB on volatile fatty acids	3.897702e-3	$\mathrm{mgCODmgCOD^{-1}}$
$f_{IC,ch,SS}$	Stoichiometry of inorganic carbon produced for aerobic chemotrophic growth of PPB on soluble organics	0.01400	$\mathrm{mgCODmgCOD^{-1}}$
$f_{IC,ch,VFA}$	Stoichiometry of inorganic carbon produced for aerobic chemotrophic growth of PPB on volatile fatty acids	0.023728	$\mathrm{mgCODmgCOD^{-1}}$
$f_{IC,an,SS}$	Stoichiometry of inorganic carbon produced for anaerobic chemotrophic growth of PPB on soluble organics	-0.02702	$\mathrm{mgCODmgCOD^{-1}}$
$f_{IC,AHB,SS}$	Stoichiometry of inorganic carbon produced for growth of AHB on soluble organics	0.01400	$\mathrm{mgCODmgCOD^{-1}}$
$f_{IC,AHB,VFA}$	Stoichiometry of inorganic carbon produced for growth of AHB on volatile fatty acids	0.023728	$\mathrm{mgCODmgCOD^{-1}}$
$f_{IC,AN,SS}$	Stoichiometry of inorganic carbon produced for growth of AN on soluble organics	-0.02702	$\mathrm{mgCODmgCOD^{-1}}$
$f_{IC,dec}$	Inorganic carbon produced from bacterial biomass decay	-1.984127e-04	$\mathrm{mmolHCO_3-CmgCOD^{-1}}$
$f_{IN,dec}$	Inorganic nitrogen produced from bacterial biomass decay	0.058	$\mathrm{mgNH_3-NmgCOD^{-1}}$
$f_{IP,dec}$	Inorganic phosphorus produced from bacterial biomass decay	0.01	$\mathrm{mgPO_4-PmgCOD^{-1}}$
$f_{SIC,XS}$	Suspended solids produced from hydrolysis	1.303971e-06	$\mathrm{mmolHCO_3-CmgCOD^{-1}}$
$f_{SS,XS}$	Soluble organics produced from hydrolysis	1.638241-01	$\mathrm{mgCODmgCOD^{-1}}$
$f_{SH2,XS}$	Hydrogen produced from hydrolysis	8.442468e-02	$\mathrm{mmolHCO_3-CmgCOD^{-1}}$
$f_{SIN,XS}$	Inorganic nitrogen produced from hydrolysis	1.162246-02	$\mathrm{mgNH_3-NmgCOD^{-1}}$
$f_{SIP,XS}$	Inorganic phosphorus produced from hydrolysis	2.075440e-03	$\mathrm{mgPO_4-PmgCOD^{-1}}$
$f_{SI,XS}$	Inert soluble organics produced from hydrolysis	1.518208e-01	$\mathrm{mgCODmgCOD^{-1}}$
$f_{XI,XS}$	Inert suspended solids produced from hydrolysis	4.330911e-01	$\mathrm{mgCODmgCOD^{-1}}$
$f_{VFA,AN,SS}$	Fraction of VFA produced during acidogenic fermentation	0.7728	$\mathrm{mgCODmgCOD^{-1}}$
$f_{H2,AN}$	Fraction of hydrogen produced during acidogenic fermentation	0.0304	$\mathrm{mgCODmgCOD^{-1}}$
$Y_{N,PB}$	Nitrogen content of PPB	-0.0860	$\mathrm{mgNmgCOD^{-1}}$
$Y_{N,AHB}$	Nitrogen content of AHB	-0.0860	$\mathrm{mgNmgCOD^{-1}}$
$Y_{N,AN}$	Nitrogen content of AN	-0.0860	$\mathrm{mgNmgCOD^{-1}}$
$Y_{P,PB}$	Phosphorus content of PPB	-0.0150	$\mathrm{mgPmgCOD^{-1}}$
$Y_{P,AHB}$	Phosphorus content of AHB	-0.0150	$\mathrm{mgPmgCOD^{-1}}$
$Y_{P,AN}$	Phosphorus content of AN	-0.0150	$\mathrm{mgPmgCOD^{-1}}$
Physico-chemical parameters			
ϵ	Light extinction coefficient	0.07	
σ	Light absorbance and scattering factor	1.15	
S_{E0}	Light intensity	54	$\mathrm{W\,m^{-2}}$
$P_{ka_{CO_2}}$	Acid-base equilibrium coefficient for inorganic carbon	6.37	
$P_{ka_{NH_4}}$	Acid-base equilibrium coefficient for inorganic nitrogen	9.25	
Kla_{O2}	Oxygen gas-liquid transfer coefficient	1	$\mathrm{h^{-1}}$
Kla_{CO2}	Carbon dioxide gas-liquid transfer coefficient	0.0127	$\mathrm{h^{-1}}$
Kla_{NH3}	Ammonia gas-liquid transfer coefficient	0.533186	$\mathrm{h^{-1}}$
Kla_{H2}	Hydrogen gas-liquid transfer coefficient	1.6	$\mathrm{h^{-1}}$
O_2^{sat}	Saturated oxygen	7.85	$\mathrm{mgO_2L^{-1}}$
CO_2^{sat}	Saturated carbon dioxide	0.0127	$\mathrm{mmolHCO_3^-\,L^{-1}}$
NH_3^{sat}	Saturated ammonia	0.533186	$\mathrm{mgNL^{-1}}$

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Symbol	Definition	Value	Unit
H_2^{sat}	Saturated hydrogen	1.6	mgH_2L^{-1}
$f_{O2,PB}$	Oxygen uptake chemoheterotrophy of PPB	$\frac{-(1-Y_{PB,ch})}{Y_{PB,ch}}$	$mgO2mgCOD^{-1}$
$f_{O2,AHB}$	Oxygen uptake chemoheterotrophy of AHB	$\frac{-(1-Y_{AHB})}{Y_{AHB}}$	$mgO2mgCOD^{-1}$
Reactor geometry			
V	Volume	100	L
A	Area	0.5	m
$f_{H/S}$	Fraction of removed particles	$\frac{HRT}{SRT}$	

Table S.3: Different versions of mechanistic models simulating the utilization of PPB in WWT.

Name	PAnM	PBM	ePAnM
Conditions	Anaerobic	Semi-aerobic	Aerobic
Processes	6	16	30
PPB-based	*5*	*6*	*11*
Other biomass	-	*5*	*19*
Hydrolysis	*1*	*1*	*1*
Physical processes	-	*4*	*2*
State variables	10	15	21
PBB-based	*1*	*3*	*1*
Substrate	Acetate Other organics	VFAs Other organics	Acetate Other VFAs Other organics
Biomass	PPB	Photoheterotrophic PPB (An)aerobic chemoheterotrophic PBB Aerobic heterotropic Acidogenic	PBB Aerobic heterotropic Acidogenic Acetogenic Aerobic predators Heterotrophic sulphate reducing bacteria Autotrophic sulphate reducing bacteria Microalgae biomass
PPB metabolisms	Photoheterotrophic Photoautotrophic Anaerobic chemoheterotrophic	Photoheterotrophic (An)aerobic chemoheterotrophic	Photoheterotrophic Photoautotrophic (An)aerobic chemoheterotrophic Fermentative
Inhibition functions	Competitive inhibitions Inorganic nitrogen Inorganic phosphor Free amonia Light	Competitive inhibitions Inorganic nitrogen Inorganic phosphor Photoheterotrophic light Chemoheterotrophic light Photoheterotrophic oxygen Chemoheterotrophic oxygen	Inorganic nitrogen Inorganic phosphor Free amonia Light Oxygen pH Temperature
Physical processes	-	Carbon dioxide dissolution/stripping Oxygen dissolution/stripping Stripping of hydrogen Stripping of ammonium	Carbon dioxide loses Oxygen supply
Operational mode	Continuous	SBR/Constant	Continuous
pH	Dynamic	Constant	Dynamic
Temperature	Constant	Constant	Cardial temperature model
Light	Constant	Lambert-Beer's law	Lambert-Beer's law