

Bio-electrochemical system depollution capabilities and monitoring applications: Models, applicability, advanced bio-based concept for predicting pollutant degradation and microbial growth kinetics via gene regulation modelling

Table S1: Nomenclature and model parameter values of Tsipa et al. model

Symbols	Description	Estimated value	Units
α_{BenB}	BenB degradation and dilution due to cellular volume increase	33.352	h^{-1}
α_{BenRi}	BenRi degradation and dilution due to cellular volume increase	60	h^{-1}
α_{Pm}	mRNA degradation rate of <i>Pm</i>	1.613	h^{-1}
α_{PbenA}	mRNA degradation rate of <i>PbenA</i>	5.583	h^{-1}
α_{PbenR}	mRNA degradation rate of <i>PbenR</i>	5.865	h^{-1}
α_{Pr}	mRNA degradation rate of <i>Pr</i>	2.483	h^{-1}
α_{Ps}	mRNA degradation rate of <i>Ps</i>	2.107	h^{-1}
α_{Pu}	mRNA degradation rate of <i>Pu</i>	2.528	h^{-1}
α_{XylM}	XylM degradation and dilution due to cellular volume increase	60	h^{-1}
α_{XylRi}	XylRi degradation and dilution due to cellular volume increase	60	h^{-1}
α_{XylSi}	XylSi degradation and dilution due to cellular volume increase	6	h^{-1}
α_{XylU}	XylU degradation and dilution due to cellular volume increase	0.056	h^{-1}
β_b	maximum specific growth rate of biomass based on XylM	0.087	h^{-1}
β_{BenB}	translation rate based on <i>PbenA</i> mRNA	9.11×10^2	$mM h^{-1}$
β_{BenRi}	maximal translation rate of BenRi	24.58×10^2	$mM h^{-1}$
β_{PbenA}	maximal mRNA expression of <i>PbenA</i>	52.887	h^{-1}
β_{PbenR}	maximal mRNA expression of <i>PbenR</i>	4.212	h^{-1}
β_{Pm}	maximal expression level of <i>Pm</i>	0.927	h^{-1}
β_{Pr}	maximal expression level of <i>Pr</i>	0.343	h^{-1}
β_{Ps}	maximal expression level of <i>Ps</i>	28.47	h^{-1}
β_{Pu}	maximal expression level of <i>Pu</i>	44.812	h^{-1}
β_{XylM}	translation rate based on <i>Pm</i> mRNA	0.002	$mM h^{-1}$
β_{XylSi}	translation rate based on <i>Ps</i> mRNA	10.69×10^2	$mM h^{-1}$
β_{XylRi}	maximal translation rate of <i>Pr</i> mRNA	5.7×10^2	$mM h^{-1}$
β_{XylU}	translation rate based on <i>Pu</i> mRNA	16.98×10^2	$mM h^{-1}$
$\beta_{XylU,m-xyl}$	maximum <i>m</i> -xylene metabolic quotient based on XylU	0.018	$g_{tol} g_{biomass} h^{-1}$
$\beta_{XylU,tol}$	maximum toluene metabolic quotient based on XylU	0.018	$g_{tol} g_{biomass} h^{-1}$
$K_{BenB,b}$	saturation constant of BenB	19.543	mM
$K_{BenRa,PbenA}$	activation coefficient of <i>PbenA</i> by BenRa	2.02	mM
$K_{BenRa,PbenR}$	activation coefficient of <i>PbenR</i> by BenRa	1.645	mM
$K_{BenRa,Pm}$	activation coefficient of <i>Pm</i> by BenR	9.208	mM
$K_{XylM,b}$	saturation constant of XylM	25.103	mM

K_{XylSi}	activation coefficient of <i>Pm</i> by XylSi	17.984	mM
$K_{XylRa,Ps}$	activation coefficient of <i>Ps</i> by XylRa	5.44	mM
$K_{XylRa,Pu}$	activation coefficient of <i>Pu</i> by XylRa	3.626	mM
K_{XylRi}	repression coefficient of <i>Pr</i>	11.035	mM
$K_{XylU,m-xyl}$	saturation constant for XylU due to <i>m</i> -xylene	3.863	mM
$K_{XylU,tol}$	saturation constant for XylU due to toluene	3.863	mM
MW_{m-xyl}	molecular weight of <i>m</i> -xylene	106.2	g mol ⁻¹
MW_{tol}	molecular weight of toluene	92.14	g mol ⁻¹
$\Gamma_{R,BenR}$	dissociation constant of BenR	53.46	h ⁻¹
$\Gamma_{R,XylS}$	dissociation constant of XylS	37.88	h ⁻¹
$\Gamma_{R,XylR}$	dissociation constant of XylR	4.2 x10 ²	h ⁻¹

Table S2: Parameter values estimated for the double Monod, Mankad and Bungay, SKIP and the sum kinetics with competitive enzymatic interactions models using.

Symbols	Description	Double Monod	Mankad and Bungay	SKIP	Competitive enzymatic interactions	Units
$I_{m-xyl,tol}$	degree of inhibition of <i>m</i> -xylene to toluene	-	-	0.004	-	-
$I_{tol,m-xyl}$	degree of inhibition of toluene to <i>m</i> -xylene	-	-	0.0003	-	-
K_{m-xyl}	saturation constant of <i>m</i> -xylene	0.1	0.7	0.7	0.7	(mM)
K_{tol}	saturation constant of toluene	0.1	0.46	0.035	0.45	(mM)
μ_{max}	maximal specific growth rate	0.033	0.079	-	-	(h ⁻¹)
$\mu_{max,tol}$	maximal specific growth rate of toluene	-	-	0.018	0.097	(h ⁻¹)
$\mu_{max,m-xyl}$	maximal specific growth rate of <i>m</i> -xylene	-	-	0.093	0.042	(h ⁻¹)
Y_{m-xyl}	yield coefficient of <i>m</i> -xylene	0.99	0.99	0.99	0.99	(g/g)
Y_{tol}	yield coefficient of toluene	0.99	0.99	0.99	0.99	(g/g)