

Supporting Information for

An agile benchmarking framework for wastewater resource recovery technologies

Xinyi Zhang^{1*}, Saumitra Rai¹, Zixuan Wang¹, Yalin Li^{2*}, Jeremy S. Guest^{1,3*}

¹ The Grainger College of Engineering, Department of Civil and Environmental Engineering, University of Illinois Urbana-Champaign, 3221 Newmark Civil Engineering Laboratory, Urbana, Illinois, United States of America

² Department of Civil and Environmental Engineering, Rutgers, The State University of New Jersey, Piscataway, New Jersey, United States of America

³ Institute for Sustainability, Energy, and Environment, University of Illinois Urbana-Champaign, Urbana, Illinois, United States of America

*Corresponding authors: xinyiz6@illinois.edu (XZ); yalin.li@rutgers.edu (YL); jsquest@illinois.edu (JSG)

Table S1. Characteristics of different influent wastewater and fractionation assumptions. Low-strength, medium-strength, and high-strength wastewaters are alternatives based on [1].

Unit		Raw wastewater			
		Default	Low strength	Medium strength	High strength
Composite variables					
Q	MGD	10.0	10.0	10.0	10.0
COD	mg·L ⁻¹	358.0	339.0	508.0	1016
BOD	mg·L ⁻¹	172.1	136.4	204.3	408.7
TSS	mg·L ⁻¹	165.4	135.6	203.2	406.5
TN	mg·L ⁻¹	40.0	23.9	34.9	70.7
TP	mg·L ⁻¹	7.0	3.7	5.6	11.0
State variables					
S_{NH_4}	mg-N·L ⁻¹	25.9	14.0	20.0	41.0
S_{PO_4}	mg-P·L ⁻¹	5.0	1.6	2.4	4.7
S_F	mg-COD·L ⁻¹	111.0	81.4	121.9	243.8
S_A	mg-COD·L ⁻¹	8.6	17.0	25.4	50.8
S_I	mg-COD·L ⁻¹	17.9	25.4	38.1	76.2
S_{IC}	mg-C·L ⁻¹	84.0	84.0	84.0	84.0
S_K	mg·L ⁻¹	28.0	11.0	16.0	32.0
S_{Mg}	mg·L ⁻¹	50.0	50.0	50.0	50.0
X_I	mg-COD·L ⁻¹	71.6	101.7	152.4	304.8
X_S	mg-COD·L ⁻¹	148.9	113.6	170.2	340.4
S_{Ca}	mg·L ⁻¹	140.0	140.0	140.0	140.0
S_{Na}	mg·L ⁻¹	87.0	87.0	87.0	87.0
S_{Cl}	mg·L ⁻¹	425.0	39.0	59.0	118.0
COD fractionation					
S_F	-	0.31	0.24	0.24	0.24
S_A	-	0.024	0.05	0.05	0.05
S_I	-	0.05	0.075	0.075	0.075
X_S	-	0.416	0.335	0.335	0.335
X_I	-	0.2	0.3	0.3	0.3
Nitrogen content					
S_F, X_S	g N·g ⁻¹ COD	0.03352	0.023464	0.023464	0.023464
S_I, X_I	g N·g ⁻¹ COD	0.06003	0.042021	0.042021	0.042021
X_H, X_{PAO}, X_{AUT}	g N·g ⁻¹ COD	0.08615	0.060305	0.060305	0.060305
Phosphorus content					
S_F, X_S	g P·g ⁻¹ COD	0.00559	0.006149	0.006149	0.006149
S_I, X_I	g P·g ⁻¹ COD	0.00649	0.007139	0.007139	0.007139
X_H, X_{PAO}, X_{AUT}	g P·g ⁻¹ COD	0.02154	0.002369	0.002369	0.002369
COD-to-mass ratio					
X_S, X_I	g mass·g ⁻¹ COD	0.75	0.63	0.63	0.63

Table S2. Default parameter values in *MetalDosage* model.

Symbol	Description	Value		Unit
		S_F	S_I	
F_{min}	Minimum metal consumption per unit soluble component	4	4	g Me·g ⁻¹ COD
F_{max}	Maximum metal consumption per unit soluble component	20	20	g Me·g ⁻¹ COD
k_a	Affinity factor for coagulation	0.5	0.5	m ³ ·g ⁻¹
f_{col}	Colloidal fraction of soluble component [†]	0.48	-	-

[†] Only a fraction of soluble organic substrate (S_F) is assumed to be colloidal and removable by coagulation/flocculation. The default colloidal fraction is consistent with the assumptions on raw wastewater composition in [2].

Table S3. *mASM2d* model state variables and default properties in QSDsan, including the way in which each component is measured in the model (“Measured As”), the elemental contents (i.e., C, N, P, COD), and i_{mass} relevant for the estimation of TSS. All default elemental compositions are consistent with assumptions in [3].

	Description	Measured As	i_{COD}	i_C	i_N	i_P	i_{mass}
g·(g “measured-as”)⁻¹							
S_{O_2}	Dissolved oxygen gas	O ₂	-1	0	0	0	1
S_{N_2}	Dissolved nitrogen gas	N ₂	-1.71	0	1	0	1
S_{NH_4}	Ammonium	N	0	0	1	0	1.288
S_{NO_3}	Nitrate	N	-4.57	0	1	0	4.427
S_{PO_4}	Orthophosphate	P	0	0	0	1	3.099
S_F	Fermentable substrate	COD	1	0.318	0.03352	0.00559	0.75
S_A	Acetate	COD	1	0.375	0	0	0.923
S_I	Soluble inert organic materials	COD	1	0.362	0.06003	0.00649	0.75
S_{IC}	Total inorganic C in forms of HCO ₃ ⁻	C	0	1	0	0	5.080
S_K	Potassium	K	0	0	0	0	1
S_{Mg}	Magnesium	Mg	0	0	0	0	1
X_I	Particulate inert organic materials	COD	1	0.362	0.06003	0.00649	0.75
X_S	Slowly biodegradable substrate	COD	1	0.318	0.03352	0.00559	0.75
X_H	Heterotrophic biomass	COD	1	0.366	0.08615	0.02154	0.9
X_{PAO}	Phosphorus-accumulating organisms	COD	1	0.366	0.08615	0.02154	0.9
X_{PP}	Polyphosphate (K _{0.33} Mg _{0.33} PO ₃) _n	P	0	0	0	1	3.225
X_{PHA}	Poly-β-hydroxyalkanoates	COD	1	0.3	0	0	0.55
X_{AUT}	Autotrophic biomass	COD	1	0.366	0.08615	0.02154	0.9
S_{Ca}	Calcium	Ca	0	0	0	0	1
X_{CaCO_3}	Calcite	CaCO ₃	0	0.120	0	0	1
X_{struv}	Struvite	NH ₄ MgPO ₄	0	0	0.05708	0.12621	1
X_{newb}	Newberyite	MgHPO ₄	0	0	0	0.17767	1
X_{ACP}	Amorphous calcium phosphate	Ca ₃ (PO ₄) ₂	0	0	0	0.19972	1
X_{MgCO_3}	Magnesite	MgCO ₃	0	0.142	0	0	1
X_{AlOH}	Aluminum hydroxide	Al(OH) ₃	0	0	0	0	1
X_{AlPO_4}	Aluminum phosphate	AlPO ₄	0	0	0	0.25398	1
X_{FeOH}	Iron hydroxide	Fe(OH) ₃	0	0	0	0	1
X_{FePO_4}	Iron phosphate	FePO ₄	0	0	0	0.20537	1
S_{Na}	Sodium, proxy for cations	Na	0	0	0	0	1
S_{Cl}	Chloride, proxy for anions	Cl	0	0	0	0	1

Table S4. Kinetic rate expressions in *mASM2d*, based on modifications by [3].

Process	Kinetic rate expression
Aerobic hydrolysis	$K_h \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{\frac{X_S}{X_H}}{K_X + \frac{X_S}{X_H}} \cdot X_H$
Anoxic hydrolysis	$K_h \cdot \eta_{NO_3} \cdot \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \cdot \frac{\frac{X_S}{X_H}}{K_X + \frac{X_S}{X_H}} \cdot X_H$
Anaerobic hydrolysis	$K_h \cdot \eta_{fe} \cdot \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \cdot \frac{\frac{X_S}{X_H}}{K_X + \frac{X_S}{X_H}} \cdot X_H$
X_H aerobic growth on S_F	$\mu_H \cdot \frac{S_{O_2}}{K_{O_2,H} + S_{O_2}} \cdot \frac{S_F}{K_F + S_F} \cdot \frac{S_F}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4,H} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_{P,H} + S_{PO_4}} \cdot X_H$
X_H aerobic growth on S_A	$\mu_H \cdot \frac{S_{O_2}}{K_{O_2,H} + S_{O_2}} \cdot \frac{S_A}{K_{A,H} + S_A} \cdot \frac{S_A}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4,H} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_{P,H} + S_{PO_4}} \cdot X_H$
Denitrification with S_F	$\mu_H \cdot \eta_{NO_3,H} \cdot \frac{K_{O_2,H}}{K_{O_2,H} + S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3,H} + S_{NO_3}} \cdot \frac{S_F}{K_F + S_F} \cdot \frac{S_F}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4,H} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_{P,H} + S_{PO_4}} \cdot X_H$
Denitrification with S_A	$\mu_H \cdot \eta_{NO_3,H} \cdot \frac{K_{O_2,H}}{K_{O_2,H} + S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3,H} + S_{NO_3}} \cdot \frac{S_A}{K_{A,H} + S_A} \cdot \frac{S_A}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4,H} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_{P,H} + S_{PO_4}} \cdot X_H$
Fermentation	$q_{fe} \cdot \frac{K_{O_2,H}}{K_{O_2,H} + S_{O_2}} \cdot \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \cdot \frac{S_F}{K_{fe} + S_F} \cdot X_H$
Lysis of X_H	$b_H \cdot \left(\frac{S_{O_2}}{K_{O_2,H} + S_{O_2}} + \eta_{NO_3,H,l} \cdot \frac{K_{O_2,H}}{K_{O_2,H} + S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3,H} + S_{NO_3}} \right) \cdot X_H$
Storage of X_{PHA}	$q_{PHA} \cdot \frac{S_A}{K_{A,PAO} + S_A} \cdot \frac{\frac{X_{PP}}{X_{PAO}}}{K_{PP} + \frac{X_{PP}}{X_{PAO}}} \cdot X_{PAO}$
Aerobic storage of X_{PP}	$q_{PP} \cdot \frac{S_{O_2}}{K_{O_2,PAO} + S_{O_2}} \cdot \frac{S_{PO_4}}{K_{PS} + S_{PO_4}} \cdot \frac{\frac{X_{PHA}}{X_{PAO}}}{K_{PHA} + \frac{X_{PHA}}{X_{PAO}}} \cdot \frac{K_{MAX} - \frac{X_{PP}}{X_{PAO}}}{K_{IPP} + K_{MAX} - \frac{X_{PP}}{X_{PAO}}} \cdot X_{PAO}$
Anoxic storage of X_{PP}	$q_{PP} \cdot \eta_{NO_3,PAO} \cdot \frac{K_{O_2,PAO}}{K_{O_2,PAO} + S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3,PAO} + S_{NO_3}} \cdot \frac{S_{PO_4}}{K_{PS} + S_{PO_4}} \cdot \frac{\frac{X_{PHA}}{X_{PAO}}}{K_{PHA} + \frac{X_{PHA}}{X_{PAO}}} \cdot \frac{K_{MAX} - \frac{X_{PP}}{X_{PAO}}}{K_{IPP} + K_{MAX} - \frac{X_{PP}}{X_{PAO}}} \cdot X_{PAO}$
X_{PAO} aerobic growth on X_{PHA}	$\mu_{PAO} \cdot \frac{S_{O_2}}{K_{O_2,PAO} + S_{O_2}} \cdot \frac{S_{NH_4}}{K_{NH_4,PAO} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_{P,PAO} + S_{PO_4}} \cdot \frac{\frac{X_{PHA}}{X_{PAO}}}{K_{PHA} + \frac{X_{PHA}}{X_{PAO}}} \cdot X_{PAO}$
X_{PAO} anoxic growth on X_{PHA}	$\mu_{PAO} \cdot \eta_{NO_3,PAO} \cdot \frac{K_{O_2,PAO}}{K_{O_2,PAO} + S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3,PAO} + S_{NO_3}} \cdot \frac{S_{NH_4}}{K_{NH_4,PAO} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_{P,PAO} + S_{PO_4}} \cdot \frac{\frac{X_{PHA}}{X_{PAO}}}{K_{PHA} + \frac{X_{PHA}}{X_{PAO}}} \cdot X_{PAO}$
Lysis of X_{PAO}	$b_{PAO} \cdot \left(\frac{S_{O_2}}{K_{O_2,PAO} + S_{O_2}} + \eta_{NO_3,PAO,l} \cdot \frac{K_{O_2,PAO}}{K_{O_2,PAO} + S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3,PAO} + S_{NO_3}} \right) \cdot X_{PAO}$
Lysis of X_{PP}	$b_{PP} \cdot \left(\frac{S_{O_2}}{K_{O_2,PAO} + S_{O_2}} + \eta_{NO_3,PP,l} \cdot \frac{K_{O_2,PAO}}{K_{O_2,PAO} + S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3,PAO} + S_{NO_3}} \right) \cdot X_{PP}$
Lysis of X_{PHA}	$b_{PHA} \cdot \left(\frac{S_{O_2}}{K_{O_2,PAO} + S_{O_2}} + \eta_{NO_3,PHA,l} \cdot \frac{K_{O_2,PAO}}{K_{O_2,PAO} + S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3,PAO} + S_{NO_3}} \right) \cdot X_{PHA}$

Table S4 (cont.). Kinetic rate expressions in *mASM2d*, based on modifications by [3].

Process	Kinetic rate expression
Aerobic growth of X_{AUT}	$\mu_{AUT} \cdot \frac{S_{O_2}}{K_{O_2,AUT} + S_{O_2}} \cdot \frac{S_{NH_4}}{K_{NH_4,AUT} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_{P,AUT} + S_{PO_4}} \cdot X_{AUT}$
Lysis of X_{AUT}	$b_{AUT} \cdot \left(\frac{S_{O_2}}{K_{O_2,AUT} + S_{O_2}} + \eta_{NO_3,AUT,l} \cdot \frac{K_{O_2,AUT}}{K_{O_2,AUT} + S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3,AUT} + S_{NO_3}} \right) \cdot X_{AUT}$
X_{AlPO_4} precipitation & redissolution	$k_{PRE,Al} \cdot S_{PO_4} \cdot X_{AlOH} - k_{RED} \cdot X_{AlPO_4} \cdot I_{alk}$
X_{FePO_4} precipitation & redissolution	$k_{PRE,Fe} \cdot S_{PO_4} \cdot X_{FeOH} - k_{RED} \cdot X_{FePO_4} \cdot I_{alk}$

$$I_{alk} = \frac{S_{ALK}}{S_{ALK} + K_{ALK,PRE}}, S_{ALK} = [CO_3^{2-}] \times 2 + [HCO_3^-]$$

Relative abundances of carbonic species (H_2CO_3 , HCO_3^- , CO_3^{2-}) are determined by pH, which by default is assumed to be constant at 7. pH can also be user-specified or estimated at each time step as a function of wastewater composition.

Table S5. New kinetic parameters in *mASM2d*. All default values below are taken from [3]. Typical values at 20°C for kinetic parameters in the original ASM2d [4] are taken as default values in *mASM2d*.

Symbol	Description	Default value	Unit
$\eta_{NO_3,H,l}$	Reduction factor for anoxic lysis of heterotrophs	0.5	-
$\eta_{NO_3,PAO,l}$	Reduction factor for anoxic lysis of PAO	0.33	-
$\eta_{NO_3,PP,l}$	Reduction factor for anoxic lysis of PP	0.33	-
$\eta_{NO_3,PHA,l}$	Reduction factor for anoxic lysis of PHA	0.33	-
$\eta_{NO_3,AUT,l}$	Reduction factor for anoxic lysis of autotrophs	0.33	-
$K_{NO_3,AUT}$	Half saturation coefficient for S_{NO_3} for autotroph lysis	0.5	mg N·L ⁻¹
$k_{PRE,Fe}$	Precipitation rate constant for FePO ₄	1.0	m ³ ·g ⁻¹ Fe(OH) ₃ ·d ⁻¹
$k_{PRE,Al}$	Precipitation rate constant for AlPO ₄	1.37	m ³ ·g ⁻¹ Al(OH) ₃ ·d ⁻¹

Table S6. *ADM1p* model state variables and default properties in QSDsan. Omitted in this list are S_K , S_{Mg} , S_{Ca} , X_{CaCO_3} , X_{struv} , X_{newb} , X_{ACP} , X_{MgCO_3} , X_{AlOH} , X_{AlPO_4} , X_{FeOH} , X_{FePO_4} , S_{Na} , and S_{Cl} , which are identical to the ones in *mASM2d* (Table S3). All default elemental compositions are consistent with assumptions in [3].

	Description	Measured As	i_{COD}	i_C	i_N	i_P	i_{mass}
g·(g “measured-as”)⁻¹							
S_{su}	Monosaccharides	COD	1	0.375	0	0	0.938
S_{aa}	Amino acids	COD	1	0.369	0.11065	0	0.738
S_{fa}	Long-chain fatty acids (LCFAs)	COD	1	0.257	0	0	0.348
S_{va}	Valerate	COD	1	0.289	0	0	0.491
S_{bu}	Butyrate	COD	1	0.3009	0	0	0.544
S_{pro}	Propionate	COD	1	0.322	0	0	0.652
S_{ac}	Acetate	COD	1	0.375	0	0	0.923
S_{h2}	Dissolved hydrogen gas	COD	1	0	0	0	0.126
S_{ch4}	Dissolved methane gas	COD	1	0.188	0	0	0.251
S_{IC}	Total inorganic C in forms of CO ₂	C	0	1	0	0	3.664
S_{IN}	Inorganic N in forms of NH ₄ ⁺	N	0	0	1	0	1.216
S_{IP}	Inorganic P in forms of orthophosphate	P	0	0	0	1	3.099
S_I	Soluble inert organic materials	COD	1	0.362	0.06003	0.00649	0.75
X_{ch}	Carbohydrates	COD	1	0.375	0	0	0.868
X_{pr}	Proteins	COD	1	0.369	0.11065	0	0.738
X_{li}	Lipids	P	1	0.263	0	0.01066	0.348
X_{su}	Sugar degraders	COD	1	0.366	0.08615	0.02154	0.9
X_{aa}	Amino acid degraders	COD	1	0.366	0.08615	0.02154	0.9
X_{fa}	LCFA degraders	COD	1	0.366	0.08615	0.02154	0.9
X_{c4}	Valerate and butyrate degraders	COD	1	0.366	0.08615	0.02154	0.9
X_{pro}	Propionate degraders	COD	1	0.366	0.08615	0.02154	0.9
X_{ac}	Acetate degraders	COD	1	0.366	0.08615	0.02154	0.9
X_{h2}	Hydrogen degraders	COD	1	0.366	0.08615	0.02154	0.9
X_I	Particulate inert organic materials	COD	1	0.362	0.06003	0.00649	0.75
X_{PHA}	Poly-β-hydroxyalkanoates	COD	1	0.300	0	0	0.55
X_{PP}	Polyphosphate (K _{0.33} Mg _{0.33} PO ₃) _n	P	0	0	0	1	3.225
X_{PAO}	Phosphorus-accumulating organisms	COD	1	0.366	0.08615	0.02154	0.9

Table S7. Stoichiometries of ADM1 biological processes in ADM1p. i_C , i_N , and i_P data from **Table S6** are used to solve for unknown stoichiometric coefficients “?” in each process based on mass conservations of carbon, nitrogen, and phosphorus, respectively. f_B^A [-] indicates the fraction of product B from the degradation of substrate A .

	S_{su}	S_{aa}	S_{fa}	S_{va}	S_{bu}	S_{pro}	S_{ac}	S_{h2}	S_{ch4}	S_{IC}	S_{IN}	S_{IP}	S_I	X_{ch}	X_{pr}	X_{li}	X_{su}	X_{aa}	X_{fa}	X_{c4}	X_{pro}	X_{ac}	X_{h2}	X_I
X_{ch} hydrolysis	1									?	?	?		-1										
X_{pr} hydrolysis		1								?	?	?			-1									
X_{li} hydrolysis	$1-f_{fa}^{li}$		f_{fa}^{li}							?	?	?				-1								
S_{su} uptake	-1				$f_{bu}^{su}(1-Y_{su})$	$f_{pro}^{su}(1-Y_{su})$	$f_{ac}^{su}(1-Y_{su})$	$f_{h2}^{su}(1-Y_{su})$?	?	?					Y_{su}							
S_{aa} uptake		-1		$f_{va}^{aa}(1-Y_{aa})$	$f_{bu}^{aa}(1-Y_{aa})$	$f_{pro}^{aa}(1-Y_{aa})$	$f_{ac}^{aa}(1-Y_{aa})$	$f_{h2}^{aa}(1-Y_{aa})$?	?	?						Y_{aa}						
S_{fa} uptake			-1				$f_{ac}^{fa}(1-Y_{fa})$	$f_{h2}^{fa}(1-Y_{fa})$?	?	?							Y_{fa}					
S_{va} uptake				-1		$f_{pro}^{va}(1-Y_{c4})$	$f_{ac}^{va}(1-Y_{c4})$	$f_{h2}^{va}(1-Y_{c4})$?	?	?								Y_{c4}				
S_{bu} uptake					-1		$f_{ac}^{bu}(1-Y_{c4})$	$f_{h2}^{bu}(1-Y_{c4})$?	?	?								Y_{c4}				
S_{pro} uptake						-1	$f_{ac}^{pro}(1-Y_{c4})$	$f_{h2}^{pro}(1-Y_{c4})$?	?	?									Y_{pro}			
S_{ac} uptake							-1		$1-Y_{ac}$?	?	?										Y_{ac}		
S_{h2} uptake								-1	$1-Y_{h2}$?	?	?											Y_{h2}	
X_{su} decay										?	?	?	f_{sl}^{xb}	f_{ch}^{xb}	f_{pr}^{xb}	f_{li}^{xb}	-1							f_{xl}^{xb}
X_{aa} decay										?	?	?	f_{sl}^{xb}	f_{ch}^{xb}	f_{pr}^{xb}	f_{li}^{xb}		-1						f_{xl}^{xb}
X_{fa} decay										?	?	?	f_{sl}^{xb}	f_{ch}^{xb}	f_{pr}^{xb}	f_{li}^{xb}			-1					f_{xl}^{xb}
X_{c4} decay										?	?	?	f_{sl}^{xb}	f_{ch}^{xb}	f_{pr}^{xb}	f_{li}^{xb}				-1				f_{xl}^{xb}
X_{pro} decay										?	?	?	f_{sl}^{xb}	f_{ch}^{xb}	f_{pr}^{xb}	f_{li}^{xb}					-1			f_{xl}^{xb}
X_{ac} decay										?	?	?	f_{sl}^{xb}	f_{ch}^{xb}	f_{pr}^{xb}	f_{li}^{xb}						-1		f_{xl}^{xb}
X_{h2} decay										?	?	?	f_{sl}^{xb}	f_{ch}^{xb}	f_{pr}^{xb}	f_{li}^{xb}							-1	f_{xl}^{xb}

Table S8. Stoichiometries and kinetic rate expressions of extended processes in ADM1p [5]. Unknown stoichiometric coefficients “?” in each process are determined by mass conservations of carbon, nitrogen, and phosphorus.

	S_{va}	S_{bu}	S_{pro}	S_{ac}	S_{IC}	S_{IN}	S_{IP}	S_I	X_{ch}	X_{pr}	X_{li}	X_I	X_{PHA}	X_{PP}	X_{PAO}	S_K	S_{Mg}	Kinetic rate expression	
S_{va} storage in X_{PHA}	-1				?	?	?					1	$-Y_{PO4}$			$Y_{PO4} \cdot K_{XPP}$	$Y_{PO4} \cdot Mg_{XPP}$	$q_{PHA} \cdot \frac{S_{VFA,i}}{K_A + S_{VFA,i}} \cdot \frac{X_{PP}}{X_{PAO} \cdot K_{PP} + \frac{X_{PP}}{X_{PAO}}} \cdot X_{PAO} \cdot \frac{S_{VFA,i}}{\sum_i S_{VFA,i}},$ $S_{VFA,i} \in \{S_{va}, S_{bu}, S_{pro}, S_{ac}\}$	
S_{bu} storage in X_{PHA}		-1			?	?	?					1	$-Y_{PO4}$			$Y_{PO4} \cdot K_{XPP}$	$Y_{PO4} \cdot Mg_{XPP}$		
S_{pro} storage in X_{PHA}			-1		?	?	?					1	$-Y_{PO4}$			$Y_{PO4} \cdot K_{XPP}$	$Y_{PO4} \cdot Mg_{XPP}$		
S_{ac} storage in X_{PHA}				-1	?	?	?					1	$-Y_{PO4}$			$Y_{PO4} \cdot K_{XPP}$	$Y_{PO4} \cdot Mg_{XPP}$		
X_{PAO} lysis					?	?	?	f_{sl}^{xb}	f_{ch}^{xb}	f_{pr}^{xb}	f_{li}^{xb}	f_{xl}^{xb}			-1			$b_{PAO}X_{PAO}$	
X_{PP} lysis					?	?	?							-1		K_{XPP}	Mg_{XPP}	$b_{PP}X_{PP}$	
X_{PHA} lysis	f_{va}^{PHA}	f_{bu}^{PHA}	f_{pro}^{PHA}	f_{ac}^{PHA}	?	?	?						-1					$b_{PHA}X_{PHA}$	

Table S9. New stoichiometric and kinetic parameters in *ADM1p*. All default values are taken from [5]. Typical values at 35°C for kinetic parameters in the original ADM1 [6] are taken as default values in *ADM1p*.

Symbol	Description	Default value	Unit
f_{sl}^{xb}	Fraction of soluble inerts from biomass	0	-
f_{ch}^{xb}	Fraction of carbohydrates from biomass	0.275	-
f_{pr}^{xb}	Fraction of proteins from biomass	0.275	-
f_{li}^{xb}	Fraction of lipids from biomass	0.350	-
f_{xl}^{xb}	Fraction of particulate inerts from biomass	0.1	-
$K_{S,IP}$	Half saturation coefficient of S_{IP} as a nutrient [†]	6.2×10^{-4}	kg P·m ⁻³
f_{va}^{PHA}	Yield of valerate on PHA	0.10	kg COD·(kg COD) ⁻¹
f_{bu}^{PHA}	Yield of butyrate on PHA	0.10	kg COD·(kg COD) ⁻¹
f_{pro}^{PHA}	Yield of propionate on PHA	0.40	kg COD·(kg COD) ⁻¹
f_{ac}^{PHA}	Yield of acetate on PHA	0.40	kg COD·(kg COD) ⁻¹
Y_{PO4}	PP requirement per PHA stored	0.40	kg P·(kg COD) ⁻¹
K_{XPP}	Potassium content of PP	0.417	kg K·(kg X_{PP} -P) ⁻¹
Mg_{XPP}	Magnesium content of PP	0.259	kg Mg·(kg X_{PP} -P) ⁻¹
q_{PHA}	PHA storage rate constant	3.0	kg COD·(kg COD) ⁻¹ ·d ⁻¹
K_A	Saturation coefficient for VFAs	0.004	kg COD·m ⁻³
K_{PP}	Saturation coefficient for PP	0.01	kg X_{PP} -P·(kg X_{PAO} -COD) ⁻¹
b_{PAO}	Lysis rate of PAOs	0.20	d ⁻¹
b_{PP}	Lysis rate of PP	0.20	d ⁻¹
b_{PHA}	Lysis rate of PHA	0.20	d ⁻¹

[†] An inhibition term, $S_{IP}/(K_{S,IP} + S_{IP})$, is applied to the kinetic rate expressions of acidogenesis, acetogenesis, and methanogenesis processes

***mASM2d* ↔ *ADM1p* interface models**

Interface models *mASM2dtoAMD1p* and *AMD1ptomASM2d* are implemented in QSDsan to perform state variable conversion from *mASM2d* to *ADM1p* and reverse. Both implementations generally follow model A1 from [5] with minor modifications to improve the numerical stability. In summary, *mASM2dtoAMD1p* performs eight steps:

- 1) Instantaneous depletion of S_{O_2} for aerobic heterotrophic growth, using S_A , then S_F , and lastly X_S as substrates, following *mASM2d* stoichiometries. By default, S_F and X_S have identical compositions. If S_A and S_F combined is insufficient for complete consumption of S_{O_2} , X_S is assumed to be hydrolyzed into S_F instantaneously to allow S_{O_2} depletion.
- 2) Instantaneous depletion of S_{NO_3} for denitrification, using S_A , then S_F , and lastly X_S as substrates.
- 3) Conversion of any S_F left to S_{aa} and S_{su} . COD and N are conserved, with S_{NH_4} serving as a potential source or sink of N.
- 4) Instantaneous decay of X_H and X_{AUT} to form S_I , X_{ch} , X_{pr} , X_{li} , and X_I according to *ADM1p* biomass decay stoichiometry. By default, all biomass components in *mASM2d* and *ADM1p* have identical compositions.
- 5) Conversion of any X_S left to X_{pr} , X_{ch} , and X_{li} . COD, C, N, and P are conserved using S_{IC} , S_{NH_4} , and S_{PO_4} as sources or sinks of corresponding elements when needed.
- 6) Direct mappings from S_A , S_{IC} , S_{NH_4} , and S_{PO_4} to S_{ac} , S_{IC} , S_{IN} , and S_{IP} , respectively.
- 7) Immediate mappings of S_I , X_I , X_{PHA} , X_{PP} , X_{PAO} , S_K , S_{Mg} , S_{Ca} , X_{CaCO_3} , X_{struv} , X_{newb} , X_{ACP} , X_{MgCO_3} , X_{AlOH} , X_{AlPO_4} , X_{FeOH} , X_{FePO_4} , S_{Na} , and S_{Cl} between two models.
- 8) Resolve any negative value in S_{IC} , S_{IN} , or S_{IP} by dissolving relevant minerals proportionally to their relative abundances.

Similarly, *AMD1ptomASM2d* has 8 steps:

- 1) Instantaneous decay of X_{su} , X_{aa} , X_{fa} , X_{C4} , X_{pro} , X_{ac} , X_{h2} , X_{PAO} , X_{PHA} , and X_{PP} according to *ADM1p* stoichiometries.
- 2) Instantaneous stripping of S_{h2} and S_{ch4} .
- 3) Conversion of X_{pr} , X_{ch} , and X_{li} to X_S using S_{IC} , S_{IN} , and S_{IP} as sources or sinks of C, N, and P, respectively, when needed.
- 4) Conversion of S_{aa} , S_{fa} , and S_{su} to S_F using S_{IC} , S_{IN} , and S_{IP} as sources or sinks of C, N, and P, respectively, when needed.
- 5) Conversion of S_{ac} , S_{pro} , S_{bu} , and S_{va} to S_A using S_{IC} for C conservation.
- 6) Direct mappings from S_{IC} , S_{IN} , and S_{IP} to S_{IC} , S_{NH_4} , and S_{PO_4} , respectively.
- 7) Immediate mappings of S_I , X_I , X_{PHA} , X_{PP} , X_{PAO} , S_K , S_{Mg} , S_{Ca} , X_{CaCO_3} , X_{struv} , X_{newb} , X_{ACP} , X_{MgCO_3} , X_{AlOH} , X_{AlPO_4} , X_{FeOH} , X_{FePO_4} , S_{Na} , and S_{Cl} between two models.
- 8) Resolve any negative value in S_{IC} , S_{NH_4} , or S_{PO_4} by dissolving minerals proportionally to their relative abundances.

Table S10. Comparative summary of processes included in different models.

	ASM2d	<i>mASM2d</i>	ADM1	<i>ADM1p</i>	mantis3	Sumo2	ASDM
Simulation platform	all	QSDsan	all	QSDsan	GPS-X™	SUMO	BioWin
Hydrolysis	√	√	√	√	√	√	√
Fermentation	√	√	√	√	√	√	√
Anoxic methylotrophs					√	√	√
Algal photosynthesis						√	
Nitrification/denitrification	1-step	1-step			2-step	2-step	2-step
Anammox					√	√	√
N ₂ O gas production					√		√
PAO	√	√		√	√	√	√
GAO						√	
Methanogenesis			√	√	√	√	√
P precipitation with metal hydroxides	√	√		√	√	√	√
Mineral precipitation		Optional [†]		CaCO ₃ , ACP, MgCO ₃ , struvite, newberyite	CaCO ₃ , ACP, MgCO ₃ , struvite, newberyite	CaCO ₃ , ACP, brushite, struvite, vivianite	HDP, HAP, struvite
Alkalinity	√	√			√		√
Alkalinity inhibition on biological growth	√						
Temperature dependency			√	√	√	√	√
pH		√	√	√	√	√	√
pH inhibition			√	√			√
Liquid-gas transfer		√	√	√	√	√	√

[†] Mineral precipitation is by default enabled in the aerobic digesters across benchmark configurations, using the kinetic expressions by Kazadi Mbamba *et al.* [7,8].

Table S11. Default design and operational settings for benchmark configurations.

See attached Excel file.

Table S12. Corresponding alphanumeric coding systems of WRRF configurations. DOE liquid code uses a * prefix to indicate the presence of primary treatment and a “-p” suffix for chemical phosphorus removal in a configuration. Certain liquid treatment trains do not have a DOE code. WERF liquid code uses “-P” suffix for “prime” to indicate a variation on the mainstream process, unrelated to the standalone “P” liquid treatment train.

	WERF code (Tarallo et al. [2] and this study)	DOE code (El Abbadi et al. [9])
Liquid code	A	
	B	*A
	C	A
	O	*B
	D	*C
	E	E
	E-P	*E
	F	*E
	P	
	G	*G
	H	*G-p
	I	F
	N	D or *D
	N-P	D or *D
	L	
	M	
Solid code	1	1
	1E	1e
	2	3
	3	4
	4	2
	5	5
	6	6

DiffusedAeration algorithm

$k_L a$ = Oxygen mass transfer coefficient at field condition [d^{-1}]

$$k_L a = \alpha \cdot F \cdot \theta^{T_{water}-T_{20}} \cdot k_L a_{20}$$

T_{water} = water temperature [K]

α = wastewater correction factor, unitless

F = diffuser fouling factor, unitless

θ = temperature correction factor, unitless

$k_L a_{20}$ = Oxygen mass transfer coefficient [d^{-1}] at standard condition (20°C, clean water, new diffuser)

$$k_L a_{20} = \frac{SOTR}{V \cdot \delta \cdot DO_{sat,20}}$$

V = reactor volume [m^3]

$DO_{sat,20}$ = surface DO saturation concentration [$mg \cdot L^{-1}$] at standard condition (20°C, 1 atm, clean water)

δ = depth correction factor, unitless

$$\delta(d_{sub}) = \begin{cases} 1 + 0.03858 \times d_{sub} & \text{fine pore} \\ 0.99 + 0.0291 \times d_{sub} & \text{coarse bubble} \end{cases}$$

d_{sub} = diffuser submergence depth [m]

$SOTR$ = standard oxygen transfer rate [$g \cdot d^{-1}$]

$$SOTR = \frac{Q_{air}}{f} \cdot CF_1 \cdot SOTE$$

Q_{air} = air flowrate at field condition [$m^3 \cdot d^{-1}$]

CF_1 = oxygen gas content in standard air [$g \text{ O}_2 \cdot m^{-3} \text{ air}$]

$SOTE$ = standard oxygen transfer efficiency, unitless

f = air flowrate correction factor, unitless

$$f = \frac{T_{air}}{T_{20}} \cdot \exp\left(\frac{M_{air} \cdot g \cdot h}{R \cdot T_{air} \cdot 10^3}\right)$$

T_{air} = air temperature [K]

$T_{20} = 293.15$ [K], i.e., 20°C

M_{air} = molecular weight of dry air [$g \cdot mol^{-1}$]

g = gravitational acceleration [$m \cdot s^{-2}$]

R = universal gas constant [$J \cdot mol^{-1} \cdot K^{-1}$]

h = diffuser elevation [m]

$$\therefore k_L a = \frac{\alpha F \theta^{T_{water}-T_{20}} \cdot SOTE \cdot CF_1}{\frac{T_{air}}{T_{20}} \cdot \exp\left(\frac{M_{air} g h}{R T_{air} \cdot 10^3}\right) \cdot \delta(d_{sub}) \cdot DO_{sat,20}} \cdot \frac{Q_{air}}{V}$$

where g , R , T_{20} are constants, T_{air} , T_{water} , V , h , d_{sub} are system-specific model inputs, and α , F , θ , $SOTE$, M_{air} , $DO_{sat,20}$, CF_1 are user-specified parameters.

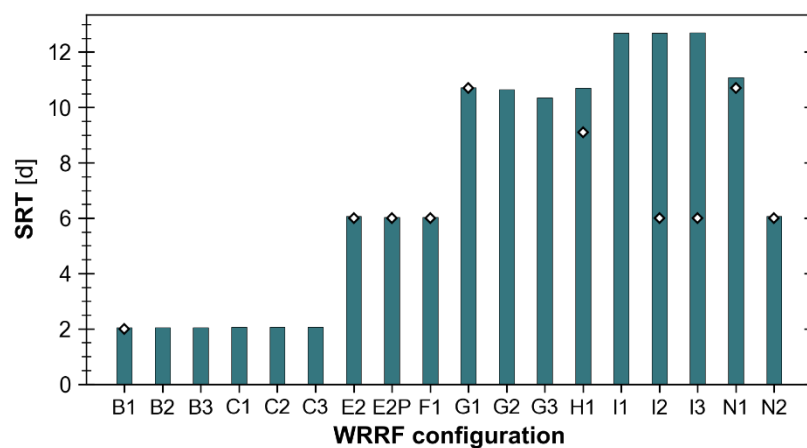


Figure S2. Steady-state SRTs of secondary treatment across benchmark configurations. Vertical bars represent simulations with QSDsan (this study). Diamond markers represent simulations with the original GPS-X models by Tarallo *et al.* [2].

References

1. Metcalf & Eddy, Inc. Wastewater Engineering: Treatment and Resource Recovery [Internet]. 5th ed. NY, UNITED STATES: McGraw-Hill Higher Education; 2013 [cited 2025 Feb 23]. Available from: <http://ebookcentral.proquest.com/lib/uiuc/detail.action?docID=5662641>
2. Tarallo S, Shaw A, Kohl P, Eschborn R. A Guide to Net-Zero Energy Solutions for Water Resource Recovery Facilities [Internet]. The Water Environment Research Foundation; 2015 Aug [cited 2024 Oct 29]. Available from: <https://iwaponline.com/ebooks/book/293/>
3. Solon K, Flores-Alsina X, Kazadi Mbamba C, Ikumi D, Volcke EIP, Vaneeckhaute C, et al. Plant-wide modelling of phosphorus transformations in wastewater treatment systems: Impacts of control and operational strategies. *Water Res.* 2017 Apr;113:97–110.
4. Henze M, Gujer W, Mino T, Matsuo T, Wentzel MC, Marais G v. R, et al. Activated Sludge Model No.2d, ASM2D. *Water Sci Technol.* 1999 Jan 1;39(1):165–82.
5. Flores-Alsina X, Solon K, Kazadi Mbamba C, Tait S, Gernaey KV, Jeppsson U, et al. Modelling phosphorus (P), sulfur (S) and iron (Fe) interactions for dynamic simulations of anaerobic digestion processes. *Water Res.* 2016 May 15;95:370–82.
6. Batstone DJ, Keller J, Angelidaki I, Kalyuzhnyi SV, Pavlostathis SG, Rozzi A, et al. The IWA Anaerobic Digestion Model No 1 (ADM1). *Water Sci Technol.* 2002 May 1;45(10):65–73.
7. Kazadi Mbamba C, Batstone DJ, Flores-Alsina X, Tait S. A generalised chemical precipitation modelling approach in wastewater treatment applied to calcite. *Water Res.* 2015 Jan 1;68:342–53.
8. Kazadi Mbamba C, Tait S, Flores-Alsina X, Batstone DJ. A systematic study of multiple minerals precipitation modelling in wastewater treatment. *Water Res.* 2015 Nov 15;85:359–70.
9. El Abbadi SH, Feng J, Hodson AR, Amouamouha M, Busse MM, Polcuch C, et al. Benchmarking Greenhouse Gas Emissions from U.S. Wastewater Treatment for Targeted Reduction. *Nature Water.* *In press.*