Appendix 2

Definitions for Model Integration

I. DEFINITIONS FOR MODEL PARAMETERS, CONSTANTS, AND COEFFICIENTS

ADM1 model:

Variable	Definition	Units
C_i	Carbon content of component i	kmoleC $kgCOD^{-1}$
N_i	Nitrogen content of component i	kmoleN $kgCOD^{-1}$
$v_{i,j}$	Rate coefficients for component i on process j	Nominally kgCOD m^{-3}
$f_{product,substrate}$	Yield (catabolism only) of product on substrate	kgCOD $kgCOD^{-1}$
H_{gas}	Gas law constant	bar M^{-1}
$K_{a,acid}$	Acid-base equilibrium coefficient	M
K_H	Henry's law coefficient	M bar^{-1}
pKa	$-\log_{10}[K_a]$	
R	Gas law constant	bar M^{-1} K^{-1}
ΔG	Free energy	J $mole^{-1}$
$k_{A/Bi}$	Acid-base kinetic parameter	M^{-1} d^{-1}
k_{dec}	First order decay rate	d^{-1}
$I_{inhibitor,process}$	Inhibition function	
$k_{process}$	First order decay rate (normally for hydrolysis)	d^{-1}
k_la	Gas-liquid transfer coefficient	d^{-1}
$K_{I,inhibit,substrate}$	50% inhibitory concentration	kgCOD m^{-3}
$k_{m,process}$	Monod maximum specific uptake rate	kgCOD_S $kgCOD\_X^{-1}$ d^{-1}
$K_{S,process}$	Half saturation value	kgCOD_S m^{-3}
ρ_j	Kinetic rate of process j	kgCOD_S m^{-3} d^{-1}
$Y_{substrate}$	Yield of biomass on substrate	kgCOD_X $kgCOD\_S^{-1}$
μ_{max}	Monod maximum specific growth rate	d^{-1}
pH	$-\log_{10}[H^+]$	
$p_{gas,i}$	Pressure of gas i	bar
P_{gas}	Total gas pressure	bar
S_i	Soluble component i	kgCOD m^{-3}
$t_{res,x}$	Extended retention of solids	d
T	Temperature	K
V	Volume	m^3
X_i	Particulate component i	kgCOD m^{-3}

ASM3 model:

Variable	Definition	Units
$i_{N,SI}$	N contet of inert soluble COD S_I	g-N g-COD^{-1}
$i_{N,SS}$	N content of readily biodegradable substrate	g-N g-COD^{-1}
$i_{N,XI}$	N content of inert particulate COD X_I	g-N g-COD^{-1}
$i_{N,XS}$	N content of slowly biodegradable substrate	g-N g-COD^{-1}
$i_{N,BM}$	N content of biomass X_H, X_{AOB}, X_{NOB}	g-N g-COD^{-1}
f_{SI}	Production of S_I in hydrolysis	g-COD gCOD^{-1}
f_{xI}	Fraction of inert COD generated in biomass lysis	g-COD gCOD^{-1}
Y_{H,O_2}	Yield coefficient for heterotrophs in aerobic growth	g-COD gCOD^{-1}
Y_{H,NO_3}	Yield coefficient for heterotrophs in anoxic growth	g-COD gCOD^{-1}
Y_{H,NO_2}	Yield coefficient for heterotrophs in anoxic growth	g-COD gCOD^{-1}
Y_{STO,O_2}	Yield coefficient for X_{STO} in aerobic growth	g-COD gCOD^{-1}
Y_{STO,NO_3}	Yield coefficient for X_{STO} in anoxic growth	g-COD gCOD^{-1}
Y_{STO,NO_2}	Yield coefficient for X_{STO} in anoxic growth	g-COD g-N^{-1}
Y_{AOB}	Yield coefficient for X_{AOB}	g-COD g-N^{-1}
Y_{NOB}	Yield coefficient for X_{NOB}	d^{-1}
k_H	Hydrolysis rate coefficient	d^{-1}
k_{STO}	Maximum storage rate	d^{-1}
μ_H	Maximum growth rate on substrate of heterotrophs	d^{-1}
μ_{AOB}	Maximum growth rate of X_{AOB}	d^{-1}
μ_{NOB}	Maximum growth rate of X_{NOB}	d^{-1}
b_{H,O_2}	Aerobic end. resp. rate for X_H	d^{-1}
b_{STO,O_2}	Aerobic end. resp. rate for X_{STO}	d^{-1}
b_{AOB}	Decay rate of X_{AOB}	d^{-1}
b_{NOB}	Decay rate of X_{NOB}	d^{-1}
η_{H,NO_3}	Reduction factor for denitrification	
η_{H,NO_2}	Reduction factor for denitrification	
η_{H,end,NO_3}	Reduction factor for b_H, anoxic condition	
η_{H,end,NO_2}	Reduction factor for b_H, anoxic condition	

$\eta_{N,end}$	Reduction factor for b_{AOB} and b_{NOB}, anoxic conditions	
K_X	Hydrolysis saturation constant	g X_S g^{-1} X_H
K_{H,O_2}	Saturation coefficient for oxygen, het. Growth	g O_2 m^{-3}
$K_{H,O_2,inh}$	Inhibition coefficient for oxygen, het. Growth	g O_2 m^{-3}
$K_{H,SS}$	Saturation coefficient for readily biodegradable substrates, het. growth	g COD m^{-3}
K_{H,NH_4}	Saturation/inhibition coefficient for ammonium, het. growth	g N m^{-3}
K_{H,NO_3}	Saturation/inhibition coefficient for nitrate, het. growth	g N m^{-3}
K_{H,NO_2}	Saturation/inhibition coefficient for nitrite, het. growth	g N m^{-3}
$K_{H,ALK}$	Saturation/inhibition coefficient for alkalinity, het. growth	mol HCO_3^- m^{-3}
$K_{H,STO}$	Saturation coefficient for storage products	g COD m^{-3}
K_{AOB,O_2}	Saturation coefficient for oxygen, AOB	g O_2 m^{-3}
K_{NOB,O_2}	Saturation coefficient for oxygen, NOB	g O_2 m^{-3}
K_{AOB,NH_4}	Saturation coefficient for ammonium, AOB	g N m^{-3}
K_{NOB,NO_2}	Saturation coefficient for nitrite, NOB	g N m^{-3}
$K_{N,ALK}$	Saturation/inhibition coefficient for alkalinity, aut. Growth	mol HCO_3^- m^{-3}

Algae model:

μ_{ALG}	Maximum growth rate of microalgae	d^{-1}
$k_{resp,ALG}$	Endogenous respiration constant	d^{-1}
$k_{death,ALG}$	Inactivation constant	d^{-1}
$K_{C,ALG}$	Affinity constant of microalgae on carbon species	gC m^{-3}
$I_{CO2,ALG}$	CO_2 inhibition constant of microalgae	gC m^{-3}
$K_{N,ALG}$	Affinity constant of microalgae on nitrogen species	gN m^{-3}
$K_{O2,ALG}$	Affinity constant of microalgae on dissolved oxygen	gO_2 m^{-3}

K_{PR}	Inhibition constant of photorespiration	
τ	Coefficient of excess dissolved oxygen	
S_{O2}^{SAT}	Saturation concentration of oxygen in the air	$gO_2\ m^{-3}$
T_{OPT}	Optimum temperature for microalgae growth	°C
s	Normalized parameter	
α	Parameter activation	$(\mu E\ m^{-2})^{-1}$
β	Parameter inhibition	$(\mu E\ m^{-2})^{-1}$
γ	Parameter production	s^{-1}
δ	Parameter recovery	s^{-1}
E_f	Photosynthetic efficiency of solar radiation	$\mu E\ J^{-1}$
א	Index atmospheric clarity	
ζ	Universal solar constant	$W\ m^{-2}$
ω	Hour angle	°
ω_s	Sunset hour angle	°
ϕ	Latitude	°
δ	Sun declination	°
$K_{a,O2}$	Mass transfer coefficient for oxygen	d^{-1}
$K_{a,CO2}$	Mass transfer coefficient for carbon dioxide	d^{-1}
$K_{a,NH3}$	Mass transfer coefficient for ammonia	d^{-1}
$K_{eq,1}$	Chemical equilibrium $CO_2 \leftrightarrow HCO_3^-$	
$K_{eq,2}$	Chemical equilibrium $HCO_3^- \leftrightarrow CO_3^{2-}$	
$K_{eq,3}$	Chemical equilibrium $NH_4^+ \leftrightarrow NH_3$	
$K_{eq,w}$	Chemical equilibrium $H^+ \leftrightarrow OH^-$	
$k_{eq,1}$	Dissociation constant $CO_2 \leftrightarrow HCO_3^-$	d^{-1}
$k_{eq,2}$	Dissociation constant $HCO_3^- \leftrightarrow CO_3^{2-}$	d^{-1}
$k_{eq,3}$	Dissociation constant $NH_4^+ \leftrightarrow NH_3$	d^{-1}
$k_{eq,w}$	Dissociation constant $H^+ \leftrightarrow OH^-$	$g\ m^{-1}\ d^{-1}$
$i_{C,ALG}$	Fraction of carbon in microalgae	$gC\ gCOD^{-1}$
$i_{H,ALG}$	Fraction of hydrogen in microalgae	$gH\ gCOD^{-1}$
$i_{O,ALG}$	Fraction of oxygen in microalgae	$gO_2\ gCOD^{-1}$

$i_{N,ALG}$	Fraction of nitrogen in microalgae	gN $gCOD^{-1}$
ρ_{1a}	Microalgae growth rate on ammonia	M L^{-3} T^{-1}
ρ_{1b}	Microalgae growth rate on nitrate	M L^{-3} T^{-1}
ρ_2	Microalgae endogenous respiration rate	M L^{-3} T^{-1}
ρ_3	Microalgae inactivation rate	M L^{-3} T^{-1}
ρ_4	Chemical equilibrium $CO_2 \leftrightarrow HCO_3^-$	M L^{-3} T^{-1}
ρ_5	Chemical equilibrium $HCO_3^- \leftrightarrow CO_3^{2-}$	M L^{-3} T^{-1}
ρ_6	Chemical equilibrium $NH_4^+ \leftrightarrow NH_3$	M L^{-3} T^{-1}
ρ_7	Chemical equilibrium $H^+ \leftrightarrow OH^-$	M L^{-3} T^{-1}
ρ_{O2}	Oxygen transfer rate to the atmosphere	M L^{-3} T^{-1}
ρ_{CO2}	Cardon dioxide transfer rate to the atmosphere	M L^{-3} T^{-1}
ρ_{NH3}	Ammonia transfer rate to the atmosphere	M L^{-3} T^{-1}

II. DEFINITIONS FOR MODEL OUTPUTS:

ADM1 model:

Variable	Definition	Units
X_c	Composite	kgCOD m^{-3}
X_{ch}	Carbohydrates	kgCOD m^{-3}
X_{pr}	Proteins	kgCOD m^{-3}
X_{li}	Lipids	kgCOD m^{-3}
X_I	Particulate inerts	kgCOD m^{-3}
S_I	Soluble inerts	kgCOD m^{-3}
S_{su}	Monosaccharides	kgCOD m^{-3}
S_{aa}	Amino acids	kgCOD m^{-3}
S_{fa}	Total LCFA	kgCOD m^{-3}
S_{va}	Total valerate	kgCOD m^{-3}
S_{bu}	Total butyrate	kgCOD m^{-3}
S_{pro}	Total propionate	kgCOD m^{-3}
S_{ac}	Total acetate	kgCOD m^{-3}
S_{h2}	Hydrogen	kgCOD m^{-3}

S_{ch4}	Methane	kgCOD m^{-3}
S_{IC}	Inorganic carbon	M
S_{IN}	Inorganic nitrogen	M
X_{su-h2}	Biomass	kgCOD m^{-3}
S_{cat}	Cations	M
S_{an}	Anions	M

ASM3 model:

Variable	Definition	Units
S_{O_2}	Dissolved oxygen	gO_2 m^{-3}
S_S	Soluble substrate	gCOD m^{-3}
S_{NH_4}	Ammonium	gN m^{-3}
S_{NO_2}	Nitrite	gN m^{-3}
S_{NO_3}	Nitrate	gN m^{-3}
S_{N_2}	Nitrogen	gN m^{-3}
S_{ALK}	Alkalinity	mole HCO_3^- m^{-3}
S_I	Soluble inert organics	gCOD m^{-3}
X_I	Particulate inerts	gCOD m^{-3}
X_H	Heterotrophic biomass	gCOD m^{-3}
X_S	Slowly biodegradable substrate	gCOD m^{-3}
X_{STO}	Organics stored by heterotrophs	gCOD m^{-3}
X_{AOB}	Ammonium-oxidizing bacteria	gCOD m^{-3}
X_{NOB}	Nitrite-oxidizing bacteria	gCOD m^{-3}

Algae model:

Variable	Definition	Units
S_{NH_4}	Ammonium nitrogen	gNH_4^+-N m^{-3}
S_{NH_3}	Ammonia nitrogen	gNH_3-N m^{-3}
S_{NO_3}	Nitrate nitrogen	gNO_3^-N m^{-3}
S_{O_2}	Dissolved oxygen	gO_2 m^{-3}
S_{CO_2}	Carbon dioxide	gCO_2-C m^{-3}
S_{HCO_3}	Bicarbonate	$gHCO_3^-$-C m^{-3}
S_{CO_3}	Carbonate	gCO_3^{2-}-C m^{-3}
S_H	Hydrogen ions	gH m^{-3}
S_{OH}	Hydroxide ions	gOH^--H m^{-3}
X_{ALG}	Microalgae biomass	gCOD m^{-3}

III. Conversions for Model Integration

Summary of Key Integration Variables for Each Model:

ADM1	ASM3	Algae
Ssu	SO2	SNH4_alg
Saa	SS	SNH3
Sfa	SNH4_asm3	SNO3
Sva	SNO2	SO2
Sbu	SNO3	SCO2
Spro	SN2	SHCO3
Sac	SALK	SH
Sh2	SI_asm3	SOH
Sch4	XI_asm3	Xalg
Sic	XH	
Sin	XS	
Si	XSTO	
Xc	XAOB	
Xch	XNOB	
Xpr		
Xli		
Xsu		
Xaa		
Xfa		
Xc4		
Xpro		
Xac		
Xh2		
Xi		
Sva_m		
Sbu_m		
Spro_m		
Sac_m		
Shco3_m		
Snh3_m		
Sgas_h2		
Sgas_ch4		
Sgas_co2		

Response Variables Conversions:

Since all of the models ADM1, ASM3 and Algae model follow the same mathematical structures of defining the dynamics of the bioprocesses, the integration of the three models eventually became a simple set of basic operations as follows.

1. From ADM1 to ASM3:

XS = 1000*(Xc + Xch + Xpr + Xli + Xsu + Xaa + Xfa + Xc4 + Xpro + Xac + Xh2)
SS = 1000*(Ssu + Saa + Sfa + Sva + Sbu + Spro + Sac)
$\mathrm{SALK} = 1000 * (\mathrm{Sva} + \mathrm{Sbu} + \mathrm{Spro} + \mathrm{Sac} + \mathrm{Sic} + \mathrm{Sin})$

2. From ASM3 to Algae:

SNH4_alg = SNH4_asm3
SNO3 = SNO3
SO2 = SO2