Mathematical Modelling of Wastewater Treatment Plants

Part III: Dynamic Modelling of the Activated Sludge Process

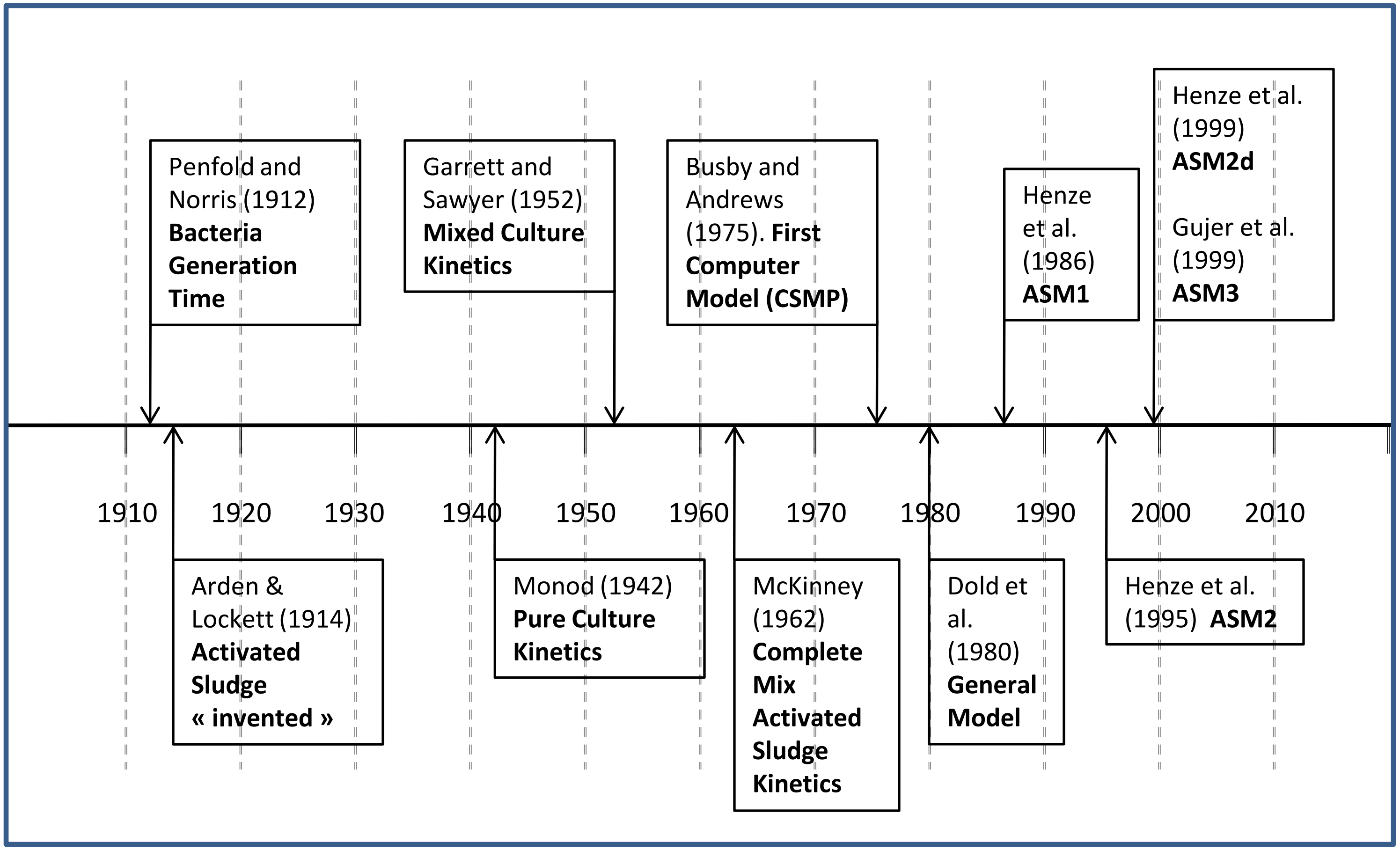
Gilles G. Patry
University of Ottawa

Outline

- Introduction
- Notation used by the Task Group (applies to all ASM models)
- ASM1 Model Development
  - ASM1 Model Structure
  - Processes
    - Aerobic growth of heterotrophs
    - Anoxic growth of heterotrophs
    - Aerobic growth of autotrophs
    - Decay of heterotrophs
    - Decay of autotrophs
    - Ammonification of soluble organic nitrogen
    - Hydrolysis of entrapped organics
    - Hydrolysis of entrapped organic nitrogen
  - Petersen matrix formulation of ASM1
- Formulating the differential equations

Activated Sludge Modelling Timeline

(adapted from Bruce Johnson, CH2M Hill)



Penfold and Norris (1912) **Bacteria Generation Time**

Arden & Lockett (1914) **Activated Sludge « invented »**

Monod (1942) **Pure Culture Kinetics**

Garrett and Sawyer (1952) **Mixed Culture Kinetics**

McKinney (1962) **Complete Mix Activated Sludge Kinetics**

Busby and Andrews (1975). **First Computer Model (CSMP)**

Dold et al. (1980) **General Model**

Henze et al. (1986) **ASM1**

Henze et al. (1995) **ASM2**

Henze et al. (1999) **ASM2d**

Gujer et al. (1999) **ASM3**

Empirical Design, Piloting & Guesswork

Kinetics-Based Design

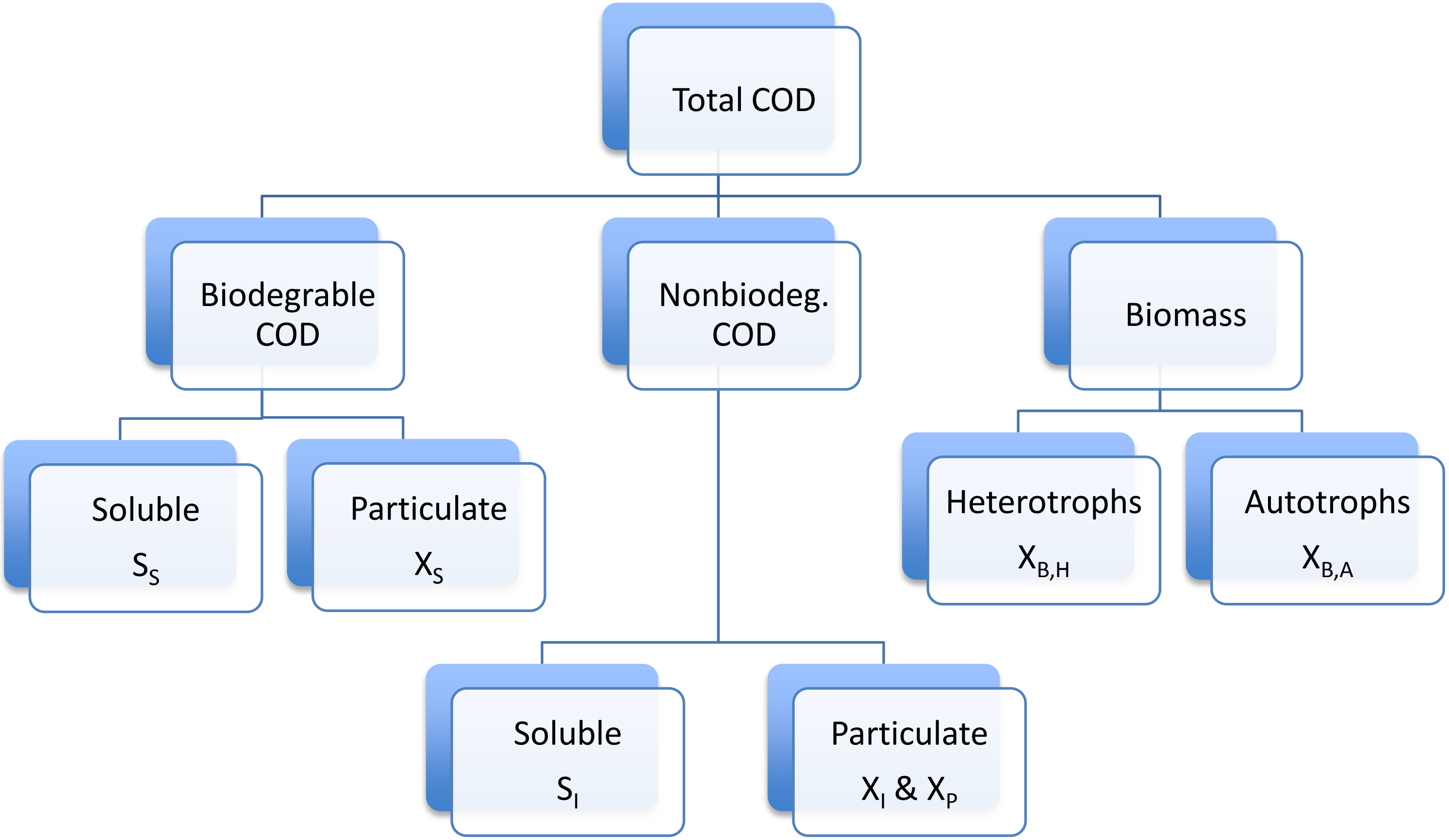
Whole Plant Simulators

Activated Sludge Model No. 1 (ASM1)

- Introduced in 1987 as IAWQ Model no. 1 (ASM1) - IAWQ Task Group on Activated Sludge Modeling
- ASM1 is a simple model consisting of:
  - 8 processes
  - 13 state variables or components
  - 19 parameters
- Model enhanced several times to address specific shortcomings of ASM1
  - ASM No. 2
  - ASM No. 2d
  - ASM No. 3
  - others

Henze, M., Grady Jr., C.P.L., Gujer, W., Marais, G.v.R., Matsuo, T. (1987). "Activated Sludge Model No.1" *IAWQ Scientific and Technical Report No.1,* IAWQ, London, Great Britain.

Carbonaceous Components



Total COD

Biodegrable COD

Nonbiodeg. COD

Biomass

Soluble S_S

Particulate X_S

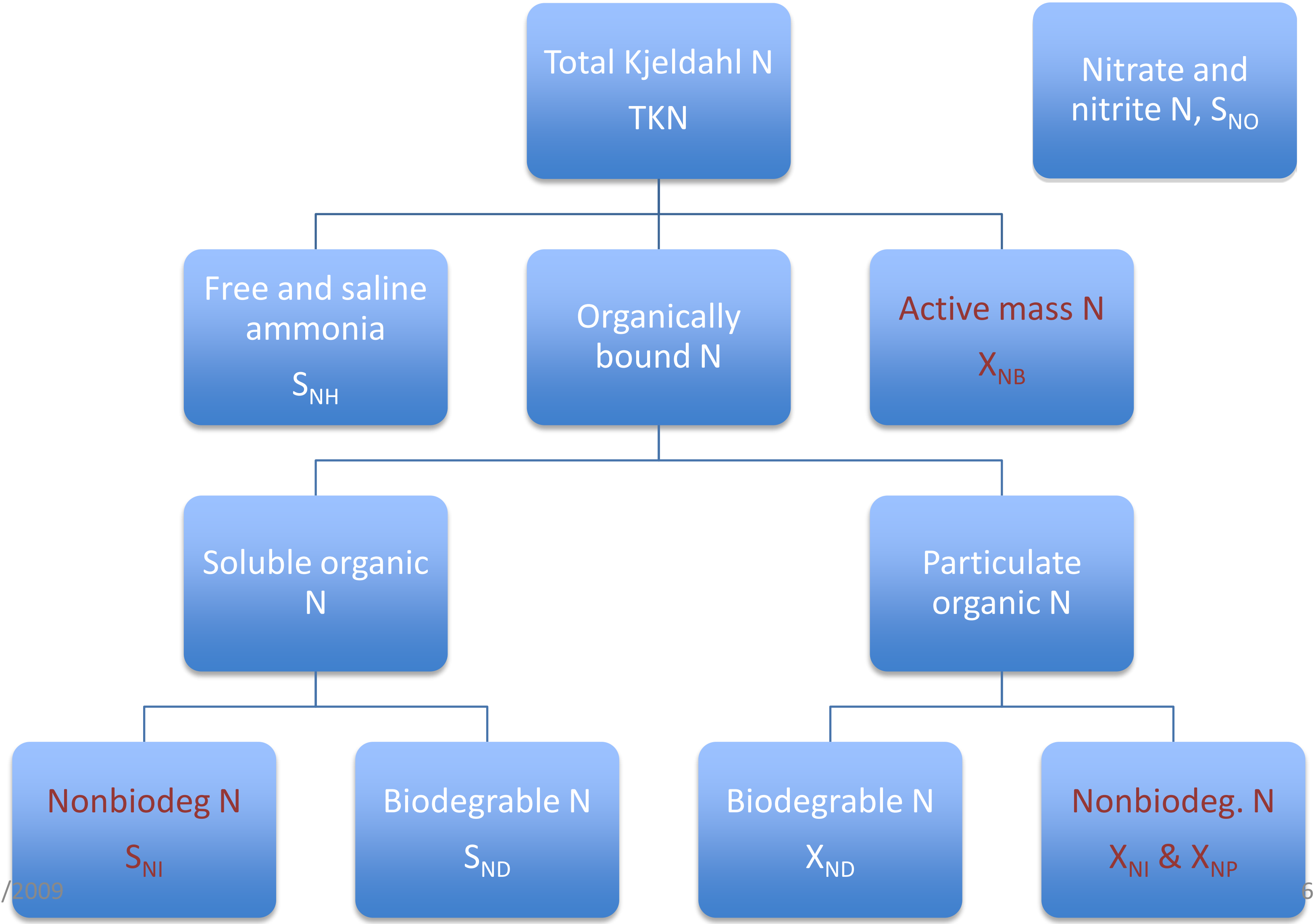
Heterotrophs $X_{B,H}$

Autotrophs $X_{B,A}$

Soluble S_I

Particulate X_I & X_P

Nitrogenous Components



Total Kjeldahl N

TKN

Nitrate and nitrite N, S_{NO}

Free and saline ammonia

S_{NH}

Organically bound N

Active mass N

X_{NB}

Soluble organic N

Particulate organic N

Nonbiodeg N

S_{NI}

Biodegradable N

S_{ND}

Biodegradable N

X_{ND}

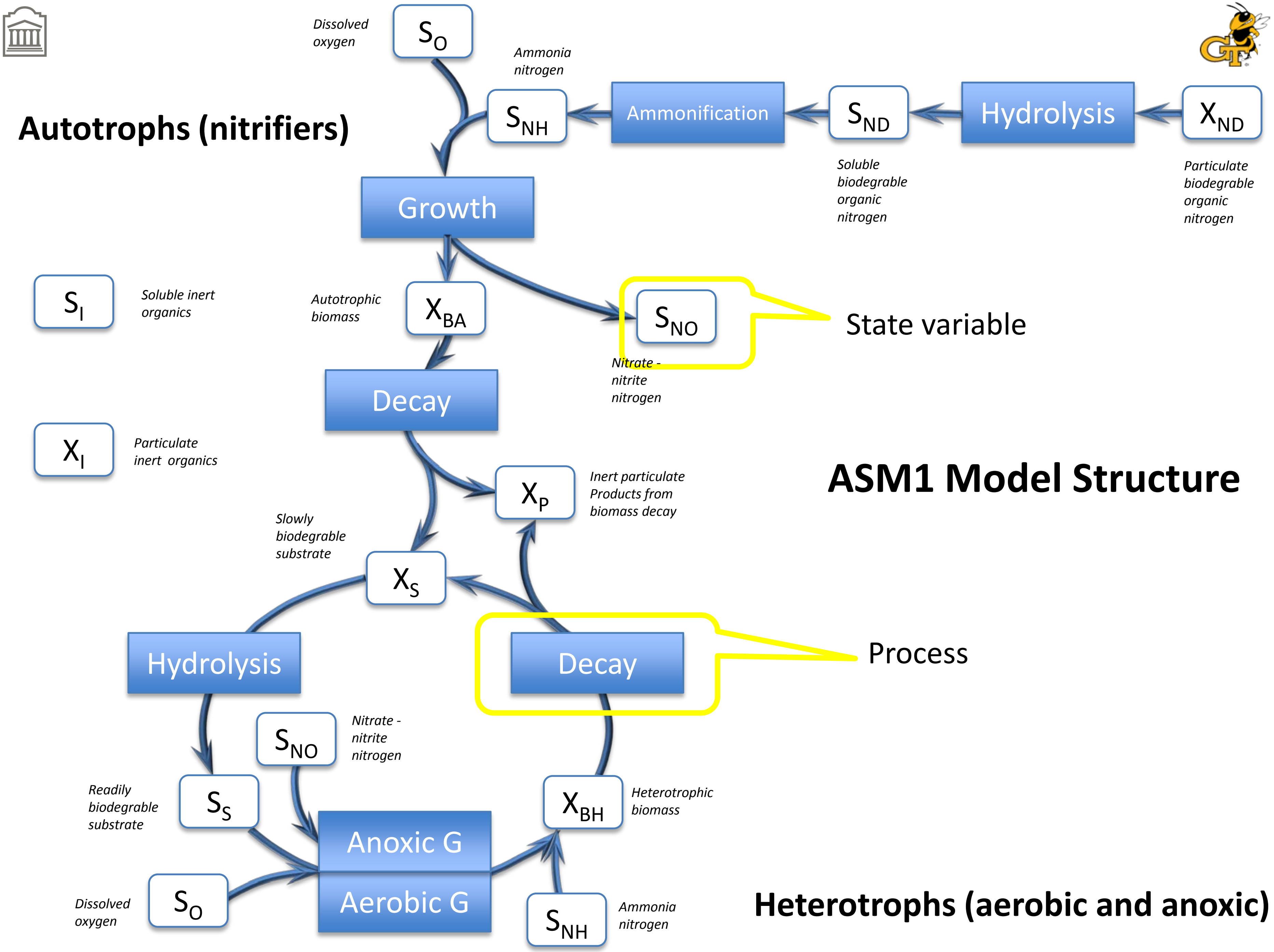
Nonbiodeg. N

X_{NI} & X_{NP}

Processes in ASM1

- Aerobic growth of heterotrophs
- Anoxic growth of heterotrophs
- Aerobic growth of autotrophs
- Decay of heterotrophs
- Decay of autotrophs
- Ammonification of soluble organic nitrogen
- Hydrolysis of entrapped organics
- Hydrolysis of entrapped organic nitrogen

ASM1 Model Structure



Autotrophs (nitrifiers)

S_O *Dissolved oxygen*

S_{NH} *Ammonia nitrogen*

Ammonification

S_{ND} *Soluble biodegrable organic nitrogen*

Hydrolysis

X_{ND} *Particulate biodegrable organic nitrogen*

Growth

S_I *Soluble inert organics*

X_{BA} *Autotrophic biomass*

S_{NO} *Nitrate - nitrite nitrogen*

State variable

Decay

X_I *Particulate inert organics*

X_P *Inert particulate Products from biomass decay*

X_S *Slowly biodegrable substrate*

Hydrolysis

Decay

Process

S_{NO} *Nitrate - nitrite nitrogen*

S_S *Readily biodegrable substrate*

Anoxic G

Aerobic G

X_{BH} *Heterotrophic biomass*

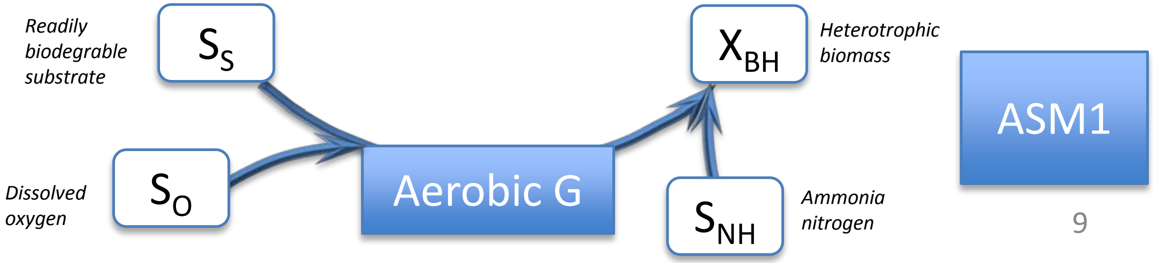
S_O *Dissolved oxygen*

S_{NH} *Ammonia nitrogen*

Heterotrophs (aerobic and anoxic)

Aerobic Growth of Heterotrophs

- A fraction of the readily biodegradable substrate is used for growth of heterotrophic biomass and the balance is oxidized for energy.
- Growth model used Monod kinetics
- Ammonia is used as nitrogen source and is incorporated in cell mass
- Both the substrate (S_S) and oxygen (S_O) may be rate limiting for the growth process and removal of COD
- Dissolved oxygen switching function is introduced
- Alkalinity change



Aerobic Growth – Heterotrophs

- Process Rate:

$$\hat{\mu}_{\mathrm{H}}\left(\frac{S_{\mathrm{S}}}{K_{\mathrm{S}}+S_{\mathrm{S}}}\right)\boxed{\left(\frac{S_{\mathrm{O}}}{K_{\mathrm{O,H}}+S_{\mathrm{O}}}\right)}X_{\mathrm{B,H}}$$

Switching Function

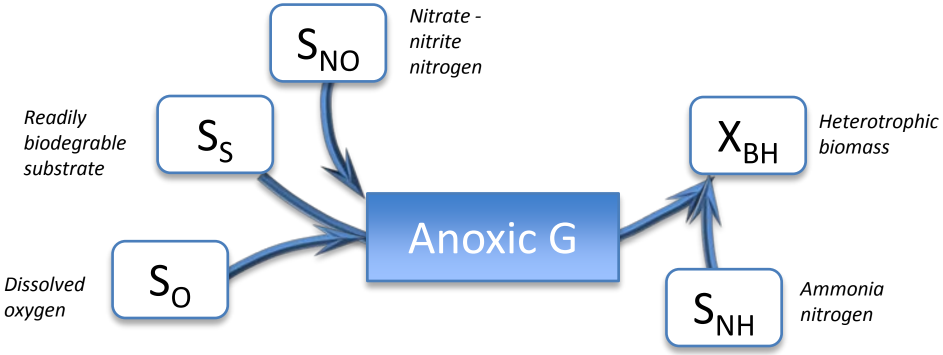
where $\hat{\mu}_{\mathrm{H}}$ = heterotrophic maximum specific growth rate, d^{-1}

K_{S} = half saturation coefficient for heterotrophs, g COD m^{-3}

$K_{\mathrm{O,H}}$ = oxygen half saturation coefficient for heterotrophs, g $\mathrm{O_2}$ m^{-3}

ASM1

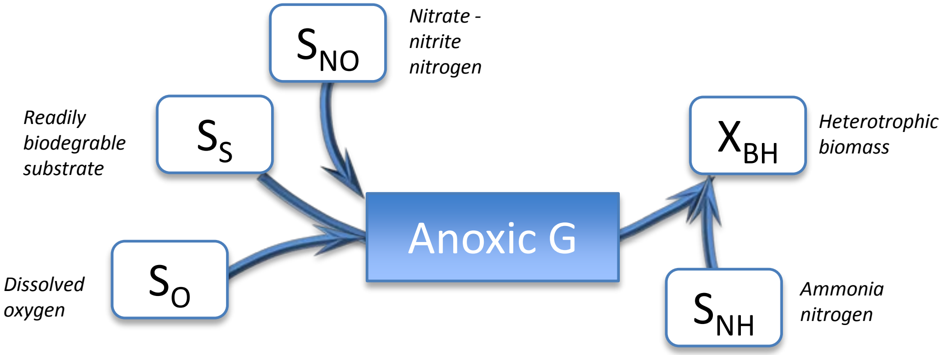
Anoxic Growth of Heterotrophs



- In the absence of oxygen, the heterotrophic organisms are capable of using nitrate as the terminal electron acceptor with S_S as the substrate
- Leads to production of heterotrophic biomass and nitrogen gas (as a result of the reduction of nitrate with associated alkalinity change)
- Growth modeled using same Monod kinetics as aerobic growth except that kinetic rate is multiplied by η_g (< 1)
  - Why $\eta_g < 1$?
    - Lower maximum growth rate under anoxic conditions OR
    - Only a fraction of the heterotrophic biomass is able to function with nitrate as electron acceptor
- Ammonia serves as nitrogen source for cell synthesis, which affects alkalinity

ASM1

Anoxic Growth of Heterotrophs



- Process rate:

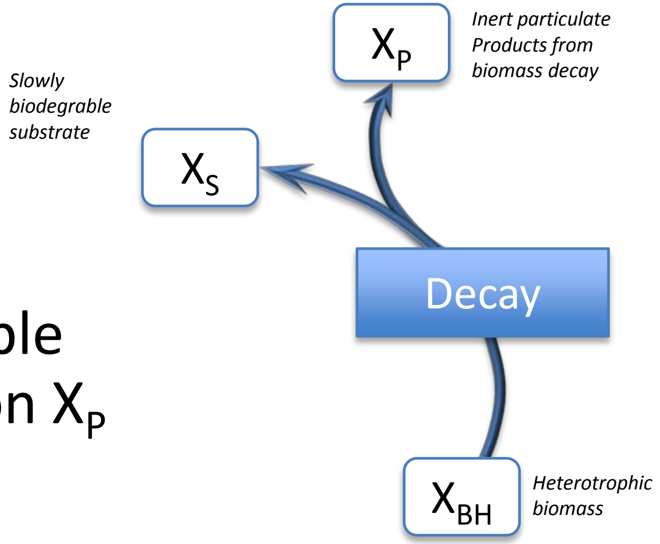
$$\hat{\mu}_{\mathrm{H}}\left(\frac{S_{\mathrm{S}}}{K_{\mathrm{S}}+S_{\mathrm{S}}}\right)\left(\frac{K_{\mathrm{O,H}}}{K_{\mathrm{O,H}}+S_{\mathrm{O}}}\right)\left(\frac{S_{\mathrm{NO}}}{K_{\mathrm{NO}}+S_{\mathrm{NO}}}\right)\eta_{\mathrm{g}}X_{\mathrm{B,H}}$$

where η_g = correction factor for anoxic growth of heterotrophs

K_{NO} = nitrate half saturation coefficient for denitrifying heterotrophs, g NO_3 - N m^{-3}

ASM1

Decay of Heterotrophs



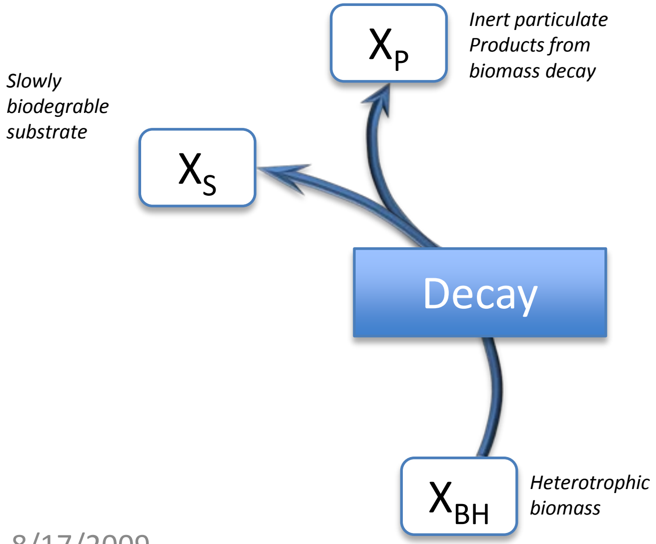
- Organisms die at a certain rate and
  - a portion of the material is considered to be non-biodegradable and adds to the particulate fraction X_P
  - the remainder adds to the pool of slowly biodegradable substrate
- Organic nitrogen in particulate substrate (X_S) becomes available as particulate organic nitrogen
- Process is assumed to take place at same rate under aerobic, anoxic or anaerobic conditions

ASM1

Decay of Heterotrophs

- Process rate:

$$b_H X_{B,H}$$



X_P

Inert particulate Products from biomass decay

Slowly biodegradable substrate

X_S

Decay

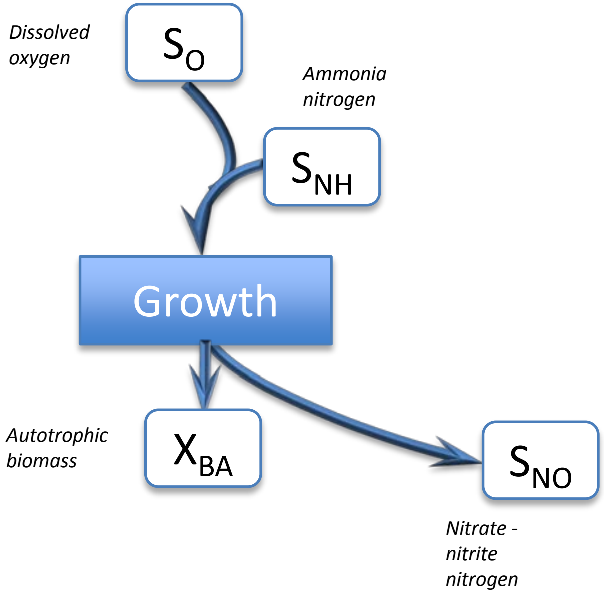
X_{BH}

Heterotrophic biomass

where $b_H =$ heterotrophic decay rate, d^{-1}

ASM1

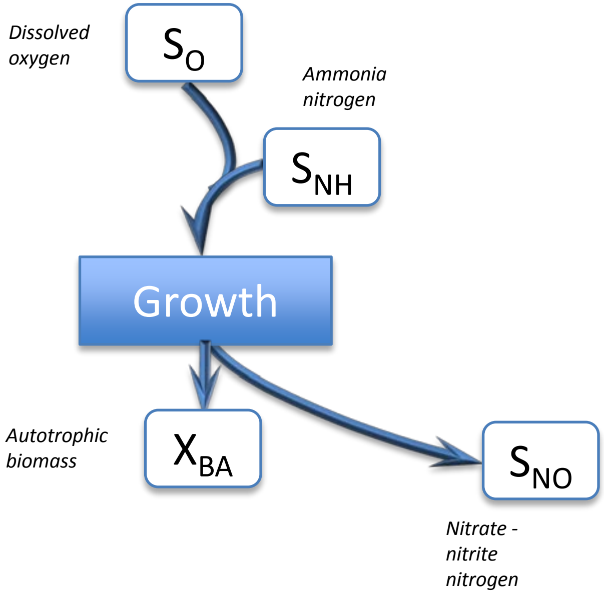
Aerobic Growth of Autotrophs



- Ammonia is oxidized to nitrate (single step process) resulting in production of autotrophic biomass and associated oxygen demand
- Ammonia is also used as nitrogen source for synthesis and incorporated in cell mass
- Process has an effect on alkalinity and total oxygen demand
- Amount of biomass formed is generally small because of the low yield autotrophic nitrifiers
- Growth rate modeled using Monod kinetics

ASM1

Aerobic Growth of Autotrophs



- Process rate:

$$\hat{\mu}_{\mathrm{A}}\left(\frac{S_{\mathrm{NH}}}{K_{\mathrm{NH}}+S_{\mathrm{NH}}}\right)\left(\frac{S_{\mathrm{O}}}{K_{\mathrm{O,A}}+S_{\mathrm{O}}}\right)X_{\mathrm{B,A}}$$

where $\hat{\mu}_{\mathrm{A}}$ = autotrophic maximum specific growth rate, d^{-1}

K_{NH} = ammonia half saturation coefficient for autotrophs, g COD m^{-3}

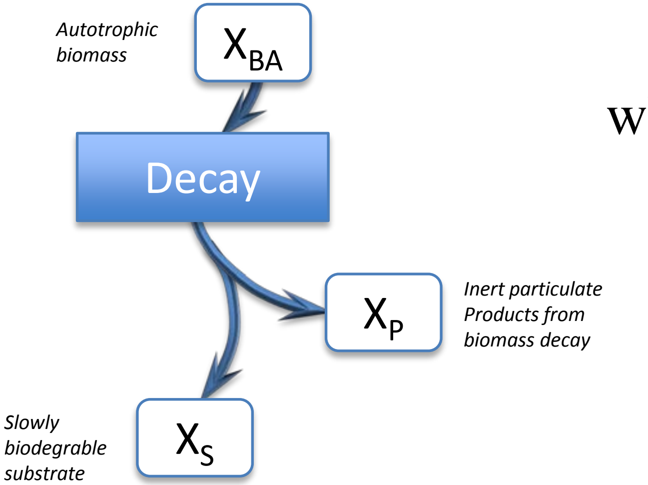
K_{OA} = oxygen half saturation coefficient for autotrophs, g O_2 m^{-3}

ASM1

Decay of Autotrophs

- Modeled in same way as decay of heterotrophs
- Process rate:

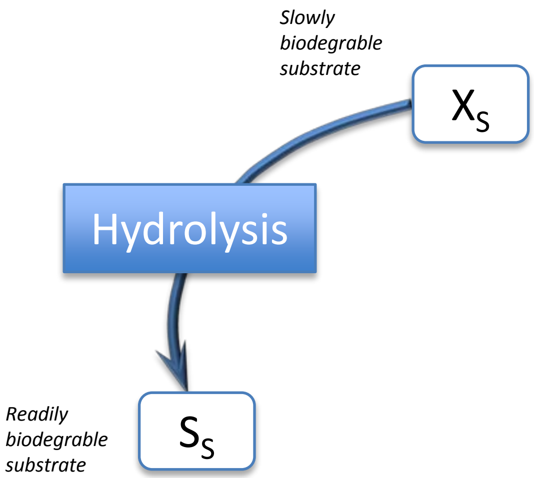
$$b_A X_{B,A}$$



where $b_A =$ autotrophic decay rate, d^{-1}

ASM1

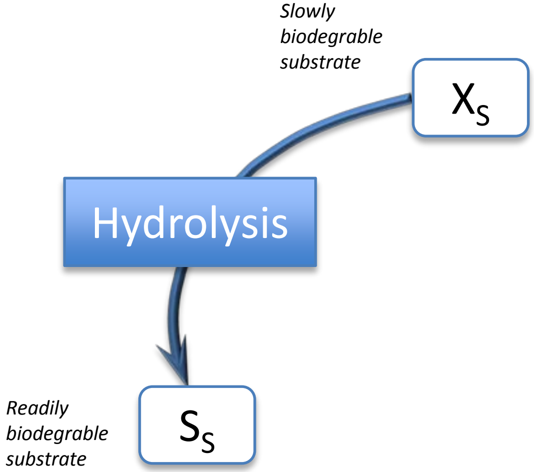
Hydrolysis of Entrapped Organics



- Slowly biodegradable substrate enmeshed in sludge mass is broken down extracellularly, producing readily biodegradable substrate available to organisms for growth
- Process modeled on basis of surface reaction kinetics
- Process occurs under aerobic and anoxic conditions
- Rate of hydrolysis is reduced under anoxic conditions by a factor η_h (< 1)
- Rate is first-order wrt heterotrophic biomass and saturates as the amount of entrapped organics becomes large

ASM1

Hydrolysis of Entrapped Organics



Slowly biodegrable substrate

X_S

Hydrolysis

Readily biodegrable substrate

S_S

- Process rate:

$$k_h \left(\frac{\dfrac{X_S}{X_{B,H}}}{K_X + \left(\dfrac{X_S}{X_{B,H}} \right)} \right) \left\{ \left(\frac{S_O}{K_{O,H} + S_O} \right) + \eta_h \left(\frac{K_{O,H}}{K_{O,H} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}} \right) \right\} X_{B,H}$$

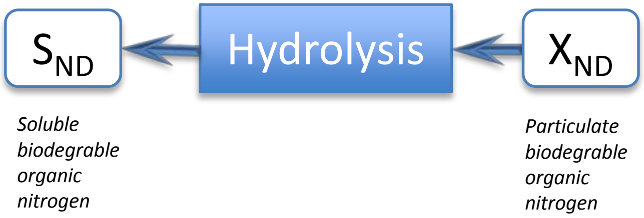
where k_h = maximum specific hydrolysis rate, g slowly biodeg. COD $(\text{g cell COD day})^{-1}$

K_X = half saturation coefficient for hydrolysis of slowly biodeg. substrate, g slowly biodeg. COD $(\text{g cell COD day})^{-1}$

η_h = correction factor for anoxic hydrolysis

ASM1

Hydrolysis of Entrapped Organic Nitrogen


S_{ND} ← Hydrolysis ← X_{ND}

Soluble biodegrable organic nitrogen

Particulate biodegrable organic nitrogen

- Biodegradable particulate organic nitrogen is broken down into soluble organic nitrogen at a rate defined by the hydrolysis reaction for entrapped organics

ASM1

Hydrolysis of Entrapped Organic Nitrogen

- Process rate:

Soluble biodegrable organic nitrogen

Particulate biodegrable organic nitrogen

$$\rho_7 \frac{X_{\mathrm{ND}}}{X_{\mathrm{S}}}$$

where ρ_7 is given by:

$$k_{\mathrm{h}}\left(\frac{\dfrac{X_{\mathrm{S}}}{X_{\mathrm{B,H}}}}{K_{\mathrm{X}}+\left(\dfrac{X_{\mathrm{S}}}{X_{\mathrm{B,H}}}\right)}\right)\left\{\left(\frac{S_{\mathrm{O}}}{K_{\mathrm{O,H}}+S_{\mathrm{O}}}\right)+\eta_{\mathrm{h}}\left(\frac{K_{\mathrm{O,H}}}{K_{\mathrm{O,H}}+S_{\mathrm{O}}}\right)\left(\frac{S_{\mathrm{NO}}}{K_{\mathrm{NO}}+S_{\mathrm{NO}}}\right)\right\}X_{\mathrm{B,H}}$$

ASM1

Ammonification of Soluble Organic Nitrogen

- Biodegradable soluble organic nitrogen is converted to free and saline ammonia using first-order process mediated by active heterotrophs
- Hydrogen ions consumed in the process resulting in an alkalinity change

ASM1

Ammonification of Soluble Organic Nitrogen

- Process rate:

$$k_{\mathrm{a}} S_{\mathrm{ND}} X_{\mathrm{B,H}}$$

where k_{a} = ammonification rate, $\mathrm{m}^3\ (\mathrm{g\ COD\ day})^{-1}$

Ammonia nitrogen

S_{NH}

Ammonification

S_{ND}

Soluble biodegrable organic nitrogen

ASM1

ASM1 State Variables

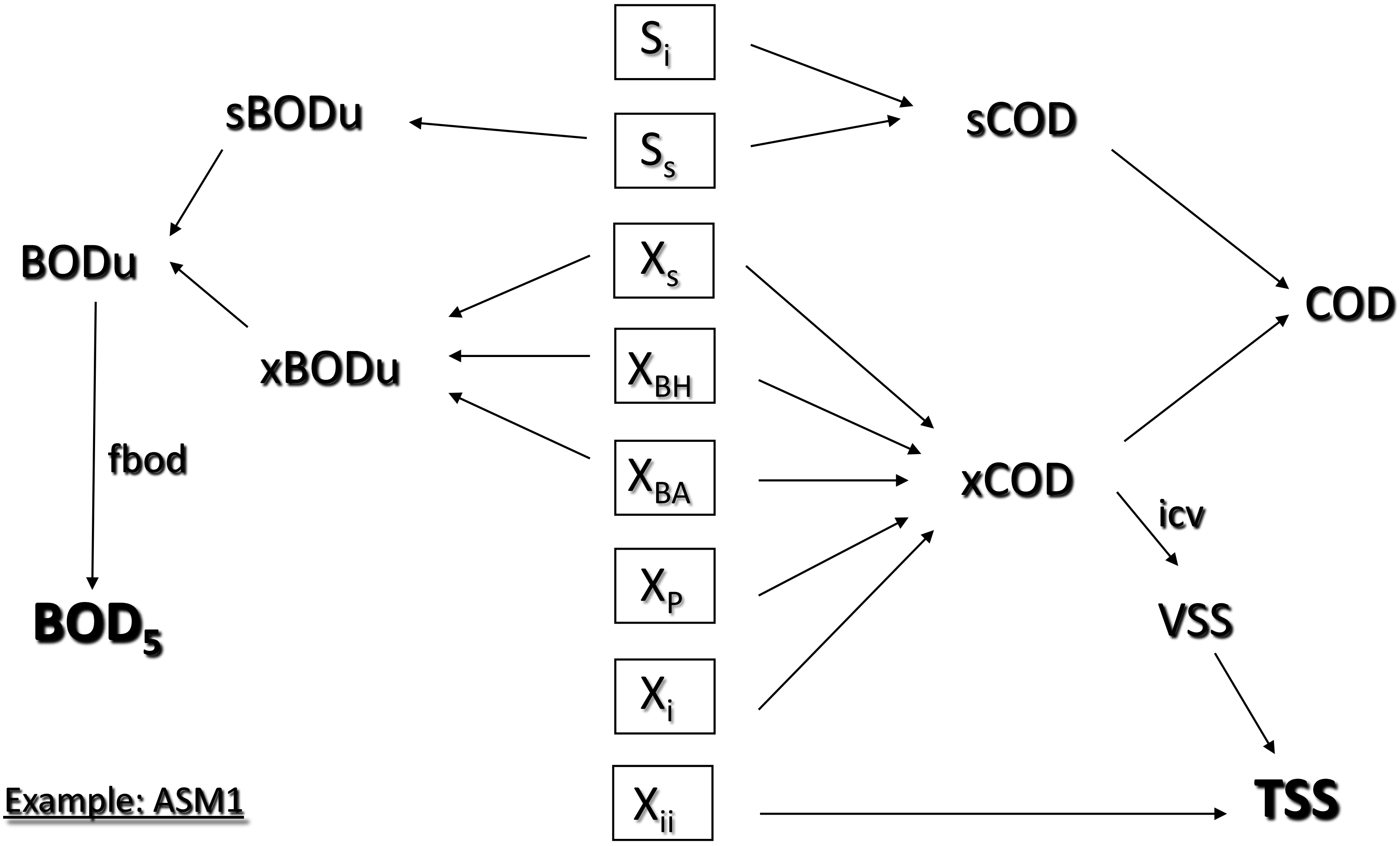
Si	Soluble inert organics	g COD/m3
Ss	Readily biodegradable (soluble) substrate	g COD/m3
Xi	Particulate inert organics	g COD/m3
Xs	Slowly biodegradable (particulate) substrate	g COD/m3
Xbh	Active heterotrophic biomass	g COD/m3
Xba	Active autotrophic biomass	g COD/m3
Xp	Unbiodegrad. particulates from cell decay	g COD/m3
So	Dissolved oxygen	g O2/m3
Sno	Nitrate and nitrite	g N/m3
Snh	Free and ionized ammonia	g N/m3
Snd	Soluble biodegradable organic nitrogen (in ss)	g N/m3
Xnd	Particulate biodegradable organic N (in xs)	gN/m3
Xii	Inert inorganic suspended solids	g/m3

S - Soluble Components

X - Particulate Components

Adapted from Hydromantis, Inc.

Mapping of State Variables to Composite Variables



S_i

S_s

X_s

X_{BH}

X_{BA}

X_P

X_i

X_{ii}

sBODu

BODu

xBODu

fbod

BOD_5

sCOD

COD

xCOD

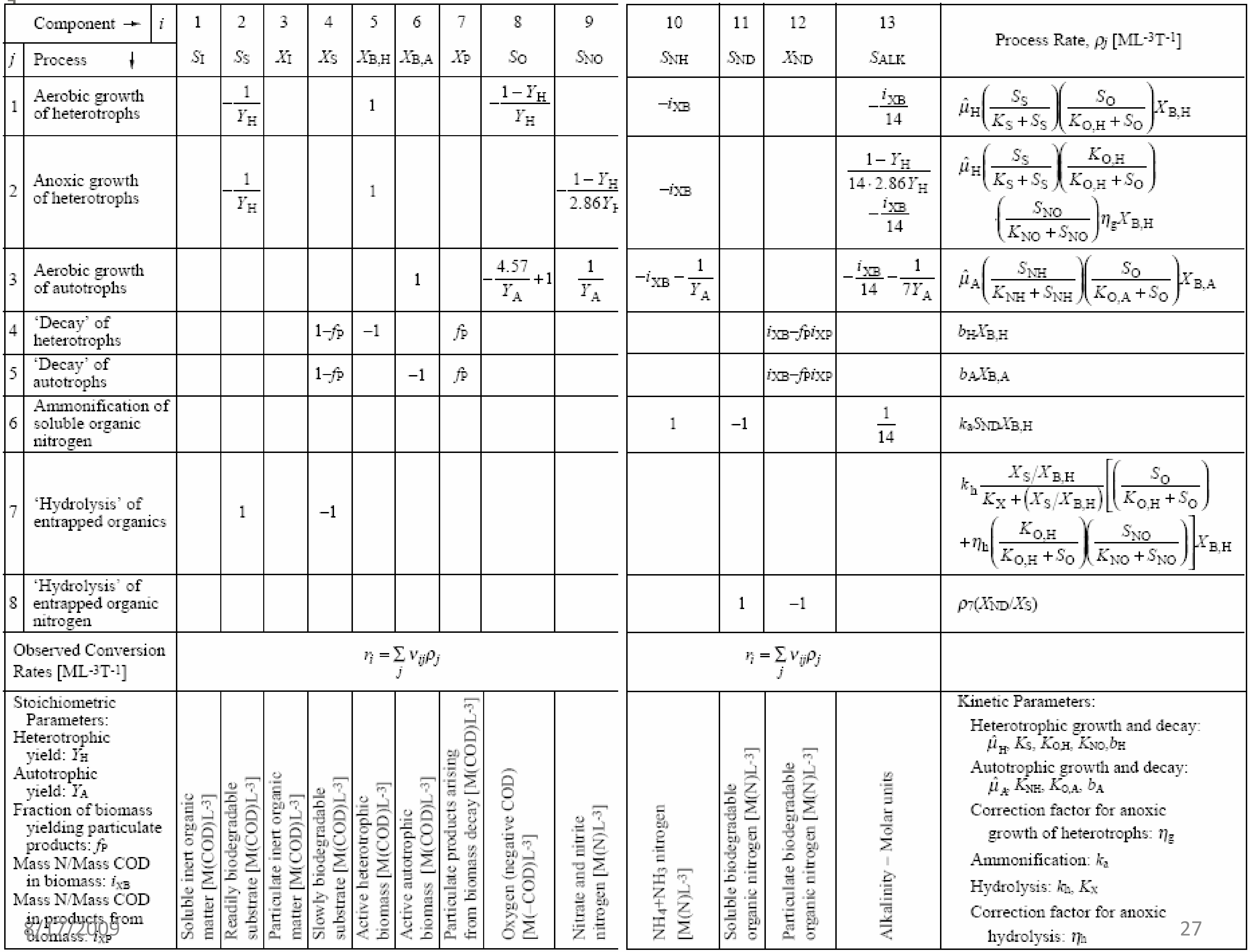
icv

VSS

TSS

Example: ASM1

Adapted from Hydromantis, Inc.



Component →	i	1	2	3	4	5	6	7	8	9	10	11	12	13	Process Rate, ρ_j [ML^{-3}T^{-1}]
j	Process ↓	S_I	S_S	X_I	X_S	$X_{B,H}$	$X_{B,A}$	X_P	S_O	S_{NO}	S_{NH}	S_{ND}	X_{ND}	S_{ALK}	
1	Aerobic growth of heterotrophs		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$			$-\frac{i_{XB}}{14}$	$\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_O}{K_{O,H}+S_O}\right)X_{B,H}$
2	Anoxic growth of heterotrophs		$-\frac{1}{Y_H}$			1				$-\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$			$\frac{1-Y_H}{14\cdot 2.86Y_H}-\frac{i_{XB}}{14}$	$\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\cdot\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_g X_{B,H}$
3	Aerobic growth of autotrophs						1		$-\frac{4.57}{Y_A}+1$	$\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$			$-\frac{i_{XB}}{14}-\frac{1}{7Y_A}$	$\hat{\mu}_A\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A}$
4	'Decay' of heterotrophs				$1-f_P$	-1		f_P					$i_{XB}-f_P i_{XP}$		$b_H X_{B,H}$
5	'Decay' of autotrophs				$1-f_P$		-1	f_P					$i_{XB}-f_P i_{XP}$		$b_A X_{B,A}$
6	Ammonification of soluble organic nitrogen										1	-1		$\frac{1}{14}$	$k_a S_{ND} X_{B,H}$
7	'Hydrolysis' of entrapped organics		1		-1										$k_h\frac{X_S/X_{B,H}}{K_X+(X_S/X_{B,H})}\left[\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_h\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right]X_{B,H}$
8	'Hydrolysis' of entrapped organic nitrogen											1	-1		$\rho_7(X_{ND}/X_S)$
	Observed Conversion Rates [ML^{-3}T^{-1}]	$r_i=\sum_j \nu_{ij}\rho_j$									$r_i=\sum_j \nu_{ij}\rho_j$				
	Stoichiometric Parameters: Heterotrophic yield: Y_H Autotrophic yield: Y_A Fraction of biomass yielding particulate products: f_P Mass N/Mass COD in biomass: i_{XB} Mass N/Mass COD in products from biomass: i_{XP}	Soluble inert organic matter [M(COD)L-3]	Readily biodegradable substrate [M(COD)L-3]	Particulate inert organic matter [M(COD)L-3]	Slowly biodegradable substrate [M(COD)L-3]	Active heterotrophic biomass [M(COD)L-3]	Active autotrophic biomass [M(COD)L-3]	Particulate products arising from biomass decay [M(COD)L-3]	Oxygen (negative COD) [M(–COD)L-3]	Nitrate and nitrite nitrogen [M(N)L-3]	NH$_4$+NH$_3$ nitrogen [M(N)L-3]	Soluble biodegradable organic nitrogen [M(N)L-3]	Particulate biodegradable organic nitrogen [M(N)L-3]	Alkalinity – Molar units	Kinetic Parameters: Heterotrophic growth and decay: $\hat{\mu}_H$, K_S, $K_{O,H}$, K_{NO}, b_H Autotrophic growth and decay: $\hat{\mu}_A$, K_{NH}, $K_{O,A}$, b_A Correction factor for anoxic growth of heterotrophs: η_g Ammonification: k_a Hydrolysis: k_h, K_X Correction factor for anoxic hydrolysis: η_h

Model

- For a completely mixed reactor ASM1 results in 13 nonlinear ordinary differential equations (NODE)
- Given a set of initial conditions, solve these using numerical methods techniques, i.e.,
  - General solvers such as Matlab, Simulink, ACSL, etc.
  - Specialized simulators such as GPS-X, BioWin, etc. as we will see later.
- A plug flow reactor consisting for example of 10 CSTR would result in 130 NODEs – if you have 8 such reactors in parallel, this translates to more than 1000 NODEs.

ASM1, ASM2, ASM2d, ASM3, etc.

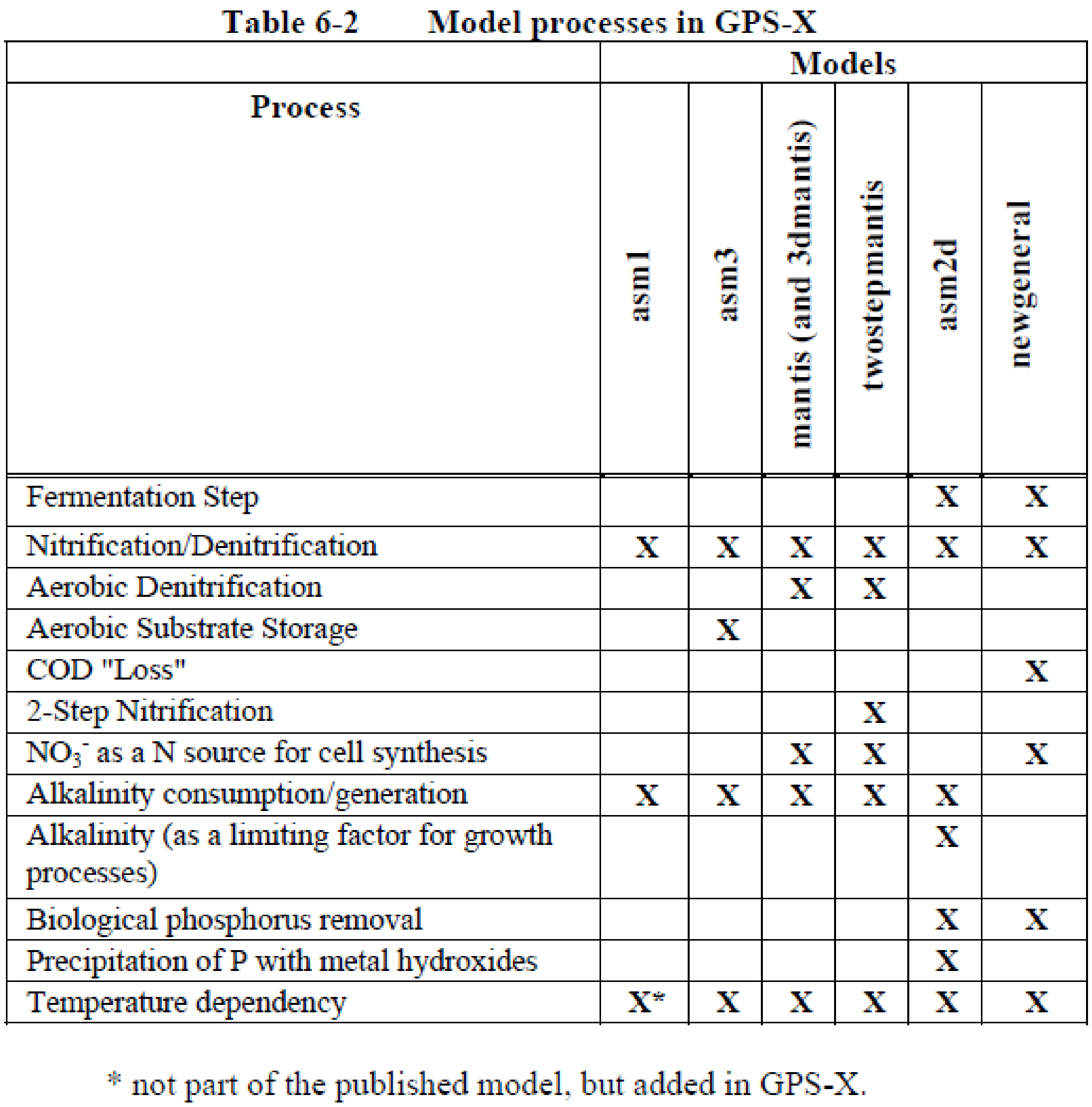
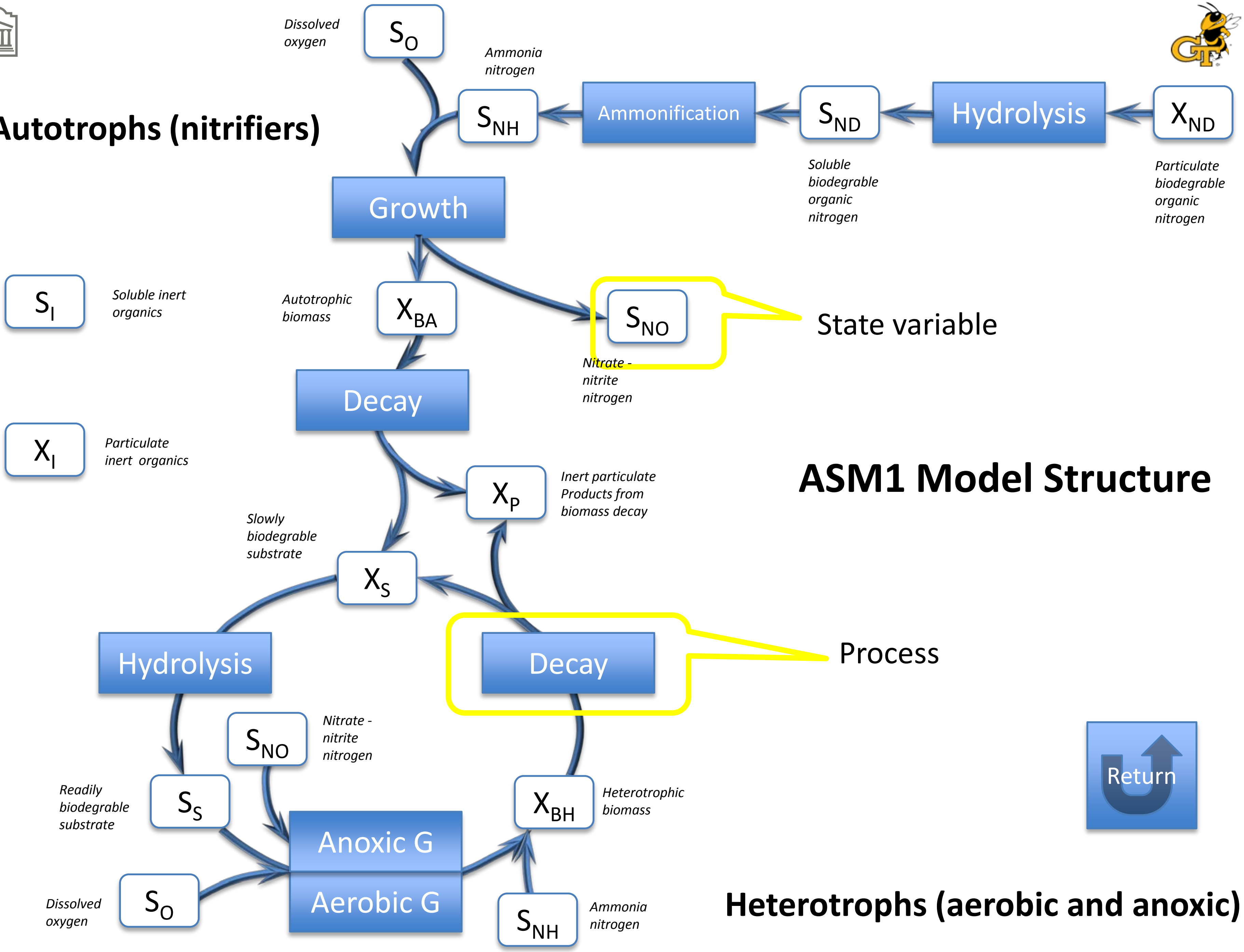


Table 6-2 Model processes in GPS-X

Process	Models					
	asm1	asm3	mantis (and 3dmantis)	twostepmantis	asm2d	newgeneral
Fermentation Step					X	X
Nitrification/Denitrification	X	X	X	X	X	X
Aerobic Denitrification			X	X		
Aerobic Substrate Storage		X				
COD "Loss"						X
2-Step Nitrification				X		
NO_3^- as a N source for cell synthesis			X	X		X
Alkalinity consumption/generation	X	X	X	X	X	
Alkalinity (as a limiting factor for growth processes)					X	
Biological phosphorus removal					X	X
Precipitation of P with metal hydroxides					X	
Temperature dependency	X*	X	X	X	X	X

* not part of the published model, but added in GPS-X.

ASM1 Model Structure



Autotrophs (nitrifiers)

S_O Dissolved oxygen

S_{NH} Ammonia nitrogen

Ammonification

S_{ND} Soluble biodegrable organic nitrogen

Hydrolysis

X_{ND} Particulate biodegrable organic nitrogen

Growth

X_{BA} Autotrophic biomass

S_{NO} Nitrate - nitrite nitrogen

State variable

Decay

S_I Soluble inert organics

X_I Particulate inert organics

X_P Inert particulate Products from biomass decay

X_S Slowly biodegrable substrate

Hydrolysis

Decay

Process

S_{NO} Nitrate - nitrite nitrogen

S_S Readily biodegrable substrate

Anoxic G

Aerobic G

X_{BH} Heterotrophic biomass

S_O Dissolved oxygen

S_{NH} Ammonia nitrogen

Heterotrophs (aerobic and anoxic)

Return