A new Schematic representation of ASM models for concepts comparison

A new schematic representation of the model processes is proposed to facilitate model concept comparison in a systematic and transparent way. For each process type, the standard processes that use the same modelling concept are represented on a single figure, and the standard processes that are different in terms of modelling concept are represented on separate figures. Different concepts are given different numbers (concept 1, concept 2…), whereas variations within the same concept are pointed out using letters (concept 1a, 1b…). The process is represented as a reaction with consumed components on the left of the figure and produced components on the right. Figure I shows the symbols used for the schematic representation:

- Models that consider the process are given by a letter (a to g).
- The electron acceptor condition of the process is indicated by a square (Ox: aerobic; Ax: anoxic; An: anaerobic), close to the corresponding model name.
- The included state variables are represented through both a shape and a background: the shape indicates whether the variable is particulate or colloidal, soluble or refers to an organism and internal storage, and the background indicates its composition in terms of ThOD (theoretical oxygen demand) (C), nitrogen (N) or phosphorus (P). The state variable name is indicated inside the shape, using the standardised notation from Corominas *et al.* (2010).
- The electron acceptor consumed in the process is represented by a square. For instance, depending on its usage, nitrate can be represented by a circle-square (electron acceptor) or by a circle only (substrate).

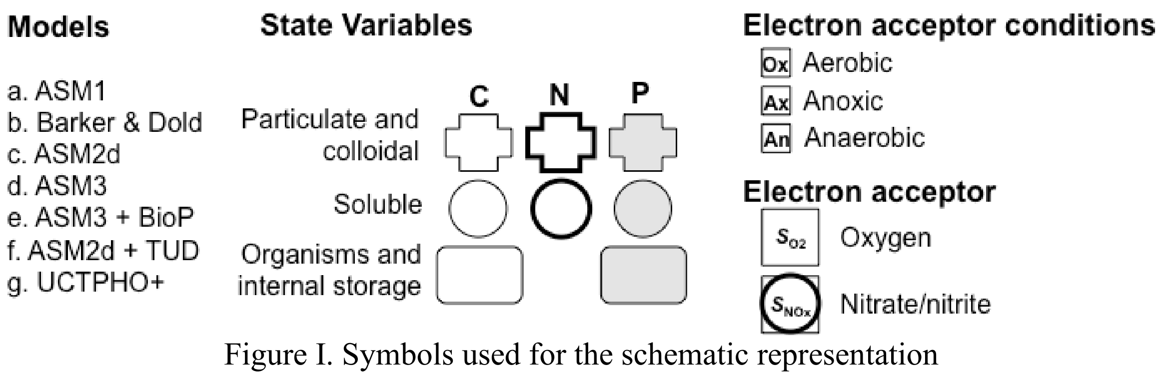


Figure I. Symbols used for the schematic representation

To simplify the graphs, alkalinity and total suspended solids are not represented. Only important stoichiometric coefficients (especially yields) are specified, as others can be calculated through conservation of ThOD, nitrogen and phosphorus (Hauduc et al. 2010).

In this process representation, the consumed and produced components of the reaction are linked by black arrows. In case state variables are not considered by all models or under all conditions, the models or conditions concerned are specified on the arrow.

The kinetic expression for the rate of reaction is also part of the concept and is therefore represented. This is also done in a condensed way by a standardised compact notation. Table I illustrates the different symbols used to keep the expression readable.

Table I. Symbols used for kinetic expressions: examples

Description	**Notation**	**Symbol**
Kinetic coefficients: maximum specific growth rate	μ_{OHO}	μ_{OHO}
Concentration of S_{NOx}	S_{NOx}	S_{NOx}
Monod function with S_B as substrate	$\frac{S_B}{K_{SB}+S_B}$	$M(S_B)$
Inhibition Monod function with S_{NOX} as electron acceptor	$\frac{K_{NOx}}{K_{NOx}+S_{NOx}}$	$IM(S_{NOx})$
Monod function with S_{PO4} as substrate, only used in models considering phosphorus removal	$\frac{S_{PO4}}{K_{PO4}+S_{PO4}}$	$\langle M(S_{PO4}) \rangle$
Electron acceptor conditions (ex: OHO growth) (aerobic or anoxic conditions)		$\left\langle \begin{matrix} M(S_{O2}) \\ \eta_{\mu OHO,Ax} M(S_{NOx}) \cdot IM(S_{O2x}) \end{matrix} \right\rangle$

N.B.: The symbol $\langle\ \rangle$ is used to indicate optional or alternative terms, one or none of the lines apply for the given condition.

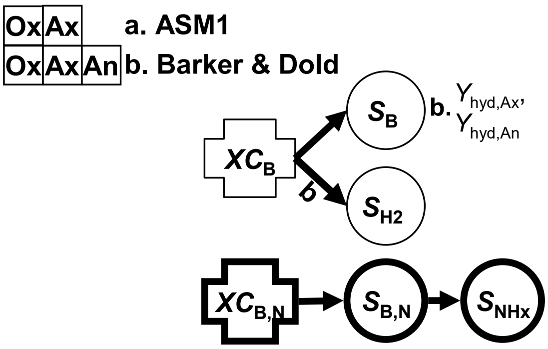
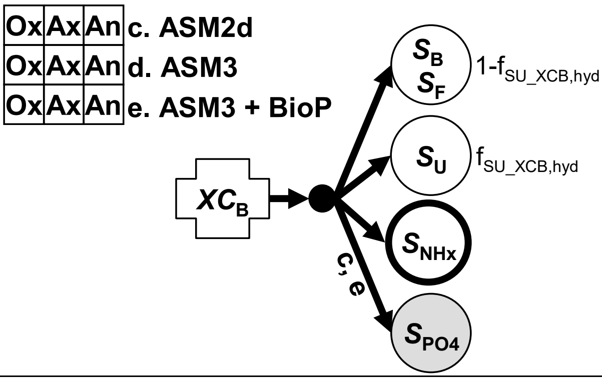
The saturation functions and inhibition functions, which have the form of a Monod expression, are expressed M() or IM(), with the component concerned in parenthesis. The symbol $\langle\ \rangle$ is used to indicate optional or alternative terms depending on the model or the environmental condition (see Table I for examples).

Nine standard processes have been identified and are listed below. These "standard processes" involve mechanisms that only differ by the environmental conditions under which they take place. For instance, aerobic and anoxic OHO growth processes are combined as one OHO standard growth process. This work is limited to biological processes, and therefore chemical phosphorus precipitation is not discussed. Besides, as OHO- and ANO-related processes of ASM2d+TUD are exactly the same as ASM2d, ASM2d+TUD will be studied only for BioP-related processes.

The nine standard processes considered are:

- Hydrolysis of particulate substrate: Table II
- Fermentation: Table III
- OHO growth: Table IV
- ANO growth: Table V
- OHO & ANO decay: Table VI
- PHA storage: Table VII
- PolyP storage: Table VIII
- PAO growth: Table IX
- PAO decay: Table X and Table XI (PAO storage pools release/consumption)

Table II. Hydrolysis of particulate substrate

Concept 1a: One step hydrolysis with organic N and C considered separately	**Concept 1b:** One step hydrolysis with N and P linked to organic matter
	

Organics:

a: $q_{XCB\_SB,hyd}\cdot M\left(\frac{XC_B}{X_{OHO}}\right)\cdot\left\langle\begin{matrix}M(S_{O2})\\ \eta_{qhyd,Ax}\cdot M(S_{NOx})\cdot IM(S_{O2})\end{matrix}\right\rangle\cdot X_{OHO}$

b, c: $q_{XCB\_SB,hyd}\cdot M\left(\frac{XC_B}{X_{OHO}}\right)\cdot\left\langle\begin{matrix}M(S_{O2})\\ \eta_{qhyd,Ax}\cdot M(S_{NOx})\cdot IM(S_{O2})\\ \eta_{qhyd,An}\cdot IM(S_{NOx})\cdot IM(S_{O2})\end{matrix}\right\rangle\cdot X_{OHO}$

d, e: $q_{XCB\_SB,hyd}\cdot M\left(\frac{XC_B}{X_{OHO}}\right)\cdot X_{OHO}$

Particulate nitrogen hydrolysis:

a, b: $q_{XCB\_SB,hyd}\cdot M\left(\frac{XC_{B,N}}{X_{OHO}}\right)\cdot\left\langle\begin{matrix}M(S_{O2})\\ \eta_{qhyd,Ax}\cdot M(S_{NOx})\cdot IM(S_{O2})\\ \eta_{qhyd,An}\cdot IM(S_{NOx})\cdot IM(S_{O2})\end{matrix}\right\rangle\cdot X_{OHO}$

Ammonification:

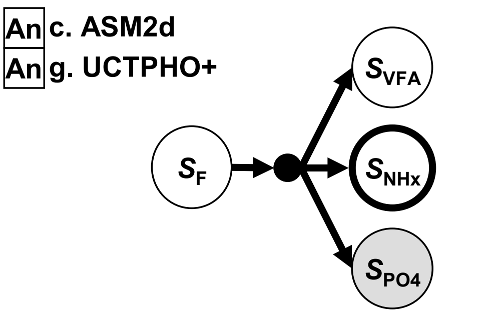
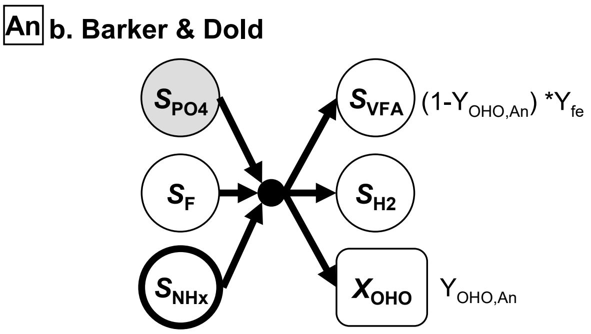
a: $q_{am}\cdot S_{B,N}\cdot X_{OHO}$

b: $q_{am}\cdot S_{B,N}\cdot(X_{OHO}+X_{PAO})$

N.B.: in UCTPHO+, hydrolysis is considered simultaneously with growth. ASM2d+TUD is identical to ASM2d.

The symbol ‹ › is used to indicate optional or alternative terms, one or none of the lines should be chosen.

Table III. Fermentation process

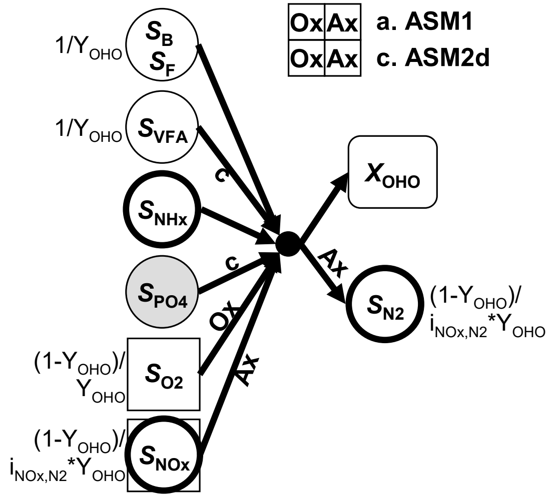
Concept 1: Transformation	**Concept 2:** Anaerobic growth process
	
c: $q_{SF\_VFA,Max}\cdot M(S_F)\cdot IM(S_{O2})\cdot IM(S_{NOx})\cdot X_{OHO}$ **g:** $q_{SF\_VFA,Max}\cdot S_F\cdot IM(S_{O2})\cdot IM(S_{NOx})\cdot X_{OHO}$	$q_{SF\_VFA,Max}\cdot M(S_F)\cdot M(S_{NHx})\cdot M(S_{PO4})\cdot IM(S_{O2})\cdot IM(S_{NOx})\cdot X_{OHO}$

N.B.: ASM2d+TUD is identical to ASM2d.

Table IV. OHO growth process concepts

<table>
<tr><td colspan="2">Concept 1: direct growth</td><td>Concept 2: storage - growth</td></tr>
<tr>
<td>

Concept 1a: S_{NHx} as only nitrogen source



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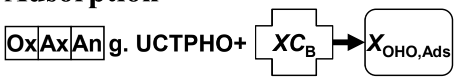
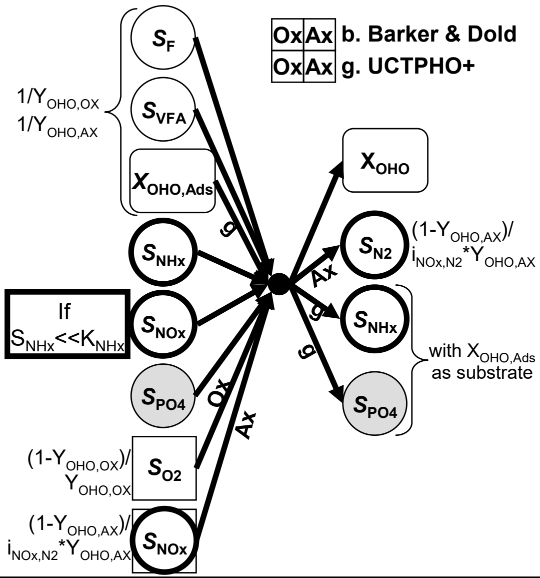
<td>

Concept 1b: S_{NHx} or S_{NOx} as nitrogen source

Adsorption



Growth



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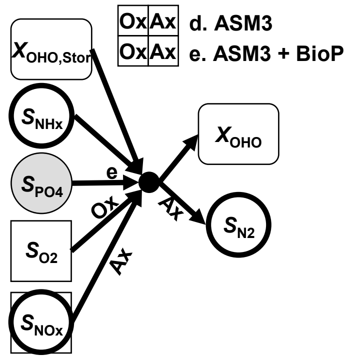
Storage

Growth



</td>
</tr>
<tr>
<td colspan="2">

Adsorption: $q_{XCB\_Ads}\cdot XC_B\left(f_{Ads\_OHO,Max}-\frac{X_{Ads}}{X_{OHO}}\right)\cdot X_{OHO}$

Growth: With S_{Sub} the considered substrate (S_B, S_F or S_{VFA})

$$\left\langle\begin{matrix}\mu_{OHO,Max}\left[M(S_{Sub})\frac{S_{Sub}}{\sum_i S_{Sub,i}}\right]\\ \mu_{Ads\_OHO,Max}\left[M\left(\frac{X_{Ads}}{X_{OHO}}\right)\frac{S_{Sub}}{\sum_i S_{Sub,i}}\right]\end{matrix}\right\rangle\cdot\left\langle\begin{matrix}M(S_{O2x})\\ \eta_{\mu OHO,Ax}M(S_{NOx})\cdot IM(S_{O2x})\end{matrix}\right\rangle\cdot\langle M(S_{PO4})\rangle\cdot\left\langle\begin{matrix}M(S_{NHx})\\ M(S_{NOx})\cdot IM(S_{NHx})\end{matrix}\right\rangle\cdot X_{OHO}$$

</td>
<td>

Storage:

$$q_{SB\_Stor}\cdot M(S_B)\cdot\left\langle\begin{matrix}M(S_{O2x})\\ \eta_{\mu OHO,Ax}M(S_{NOx})\cdot IM(S_{O2x})\end{matrix}\right\rangle\cdot X_{OHO}$$

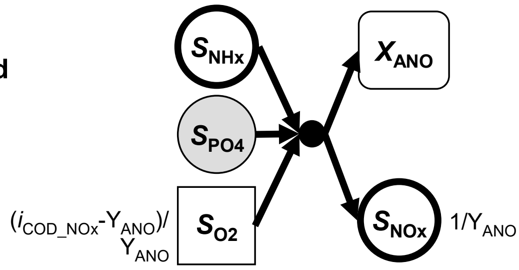
Growth:

$$\mu_{OHO,Max}\cdot M\left(\frac{X_{OHO,Stor}}{X_{OHO}}\right)\cdot\left\langle\begin{matrix}M(S_{O2x})\\ \eta_{\mu OHO,Ax}M(S_{NOx})\cdot IM(S_{O2x})\end{matrix}\right\rangle\cdot\langle M(S_{PO4})\rangle\cdot M(S_{NHx})\cdot X_{OHO}$$

</td>
</tr>
</table>

Table V. ANO growth process

Ox a. ASM1
Ox b. Barker & Dold
Ox c. ASM2d
Ox d. ASM3
Ox e. ASM3 + BioP
Ox f. ASM2d + TUD
Ox g. UCTPHO+



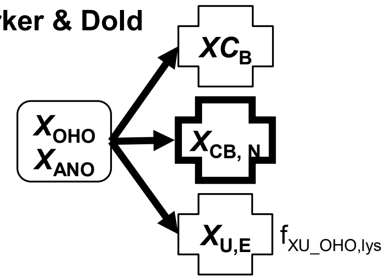
$$\mu_{ANO,Max} \cdot M(S_{NHx}) \cdot \langle M(S_{PO4}) \rangle \cdot M(S_{O2}) \cdot X_{ANO}$$

Table VI. OHO and ANO decay process concepts

Concept 1: Death-Regeneration concept

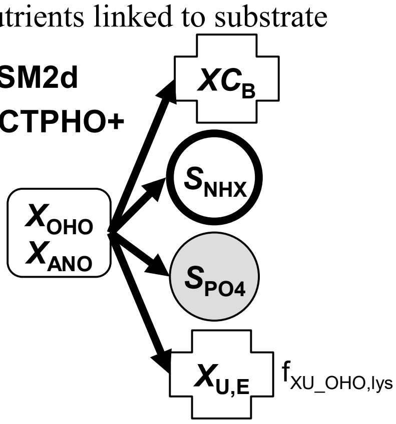
Concept 1a: nutrients considered separately from substrate

Ox Ax An a. ASM1
Ox Ax An b. Barker & Dold



Concept 1b: nutrients linked to substrate

Ox Ax An c. ASM2d
Ox Ax An g. UCTPHO+



Heterotrophs:

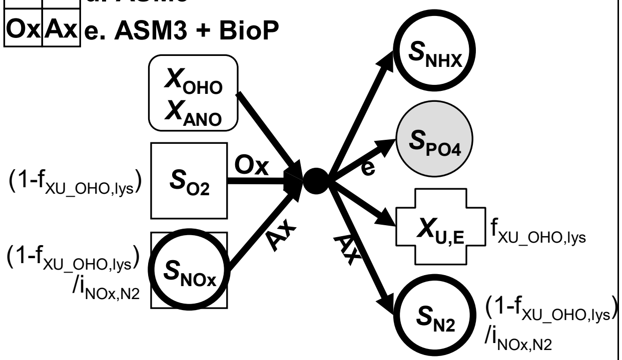
$$b_{OHO} \cdot X_{OHO}$$

Autotrophs:

$$b_{ANO} \cdot X_{ANO}$$

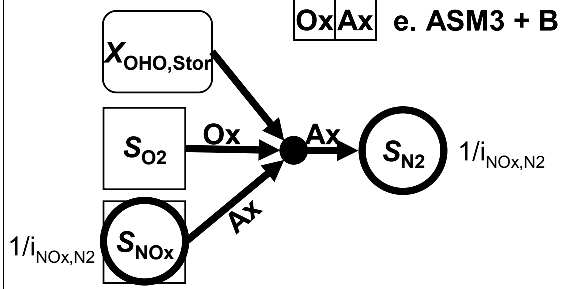
Concept 2: Endogenous respiration concept

Ox Ax d. ASM3
Ox Ax e. ASM3 + BioP



Storage lysis (OHOs only)

Ox Ax d. ASM3
Ox Ax e. ASM3 + BioP



Heterotrophs:

$$\left\langle \begin{matrix} m_{OHO,Ox} \cdot M(S_{O2}) \\ m_{OHO,Ax} \cdot M(S_{NOx}) \cdot IM(S_{O2}) \end{matrix} \right\rangle \cdot X_{OHO}$$

Storage lysis (OHOs only)

$$\left\langle \begin{matrix} m_{Stor,Ox} \cdot M(S_{O2}) \\ m_{Stor,Ax} \cdot M(S_{NOx}) \cdot IM(S_{O2}) \end{matrix} \right\rangle \cdot X_{OHO,Stor}$$

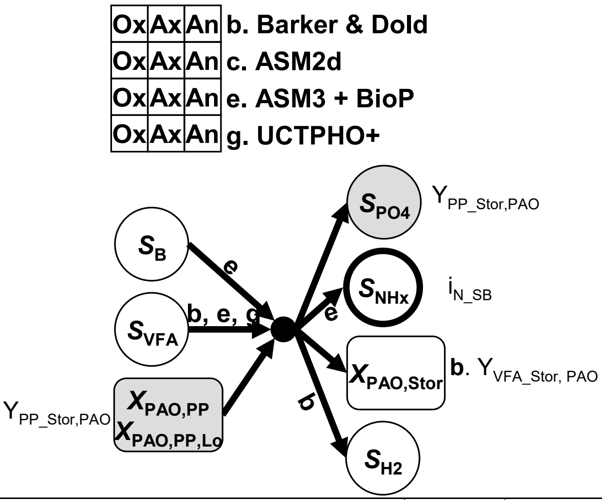
Autotrophs:

$$\left\langle \begin{matrix} m_{ANO,Ox} \cdot M(S_{O2}) \\ m_{ANO,Ax} \cdot M(S_{NOx}) \cdot IM(S_{O2}) \end{matrix} \right\rangle \cdot X_{ANO}$$

N.B.: ASM2d+TUD is identical to ASM2d.

The symbol ‹ › is used to indicate optional or alternative terms, one or none of the lines should be chosen.

Table VII. PHA storage process concept

<table>
<tr><th>Concept 1:
Energy from polyP, reducing power neglected</th><th>Concept 2: Energy from polyP, reducing power from glycogen</th></tr>
<tr><td>


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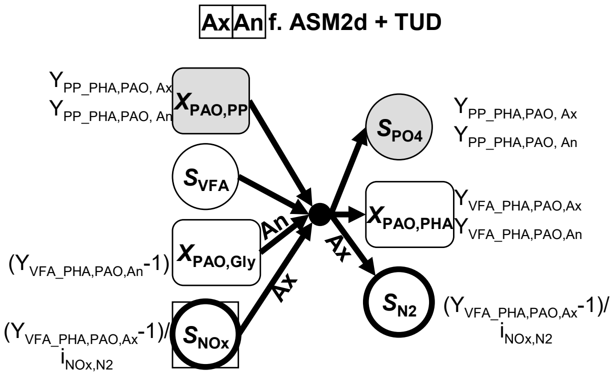
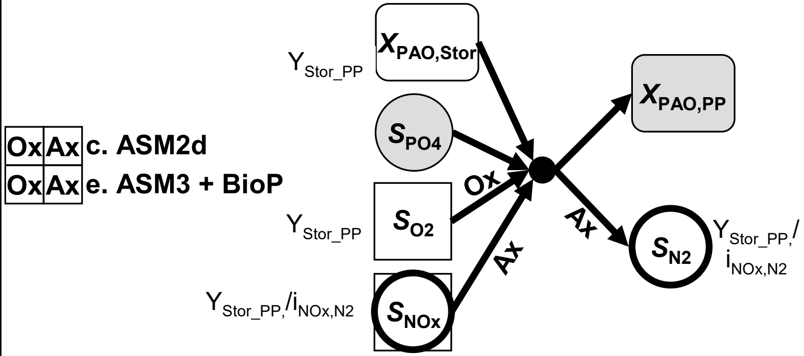
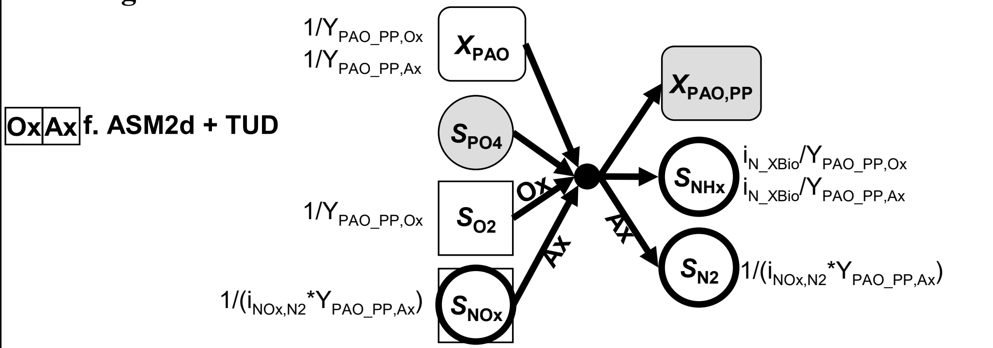


</td></tr>
<tr><td>b, g: $q_{PAO,VFA\_Stor}\cdot M(S_{VFA})\cdot M(X_{PAO,PP})\cdot X_{PAO}$
c, e:
$q_{PAO,VFA\_Stor}\cdot\left\langle\begin{matrix}M(S_{VFA})\\ M(S_B)\end{matrix}\right\rangle\cdot M(X_{PAO,PP}/X_{PAO})\cdot X_{PAO}$</td><td>$\left\langle\begin{matrix}q_{PAO,VFA\_PHA,An}\cdot IM(S_{O2})\cdot IM(S_{NOx})\cdot M(X_{PAO,Gly})\\ q_{PAO,VFA\_PHA,Ax}\cdot IM(S_{O2})\cdot M(S_{NOx})\end{matrix}\right\rangle$
$\cdot M(S_{VFA})\cdot M(X_{PAO,PP})\cdot X_{PAO}$</td></tr>
</table>

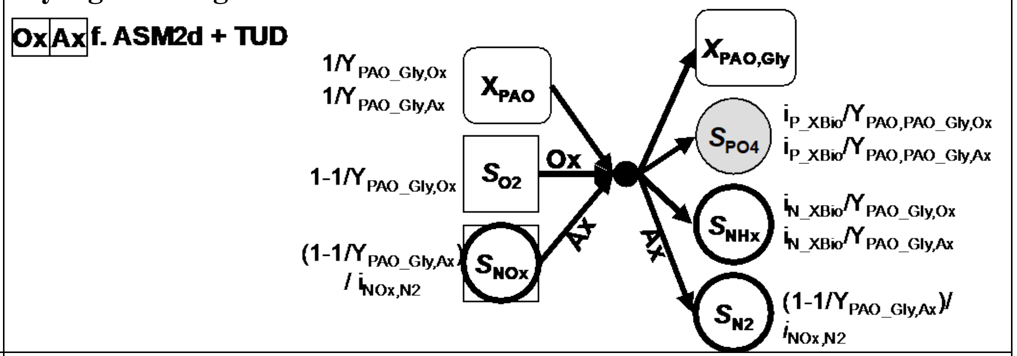
Table VIII. PolyP storage process concept

<table>
<tr><th>Concept 1: Uncoupled processes</th><th>Concept 2: Coupled processes (metabolic model)</th></tr>
<tr><td>


</td><td>
PP storage:



Glycogen storage:



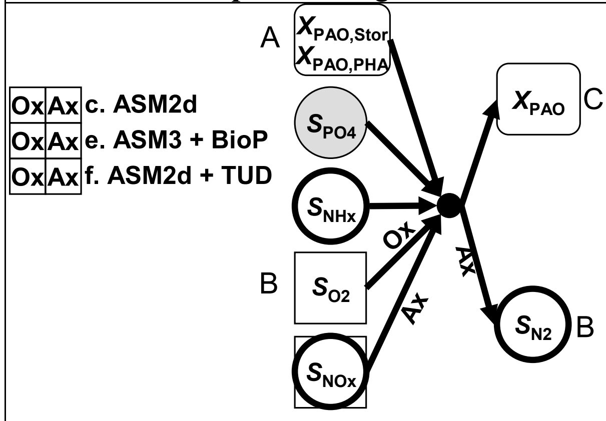
</td></tr>
<tr><td>
$$q_{PAO,PO4\_PP}\cdot\left\langle\begin{matrix}M(S_{O2})\\ \eta_{qPAO,Ax}\cdot IM(S_{O2})\cdot M(S_{NOx})\end{matrix}\right\rangle\cdot M(S_{PO4})\cdot M(X_{PAO,PHA})\cdot M(f_{PP\_PAO,Max}-X_{PAO,PP}/X_{PAO})\cdot X_{PAO}$$
</td><td>
PP storage: $$q_{PAO,PO4\_PP}\cdot\left\langle\begin{matrix}M(S_{O2})\\ \eta_{qPAO,Ax}\cdot IM(S_{O2})\cdot M(S_{NOx})\end{matrix}\right\rangle\cdot[X_{PAO}/X_{PAO,PP}]\cdot M(S_{PO4})\cdot M(X_{PAO,PHA})\cdot M(f_{PP\_PAO,Max}-X_{PAO,PP}/X_{PAO})\cdot X_{PAO}$$

Glycogen storage: $$q_{Gly}\cdot\left\langle\begin{matrix}M(S_{O2})\\ \eta_{qPAO,Ax}\cdot IM(S_{O2})\cdot M(S_{NOx})\end{matrix}\right\rangle\cdot[X_{PAO,PHA}/X_{PAO,Gly}]\cdot M(X_{PAO,PHA})\cdot M(f_{Gly\_PAO,Max}-X_{PAO,Gly}/X_{PAO})\cdot X_{PAO}$$
</td></tr>
</table>

NB: PolyP storage in the Barker & Dold and UCTPHO+ models are considered simultaneously with growth.
The symbol ‹ › is used to indicate optional or alternative terms, one or none of the lines should be chosen.

Table IX. PAO growth

Concept 1: PAO growth



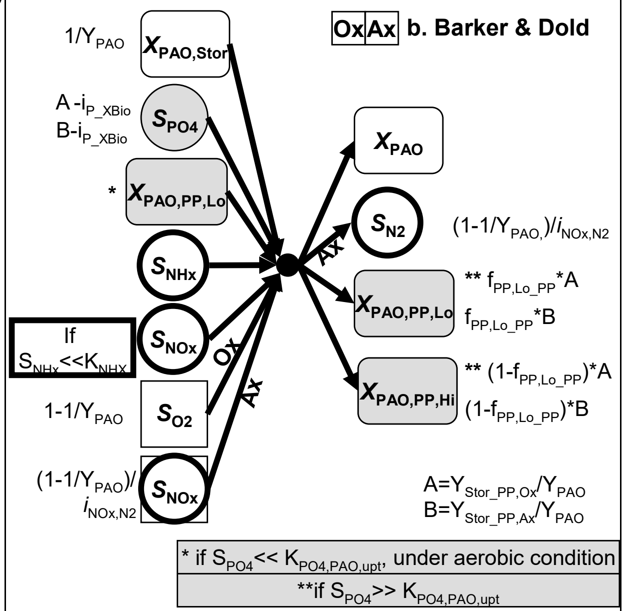
	A	B	C
c.	$1/Y_{Stor\_PAO}$	$1\text{-}1/Y_{Stor\_PAO}$	1
e.	$1/Y_{Stor\_PAO,Ox}$ $1/Y_{Stor\_PAO,Ax}$	$1\text{-}1/Y_{Stor\_PAO,Ox}$ $1\text{-}1/(i_{NOx,N2}{*}Y_{Stor\_PAO,Ax})$	1
f.	1	$1\text{-}1/Y_{Stor\_PAO,Ox}$ $1\text{-}1/(i_{NOx,N2}{*}Y_{Stor\_PAO,Ax})$	$1/Y_{Stor\_PAO,Ox}$ $1/Y_{Stor\_PAO,Ax}$

c, e: $$\mu_{PAO,Max} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ \eta_{\mu PAO} \cdot IM(S_{O2}) \cdot M(S_{NOx}) \end{matrix} \right\rangle \cdot M\left(\frac{X_{PAO,Stor}}{X_{PAO}}\right) \cdot M(S_{NHx}) \cdot M(S_{PO4}) \cdot X_{PAO}$$

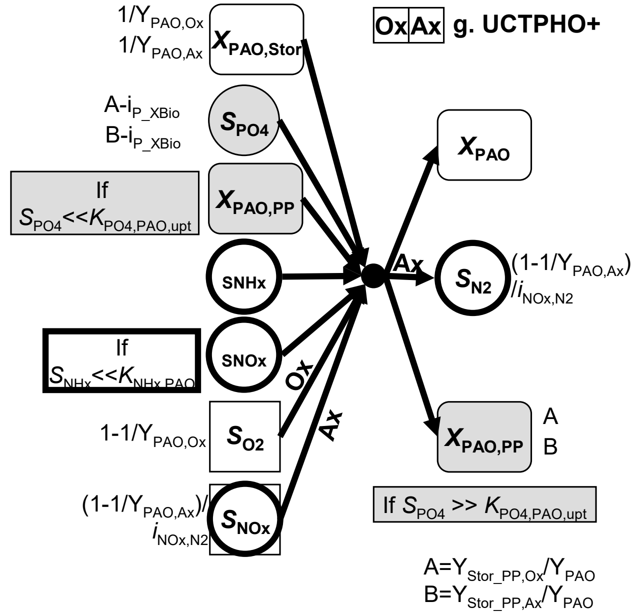
d: $$q_{PHA\_PAO} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ \eta_{\mu PAO} \cdot IM(S_{O2}) \cdot M(S_{NOx}) \end{matrix} \right\rangle \cdot M\left(\frac{X_{PAO,PHA}}{X_{PAO}}\right) \cdot M(S_{NHx}) \cdot M(S_{PO4}) \cdot X_{PAO}$$

Concept 2: Simultaneous growth and polyP storage

Concept 2a: Two polyP storage pools

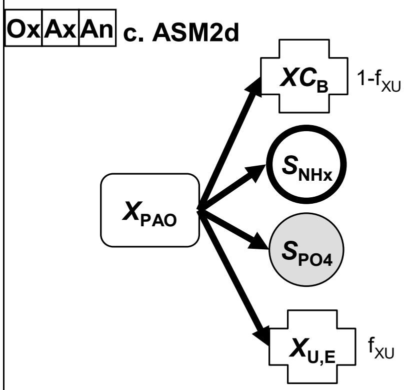
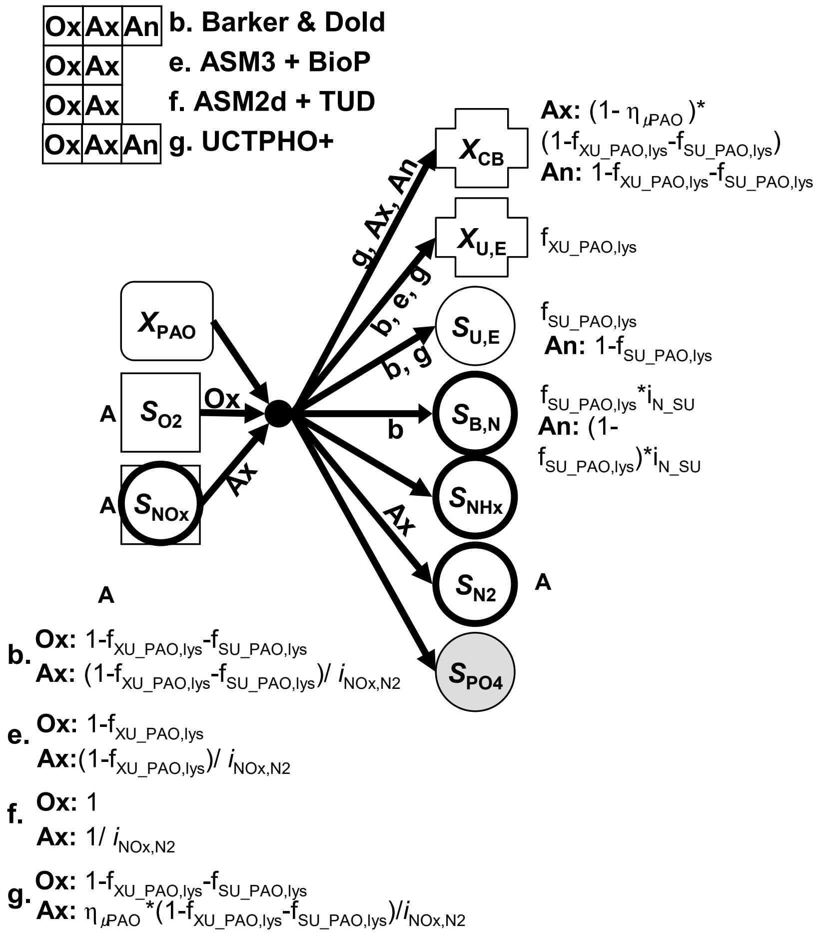


Concept 2b: Single polyP storage pools



$$\left\langle \begin{matrix} \mu_{PAO,Max} \\ \mu_{PAO,Max,P\lim} \end{matrix} \right\rangle \cdot \left\langle \begin{matrix} M(S_{O2}) \\ \eta_{\mu PAO} \cdot IM(S_{O2}) \cdot M(S_{NOx}) \end{matrix} \right\rangle \cdot M(X_{PAO,Stor} / X_{PAO}) \cdot \left\langle \begin{matrix} M(S_{NHx}) \\ IM(S_{NHx}) \cdot M(S_{NOx}) \end{matrix} \right\rangle \cdot \left\langle \begin{matrix} M(S_{PO4}) \\ IM(S_{PO4}) \cdot M(X_{PAO,PP}) \end{matrix} \right\rangle \cdot X_{PAO}$$

Table X: PAO decay process concepts

<table>
<tr><th>Concept 1: Death-regeneration concept</th><th colspan="2">Concept 2: Endogenous respiration</th></tr>
<tr><td>
</td><td colspan="2">

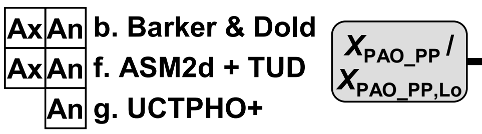
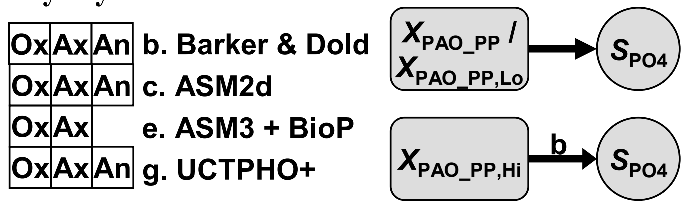
Maintenance:

</td></tr>
<tr><td rowspan="2">$b_{PAO}\cdot X_{PAO}$</td><td>Decay:</td><td>b, g: $m_{PAO}\cdot\left\langle\begin{matrix} M(S_{O2}) \\ IM(S_{O2})\cdot M(S_{NOx}) \\ IM(S_{O2})\cdot IM(S_{NOx})\end{matrix}\right\rangle\cdot X_{PAO}$
e: $m_{PAO}\cdot\left\langle\begin{matrix} M(S_{O2}) \\ \eta_{mPAO}\cdot IM(S_{O2})\cdot M(S_{NOx})\end{matrix}\right\rangle\cdot X_{PAO}$
f: $\left\langle\begin{matrix} m_{PAO,Ox}\cdot M(S_{O2}) \\ m_{PAO,Ax}\cdot IM(S_{O2})\cdot M(S_{NOx})\end{matrix}\right\rangle\cdot X_{PAO}$</td></tr>
<tr><td>Maintenance:</td><td>b: $b_{PP\_PO4}\cdot IM(S_{O2})\cdot M(X_{PAO,PP,Lo})\cdot X_{PAO}$
f: $m_{PAO,An}\cdot IM(S_{O2})\cdot IM(S_{NOx})\cdot M(X_{PAO,PP})\cdot X_{PAO}$
g:
$b_{PP\_PO4}\cdot\left\langle\begin{matrix}(1-\eta_{\mu PAO})\cdot IM(S_{O2})\cdot M(S_{NOx}) \\ IM(S_{O2})\cdot IM(S_{NOx})\end{matrix}\right\rangle\cdot M(X_{PAO,PP})\cdot X_{PAO}$</td></tr>
</table>

Table XI: PAO storage pools release/consumption during lysis

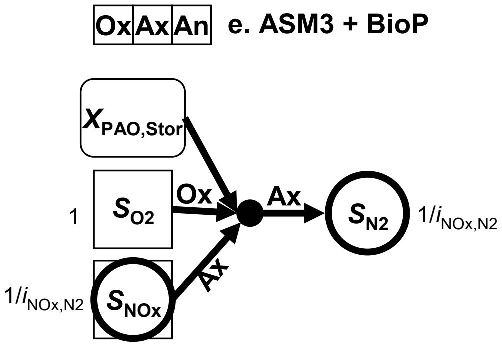
<table>
<tr><th>Concept 1:
Stored compounds are released</th><th>Concept 2:
Stored compounds are consumed</th></tr>
<tr><td>

PolyP lysis:



PHA lysis:

</td><td>



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PolyP lysis:

b, g:

$$m_{PAO} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ IM(S_{O2}) \cdot M(S_{NOx}) \\ IM(S_{O2}) \cdot IM(S_{NOx}) \end{matrix} \right\rangle \cdot \left\langle \begin{matrix} X_{PAO,PP,Lo} / X_{PAO} \\ X_{PAO,PP,Hi} / X_{PAO} \end{matrix} \right\rangle \cdot X_{PAO}$$

c: $b_{PP\_PAO} \cdot X_{PAO,PP}$

e: $b_{PP\_PAO} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ \eta_{bPP\_PAO} \cdot IM(S_{O2}) \cdot M(S_{NOx}) \end{matrix} \right\rangle \cdot X_{PAO,PP}$

PHA lysis:

b: $m_{PAO} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ IM(S_{O2}) \cdot M(S_{NOx}) \\ IM(S_{O2}) \cdot IM(S_{NOx}) \end{matrix} \right\rangle \cdot \frac{X_{PAO,Stor}}{X_{PAO}} \cdot X_{PAO}$

c: $b_{Stor\_PAO} \cdot X_{PAO,Stor}$

g:

$$m_{PAO} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ IM(S_{O2}) \cdot M(S_{NOx}) \\ IM(S_{O2}) \cdot IM(S_{NOx}) \end{matrix} \right\rangle \cdot M(S_{NHx}) \cdot M(S_{PO4}) \cdot \frac{X_{PAO,Stor}}{X_{PAO}} \cdot X_{PAO}$$

</td><td>

$m_{PAO,Stor} \cdot$

$$\left\langle \begin{matrix} M(S_{O2}) \\ \eta_{mPAO,Stor} \cdot IM(S_{O2}) \cdot M(S_{NOx}) \end{matrix} \right\rangle \cdot X_{PAO,Stor}$$

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