A new plant-wide modelling methodology for WWTPs

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PII: S0043-1354(07)00395-8
DOI: doi:10.1016/j.watres.2007.06.019
Reference: WR 6503

To appear in: *Water Research*

Received date: 23 February 2007
Revised date: 20 May 2007
Accepted date: 10 June 2007

Cite this article as: P. Grau, M. de Gracia, P.A. Vanrolleghem and E. Ayesa, A new plant-wide modelling methodology for WWTPs, *Water Research* (2007), doi:10.1016/j.watres.2007.06.019

TITLE: A NEW PLANT-WIDE MODELLING METHODOLOGY FOR WWTPs

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ABSTRACT

This paper presents a new Plant-Wide Modelling methodology for describing the dynamic behaviour of water and sludge lines in WWTPs. The methodology is based on selecting the set of process transformations needed for each specific WWTP to model all unit-process elements in the entire plant. This *"transformation-based"* approach, in comparison with the conventional *"process-based"* approach, does not require the development of specific transformers to interface the resulting unit-process models, facilitates the mass and charge continuity throughout the whole plant and is flexible enough to construct models tailored for each plant under study. As an illustrative example, a Plant-Wide model for a WWTP that includes carbon removal and anaerobic digestion has been constructed, and the main advantages of the proposed methodology for integrated modelling have been demonstrated. As a final consequence, this paper proposes a rewriting of the existing unit-process models according to the new standard *transformation-based* approach for integrated modelling purposes.

1. INTRODUCTION

Mathematical modelling and dynamic simulation of the processes in a WWTP is a useful tool in the selection of operational strategies that improve process stability, effluent quality and operational costs. Optimum solutions for the design or operation of an entire WWTP, including the mutual relationships among the different unit-process elements involved in water and sludge lines, frequently differ from the simple

compilation of solutions achieved for the design or operation of each unit-process element separately. Therefore, models used to analyze the entire WWTP must be rigorously developed taking into account the dynamic description of all the relevant processes in water and sludge lines (physico-chemical treatments, primary and secondary settling, activated sludge reactors, anaerobic digesters, etc.), and the effect of reject flows among the different lines.

Consequently, if the behaviour of the entire plant must be evaluated in order to establish optimum design and operational criteria, the construction of integrated WWTP models including water and sludge lines, is required. But obtaining integrated WWTP models that guarantee mass and charge continuity throughout the model plant is not a straightforward task (Vanrolleghem et al., 2005; Wentzel et al., 2006). The main challenges in obtaining integrated model plants arise from the incompatibilities and different descriptions of the components and transformations in standard process models. These include varying descriptions of organic carbonaceous substrates and organic nitrogen as well as pH and buffer capacity in water or sludge and the different processes considered, etc. With respect to this problem, two main plant-wide modelling approaches have been proposed so far.

The first approach is based on the construction of a *Supermodel* consisting of all the components and transformations needed to reproduce every process within the entire plant (Jones and Tákacs, 2004; Seco et al., 2004). In this model, components and transformations are common to every unit process model in the WWTP and therefore, specific transformers connecting different process models are not required. Nevertheless, the use of a unique *Supermodel* for any WWTP lacks the flexibility to add or remove components as well as transformations depending on the case study and model aims. Another significant drawback to this approach is the continuous increase of

the model size required to progressively adapt the Supermodel to reproduce new processes (Volcke et al., 2006).

The second approach, known as the *Interfaces* approach, is based on the construction of transformers among existing standard models. An illustrative example of transformers between the Activated Sludge Model ASM1 (Henze et al., 2000) and the Anaerobic Digestion Model ADM1 (Batstone et al., 2002) has been proposed by Copp et al. (2003) for the simulation of a Standard WWTP in the Benchmark study BSM2 (Jeppsson et al., 2006). In order to guarantee mass and charge continuity in the model interfaces Vanrolleghem et al. (2005) propose a general methodology (CBIM) for the interface of any two standard models (Zaher et al., 2007; Volcke et al., 2006). However, although the *Interfaces* approach facilitates the construction of integrated models tailored to the case study, there are some limitations when it comes to properly transforming the model components among existing models, guaranteeing mass and charge continuity under any dynamic condition (Grau et al., 2007).

Combining aspects from both approaches, in this paper, a new Plant Wide Modelling methodology based on the most appropriate transformations for each specific case study is proposed. This *transformation-based* approach, specially adequate for integrated modelling purposes, permits the construction of models tailored to the WWTP being studied without the need for specific transformers among process models and guarantees the mass and charge continuity at any point in the plant.

2. PLANT-WIDE MODELLING METHODOLOGY

This paper proposes a new Plant-Wide Modelling methodology for the systematic and rigorous construction of the most appropriate mathematical models for describing, in an integrated way, the dynamic behaviour of the entire WWTP under study, including the

main unit-process elements of both the water and sludge lines. The proposed methodology is based on selecting, for each specific WWTP, the set of compatible process transformations needed to model all unit-process elements throughout the entire plant. This *"transformation-based"* approach, in comparison with the conventional *"process-based"* approach, does not require the development of specific transformers to interface the resulting unit-process models and additionally facilitates the mass and charge continuity throughout the whole plant.

The proposed modelling methodology requires, as a preliminary step, the compilation of the stoichiometry and kinetics (Petersen matrix) of all the most relevant biochemical, chemical and physico-chemical transformations that can occur in a WWTP, in order to create a general *List of Transformations* (**LT**) for Plant-Wide Modelling objectives.

This List should be approved and standardized within the scientific community and serve as the common base for the building of any WWTP model. Additional transformations or alternative descriptions of the existing ones could be introduced when needed without changes in the modelling methodology.

Once the general *List of Transformations* **(LT)** has been defined and compiled, the construction of every *Plant-Wide Model* (PWM) under study is based on a systematic procedure. The compilation of the LT and the systematic procedure proposed in this paper for the construction of plant-wide models for WWTPs are described in detail in the following paragraphs.

The general List of Transformations (LT) for Plant-Wide Modelling

The basic sources for the selection of the most relevant transformations involved in WWTPs are the well-known IWA models ASM1, ASM2d, ASM3 (Henze et al., 2000) and ADM1 (Batstone et al., 2002). However, in order to obtain a standardized and

compatible LT for a PWM objective, some modifications should be made to the original models.

On the one hand, stoichiometry must be defined in order to avoid redundancies in component definition and to guarantee elemental mass (in terms of C, N, O, P and H) and charge continuity for all transformations included within the LT. With this in mind, all model components must be characterised by constant values for their elemental mass composition and charge density. Furthermore, some components must act as *source-sink* or compensation terms accounting for possible imbalances in C, N, O, P, H and charge (Reichert et al., 2001; De Gracia et al., 2006). This role of compensation is usually associated with components in their oxidation reference state (Reichert et al., 2001; Gujer et al., 1999). On the other hand, kinetic equations have to incorporate all required activation or inhibition terms in order to reproduce the appropriate activity under every possible environmental condition in a WWTP (aerobic, anoxic and anaerobic).

Figure 1 shows an example of a possible LT that can be compiled for PWM objectives. Readily and slowly biodegradable organic matter, known in the AS models as S_s and X_s, have been described as a set of different components (monomers and VFAs for soluble substrate and carbohydrates, proteins and lipids for particulates) to properly describe the biological activity under anaerobic conditions. Organic nitrogen, known in the ASM1 model as S_{nd} and X_{nd}, has been considered as part of the soluble and particulate carbonaceous substrates. Buffer capacity and pH prediction have been described by means of the component S_{h+} with a set of acid-base transformations related to inorganic carbon, nitrogen, VFAs, etc. that reproduce buffer capacity and permit a more realistic prediction of pH variations in the water line than in standard AS models (Sötemann et al., 2005). Furthermore, liquid-gas transfer and acid-base transformations have been

125 considered to guarantee mass continuity of the process throughout the whole WWTP.
126 Another modification is the decoupling of the composites and inert matter entering with
127 the influent (X_{c1}, X_i, S_i) from those obtained as decay by-products (X_{c2}, X_p, S_p), in order
128 to avoid the common discrepancies in elemental mass characterisation between both
129 groups of components (Huete et al., 2006). In addition, decay of microorganisms has
130 been described under aerobic, anoxic and anaerobic conditions to reproduce a realistic
131 behaviour of biological activity under all environmental conditions (Siegrist et al.,
132 1999). Finally, some transformations have been described in a more detailed way so that
133 more *Biological Processes* occurring in a WWTP can be modelled. For example, the
134 nitrification and denitrification described as two-step transformations will permit
135 developing models to reproduce processes for treating reject water with high nitrogen
136 content, like the *Sharon-Anammox process*.

137 The elemental mass characterisation for all the components, combined with the use of
138 source-sink components, makes it possible to calculate transformations stoichiometry
139 while guaranteeing mass and charge continuity. Table 1 includes the list of all non
140 redundant components involved in the transformations with their mass composition and
141 charge density. As C, N, O, P and H are considered to be the most relevant elements for
142 the description of the organic compounds, and X summarizes all other elements, any
143 model component can be described according to the following general formula:

$$\left[C_{(\alpha_{C,i}/12)} H_{(\alpha_{H,i})} O_{(\alpha_{O,i}/16)} N_{(\alpha_{N,i}/14)} P_{(\alpha_{P,i}/31)} X_{(\alpha_{X,i}/Mx)} \right]^{\alpha_{Ch,i}} \qquad \textbf{Equation 1}$$

where Mx is the molar mass of the element X.

144 This elemental characterisation does not imply a significant increase in model
145 complexity because the mass fractions of most model components can be reasonably
146 estimated from their known stoichiometric formula, bibliography or experimental data

(Huete et al., 2006). Additionally, the description of the model component's elemental mass permits a straightforward conversion of their mass to the Theoretical Oxygen Demand (ThOD) using, for example, the oxidation state of the elements in the compounds (Gujer et al., 1999) or the mineralization equation (Reichert et al., 2001). Components selected as source-sink components of the LT are dissolved CO_2 for C, NH_4^+ for N, HPO_4^{2-} for P, dissolved O_2 for O, H_2O for H and H^+ for charge.

The LT proposed in Figure 1, with its corresponding components shown in Table 1, are logically expandable with additional transformations and components that could be incorporated into the proposed modelling methodology without any necessary alterations. This may include those related to HPO_4^{2-} precipitation processes, for example.

A systematic procedure for constructing Plant-wide models for WWTPs

Once the general *List of Transformations* (**LT)** has been defined and compiled, the construction of every *Plant-Wide Model* (PWM) under study is based on a systematic procedure with three consecutive steps:

a) Selection of relevant transformations from the general list LT and construction of the specific *Plant Transformation Model* (**PTM)** appropriate for the case study.

b) Construction of a set of compatible *Unit Process Models* (**UPM**) describing each unit of the plant under study.

c) Construction of the integrated *Plant-Wide Model* (**PWM)** by direct interfacing between the Unit Process Models previously developed.

a) Construction of the Plant Transformations Model (**PTM**)

The construction of the *Plant Transformations Model* (**PTM**) consists of the selection of the relevant biochemical, chemical and physico-chemical transformations that should be considered to model the WWTP under study. The selection of appropriate transformations requires sufficient insight into biochemical processes and, consequently, must be systematized in order to simplify the tasks undertaken by model users. Therefore, the following procedure is proposed for easy construction of a PTM:

a.1) *Selection of Biological Processes*

In this first step, the modeller has to decide which *Biological Processes* should be included in the *Plant-Wide Model*, according to the plant configuration and model aims. Some of the most common processes that can take place in a WWTP can be listed as follows:

- Activated sludge process for Carbon removal **AS-C**
- Activated sludge process for Carbon and Nitrogen removal **AS-CN** (Example: ASM1)
- Activated sludge process for C, N and P removal **AS-CNP** (Example: ASM2)
- Acid Fermentation
- Anaerobic digestion (Example: ADM1)
- Sharon process for reject water treatment
- Anammox process for reject water treatment
- Others

a.2) *Selection of the active microorganism populations required to describe the selected Biological Processes*

192 The key to selecting process transformations in each specific plant model is the correct
193 identification of the microorganism populations involved in the biological processes. As
194 shown in Table 2, each of the *Biological Processes* implies the activity of one or more
195 microorganism population and, therefore, from the *Biological Processes* previously
196 selected by the model user, the active microorganism population for each plant under
197 study can be easily identified and selected.

198 a.3) *Selection of the biochemical transformations associated with the activity of*
199 *different microorganism populations*

200 The presence of microorganism populations in a plant involves a set of biochemical
201 transformations associated with their corresponding metabolisms under different
202 environmental conditions. Therefore, once the appropriate set of microorganism
203 populations has been selected according to Table 2, the biochemical transformations
204 which describe for each one of them the growth, decay and enzymatic hydrolysis under
205 all environmental conditions (aerobic, anoxic and anaerobic) must be selected from the
206 general *List of Transformations* (LT) and incorporated into the PTM. As an example,
207 the transformations associated with the activity of Heterotrophic bacteria X_h and
208 Anaerobic Sugar Consuming bacteria X_{su} are shown in Figure 2 according to the list LT
209 previously presented in Figure 1.

210 Once all transformations which describe the activity of the microorganisms have been
211 selected, all components involved in these transformations are easily identified.

212 a.4) *Incorporation of acid-base and liquid-gas equilibria*

213 The last step in the construction of the *Process Transformation Model* (PTM) is the
214 incorporation of the acid-base equilibria and liquid-gas transfer to the PTM constituted
215 in a.3. In this manner, when the model components selected in a.3 are involved in acid-

base or liquid-gas equilibria with their respective acid/base couples or gas phase components, these transformations must also be incorporated into the PTM and the corresponding acid/base conjugated and gas phase components must also be added to the list of selected model components. The set of resulting model components obtained will constitute the *Plant Components Vector* (PCV), which will be the common state vector used for the process description at any point of the plant and will additionally act as a common model interface between all Unit Process Models that will be described in the following section.

Once these four steps have been completed, the resulting set of transformations and the vector of model components (PCV) make up the *Plant Transformations Model* (PTM) (Figure 3). The selected transformations should be able to reproduce the biological activity in the liquid phase for the WWTP under study, including the buffer capacity of the liquid phase and the mass transfer between the liquid and gaseous phase in contact with it.

It is important to point out that the selection of *Biological Processes* considered in a.1 is the only "subjective" decision left to the modeller when constructing the PTM. The selection of active microorganisms, transformations and model components is a straightforward procedure that can be carried out automatically according to predefined rules.

b) Construction of the set of Unit Process Models (UPM) of the plant

The set of *Unit Process Models* (UPM) is the collection of mathematical models describing the most relevant units included in the water and sludge lines of the plant under study. Each UPM must incorporate the mathematical description of both the *mass*

239 *transport* and the *internal transformations* and must use, as a common model interface,
240 the *Plant Components Vector* (PCV) previously described.

241 The mathematical description of the *mass transport* in each UPM is logically quite
242 diverse for different elements of the plant (for example, CSTR reactors, primary or
243 secondary settlers, filters or other solids separation systems, etc.) and sometimes even
244 based on lumped additional variables that are usually a combination of the model
245 components included in the common PCV (a typical example of this is the use of total
246 solids concentration in the modelling of clarification or settling processes).

247 The mathematical description of the *internal transformations* for all UPMs should be, as
248 a general rule, based on the previously constructed PTM. The use of a common set of
249 transformations for all *Unit Process Models* will facilitate a coherent description of the
250 processes throughout the whole plant and guarantee mass continuity. Additionally, the
251 use of the common PCV, as the internal components vector for describing
252 transformations, allows for a direct connection between the Unit Process Models
253 without introducing specific transformers. However, in order to reduce the model
254 complexity and to increase computational efficiency, some simplifications could be
255 considered for some UPMs operating under specific conditions:

256 - The models describing a Unit Process without any significant biochemical
257 activity can be based only on *mass transport* equations. Typical examples
258 include the mathematical models commonly used for primary or secondary
259 settlers.

260 - The models describing a Unit Process that is always working under stable
261 environmental conditions can “switch-off” or eliminate transformations that are
262 irrelevant under these specific conditions. For example, anaerobic

transformations can be "switched-off" when describing conventional activated sludge reactors in the water line.

- For simplicity or computational efficiency, some UPMs could be developed based on internal "lumped" variables and transformations. Typical examples can include the use of lumped variables for the slowly (X_S) or easily (S_S) biodegradable carbonaceous substrates or lumped transformations as the one-step nitrification from Ammonia to Nitrates. However, the convenience of this kind of simplification should be carefully analysed in each case, as the resulting UPM must incorporate transformers among its internal model variables and the PCV (the common model interface within the whole plant). In many cases, the design of these transformers guaranteeing mass and charge continuity under different operating conditions is not a straightforward task (Vanrolleghem et al., 2005).

Therefore, although the modeller could develop specific unit process models, it is important to note that any UPM must guarantee mass and charge continuity for every internal process transformation and must use the PCV as the common interface with the other UPMs of the entire plant. Consequently, when computational time is not a critical restriction, the direct incorporation of the general PTM for internal transformations in all UPMs is strongly recommended in terms of modelling coherence and conceptual simplicity.

c) Construction of the Plant-Wide Model (**PWM)** for the whole plant

Once the set of UPMs has been constructed in accordance with the proposed methodology, the *Plant-Wide Model* (PWM) can be easily created, without additional transformers, by the direct connection of the mass fluxes among the UPMs. The

resulting integrated model will guarantee mass and charge conservation for all process transformations and through all UPM interfaces.

3. EXAMPLE: PWM FOR A CONVENTIONAL ACTIVATED SLUDGE PROCESS WITH ANAEROBIC DIGESTION

Once the methodology for model construction has been defined, tailored *Plant Transformations models* (PTMs) can easily be built including all the biological processes required for the description of the water and sludge lines at each specific case study, for example, carbon oxidation, nitrification, denitrification, biological phosphorus removal, fermentation or complete anaerobic digestion, etc.

As an example, this paper shows a PWM for a conventional WWTP that includes an aerated activated sludge reactor for C removal, a secondary settler and an anaerobic digester for sludge treatment.

a) PTM Construction

The PTM for the WWTP proposed in this example has been constructed following the sequential procedure indicated in Section 2.

a.1) *Selection of Biological Processes*

According to plant configuration and model objectives, the *Biological Processes* considered have been limited to the activated sludge process for Carbon removal (AS-C), which occurs mainly in the aerated activated sludge tank and the anaerobic digestion process (ADM1), which is active in the digester.

a.2) *Selection of the microorganism populations required to describe the selected Biological Processes*

As a consequence of the *Biological processes* considered in a.1, as shown in Table 2, the selected active microorganism populations are X_h, and the set of anaerobic microorganisms X_{su}, X_{aa}, X_{fa}, X_{c4}, X_{pro}, X_{ac} and X_{h2}.

a.3) *Selection of the biochemical transformations associated with the activity of the microorganism populations*

Once active microorganism populations have been determined, the biochemical transformations describing their growth, decay and enzymatic hydrolysis are selected under all environmental conditions as shown in Figure 2. In this case, the selected transformations are 1-7, 16-29, 33-40, 41, 45-51, 55, 59-65, 69, 73-79 and 89-97. In addition to these biochemical transformations, X_{c2} disintegration under aerobic, anoxic and anaerobic conditions must be selected (84, 86 and 88). Although disintegration of X_{c2} is not related to activities of the microorganisms, this transformation has been considered as an intermediate transformation between the microorganisms´ decay and the enzymatic hydrolysis as it is proposed for X_c in the ADM1. The list of all these transformations will reproduce the biological activity that occurs in the whole WWTP. However, as in this particular case, anoxic conditions do not exist at any point in the plant, transformations occurring under this specific condition (16-29, 55, 59-65, 86 and 92-94) can be eliminated.

The set of components involved in the selected transformations will correspond to the soluble substrate, the microorganism populations selected in a.2, the decay products and the particulate substrate. Furthermore, source-sink components have been considered by default to guarantee the mass and charge continuity in the biochemical transformations regardless of the components´ mass compositions. Figure 4 shows, as an illustrative example, the biochemical transformations and components involved in the X_h and X_{su} activities.

a.3) *Incorporation of acid-base and liquid-gas equilibriums*

According to the set of components selected in a.3, the required acid-base equilibria (98-105) and liquid-gas transfers (106-110, 112) have been incorporated into the PTM. Finally, additional components needed to describe these acid-base and liquid-gas equilibria have been included in the PCV. Figure 5 shows the transformations and components incorporated in this step according to the components selected for the X_h and X_{su} biological activity description (Figure 4).

The PTM obtained is presented in Tables 4, 5, 6 and 7 in terms of stoichiometry and kinetics (Petersen matrix). The stoichiometry associated with the biological activity and the physico-chemical transformations is shown in Tables 5 and 6, respectively. In Table 7, the source-sinks stoichiometric values have been expressed by a set of formulas since their exact values depend on the mass composition of the components involved in each transformation. On the other hand, the kinetic equations include the appropriate activation and inhibition terms for the environmental conditions. Therefore, when the environmental conditions change from one unit-process element to another, the conversion of non-viable microorganisms under specific conditions into decay products is described by continuous decay kinetics regulated by the specific environmental conditions prevailing at each point of the WWTP. Finally, it must be taken into account that the kinetic equations selected for the construction of the PTM, should be revised for each case study to ensure that the monod terms included in them are coherent with the components considered in the model. In some cases, if the kinetic equations were modified, the values of the parameters included in them should be readjusted.

b) Construction of the set of Unit Process Models

Once the PTM is obtained, **UPMs** for the activated sludge reactor, the secondary settler and the anaerobic digester must be constructed by means of the mass transport description and internal transformations.

Mass transport description

The description of the mass transport in the activated sludge reactor and the digester, where transformations occur in a significant way, is based on a *biological reactor model*. Since the constructed PTM includes components in liquid (dissolved and particulate) and gaseous phases, one must consider these two phases in the *biological reactor model*. The anaerobic digester consists of two continuous stirred-tank reactors (CSTRs), each one with their own interfaces, corresponding to these two phases and where liquid-gas transfers take place. Therefore, mass transport will be described by means of mass balances applied to the liquid and gaseous phases. The activated sludge reactor is composed of a CSTR that represents the liquid phase in contact with the atmosphere, in which the gaseous components present constant concentrations. In this case, the mass transport description is described by mass balances applied to the liquid phase.

On the other hand, the mass transport description of the secondary settler can be reproduced by standard models that are normally utilized (ideal settlers, layered settlers, etc.) using the *TSS* variable.

Internal transformations

As recommended in section 2, the set of internal transformations and components considered in each UPM should coincide with the PTM created in the previous step.

According to this suggestion, the PTM obtained in step A, has been utilized to describe the internal transformations in the aerated activated sludge tank and in the anaerobic

382 digester. In this manner, mass and charge continuity are guaranteed in these UPMs and
383 the PCV can act as an input-output interface without the need of transformers among
384 Specific Component Vectors and the common PCV.

385 However, with respect to the secondary settler UPM, as the mass transport is described
386 based on the lumped variable *TSS*, specific input-output transformers must be included
387 to convert particulate components of the PCV into the variable *TSS* and vice-versa.
388 Relationships between the *COD* and the mass of organic components, easily established
389 with the methodology proposed in this paper, permit a direct conversion between
390 organic particulate components and *TSS,* guaranteeing the mass continuity during
391 stationary and dynamic conditions.

392 c) Construction of the Plant-Wide Model (**PWM)** for the whole plant

393 Finally, the PWM for the WWTP proposed in this example has been created by the
394 direct connection of the mass fluxes among the UPMs. The obtained PWM, specific for
395 this WWTP, is able to reproduce all relevant process transformations and guarantees
396 mass and charge continuity throughout the whole plant without specific transformers
397 among the UPMs.

398 In addition to the example presented in this paper, other models have been constructed,
399 implemented in the simulation platform WEST (http://www.mostforwater.com) and
400 successfully validated using the methodology proposed in this paper such as the BSM2
401 PWM (Grau et al., 2007), the Anaerobic Digestion Model (Huete et al., 2006), and the
402 Composting Reactor System Model (Zurcan et al., 2005).

403 It is important to point out the advantages of the *transformation-based* approach from
404 the point of view of developing computer code for simulation platforms. The general
405 List of Transformations (LT) can be compiled as a general library from which the

406 modeller can construct tailored PWMs as simple or ascomplex as needed in each case
407 study.

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409

410 **4. CONCLUSIONS**

411 The integrated modelling of an entire WWTP, including the mutual relationships among
412 the different unit-process elements of the water and sludge lines is not as
413 straightforward as the simple connection of existing models. A rigorous model
414 development must analyze the appropriate definition of model components at each unit-
415 process element and the mass continuity among all of them.

416 The Plant Wide Modelling methodology proposed in this paper takes into account the
417 advantages and limitations of existing approaches and develops a systematic procedure
418 for the tailored construction of integrated mathematical models for WWTPs, including
419 water and sludge lines, without the need of specific transformers among Unit Process
420 Models and guarantees mass and charge continuity throughout the WWTP under any
421 dynamic condition. Additionally, the proposed *"Transformation-based"* approach
422 facilitates the development of simulation codes in an efficient modular manner.

423 The example given in this paper has illustrated the different steps of the systematic
424 procedure to construct integrated models where the mass continuity is guaranteed
425 throughout the whole plant.

426 Nowadays, it is probably time to rewrite the existing unit-process models when they are
427 used for integrated modelling objectives. From an "approved" list of process
428 transformations, agreed upon by modelling experts, a general and systematic procedure

429 can be developed to create compatible unit-process models, and integrated models
430 adapted to the specific plant under study.

431 The fact that the List of Transformations and components is open and allows the
432 incorporation of new transformations and components provides a useful and flexible
433 modelling approach that facilitates the interchange and contrast of information between
434 modelling teams.

435

436 **5. ACKNOWLEDGEMENTS**

437 The authors wish to express their gratitude to the Basque Government (SPRI) for its
438 financial support and to the Spanish Ministry of Science and Education for grant
439 CICYT DPI'2003-08580-C02.

440 Peter Vanrolleghem holds the Canada Research Chair in Water Quality Modelling.

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Table 1. *Model components included in the LT*

i	Name	Formula	Description	Stoichiometric Unit	Mass fractions and charge density $\alpha_{C,i}$	$\alpha_{H,i}$	$\alpha_{O,i}$	$\alpha_{N,i}$	$\alpha_{P,i}$	$\alpha_{Ch,i}$	$\alpha_{X,i}$
Soluble components											
1	S_{h2o}	H_2O	Water	gH_2O	---	0.1111	0.8889	---	---	---	---
2	S_{o2}	O_2	Dissolved Oxygen	gO_2/m^3	---	---	1	---	---	---	---
3	S_{h+}	H^+	Protons	gH/m^3	---	1	---	---	---	1	---
4	S_{oh-}	OH^-	Hydroxyl ions	gH/m^3	---	0.0588	0.9412	---	---	-0.0588	---
5	S_{hpo4}	HPO_4^{2-}	Hidroxy phosphate	gP/m^3	---	0.0104	0.6667	---	0.3229	-0.0208	---
6	S_{h2po4}	$H_2PO_4^-$	Dihidroxy phosphate	gP/m^3	---	0.0206	0.6598	---	0.3196	-0.0103	---
7	S_{nh4}	NH_4^+	Ammonium	gN/m^3	---	0.2222	---	0.7778	---	0.0556	---
8	S_{nh3}	NH_3	Ammonia	gN/m^3	---	0.1765	---	0.8235	---	---	---
9	S_{co2}	CO_2	Dissolved C. dioxide	gC/m^3	0.2727	---	0.7273	---	---	---	---
10	S_{hco3-}	HCO_3^-	Bicarbonate	gC/m^3	0.1967	0.0164	0.7869	---	---	-0.0164	---
11	S_{su}	$C_6H_{12}O_6$	Monosacharide	$gCOD/m^3$	0.4	0.0667	0.5333	---	---	---	---
12	S_{aa}	$C_4H_{6.1}O_{1.2}N$	Aminoacids	$gCOD/m^3$	0.5498	0.0699	0.2199	0.1604	---	---	---
13	S_{fa}	$C_{16}O_2H_{32}$	LCFAs	$gCOD/m^3$	0.75	0.125	0.125	---	---	---	---
14	S_{hva}	$C_5H_{10}O_2$	Valeric acid	$gCOD/m^3$	0.5882	0.098	0.3137	---	---	---	---
15	S_{va-}	$C_5H_9O_2^-$	Valerate	$gCOD/m^3$	0.5941	0.0891	0.3168	---	---	-0.0099	---
16	S_{hbu}	$C_4H_8O_2$	Butyric acid	$gCOD/m^3$	0.5455	0.0909	0.3636	---	---	---	---
17	S_{bu-}	$C_4H_7O_2^-$	Butyrate	$gCOD/m^3$	0.5517	0.0805	0.3678	---	---	-0.0115	---
18	S_{hpro}	$C_3H_6O_2$	Propionic acid	$gCOD/m^3$	0.4865	0.0811	0.4324	---	---	---	---
19	S_{pro-}	$C_3H_5O_2^-$	Propionate	$gCOD/m^3$	0.4932	0.0685	0.4384	---	---	-0.0137	---
20	S_{hac}	$C_2H_4O_2$	Acetic acid	$gCOD/m^3$	0.4	0.0667	0.5333	---	---	---	---
21	S_{ac-}	$C_2H_3O_2^-$	Acetate	$gCOD/m^3$	0.4068	0.0508	0.5424	---	---	-0.0169	---
22	S_{h2}	H_2	Dissolved hydrogen	$gCOD/m^3$	---	1	---	---	---	---	---
23	S_{ch4}	CH_4	Dissolved methane	$gCOD/m^3$	0.75	0.25	---	---	---	---	---
24	S_{n2}	N_2	Dissolved nitrogen	gN/m^3	---	---	---	1	---	---	---
25	S_{no2}	NO_2^-	Nitrites	gN/m^3	---	---	0.6957	0.3043	---	-0.0217	---
26	S_{no3}	NO_3^-	Nitrates	gN/m^3	---	---	0.7742	0.2258	---	-0.0161	---
27	S_{k+}	K^+	Potassium ions	gK/m^3	---	---	---	---	---	0.0256	1
28	S_{Mg2+}	Mg^{2+}	Magnesium ions	gMg/m^3	---	---	---	---	---	0.0823	1
29	S_I	--	Soluble inerts	$gCOD/m^3$	$\alpha_{C,29}$	$\alpha_{H,29}$	$\alpha_{O,29}$	$\alpha_{N,29}$	$\alpha_{P,29}$	$\alpha_{Ch,29}$	$\alpha_{X,29}$
30	S_p	--	Soluble decay products	$gCOD/m^3$	$\alpha_{C,30}$	$\alpha_{H,30}$	$\alpha_{O,30}$	$\alpha_{N,30}$	$\alpha_{P,30}$	$\alpha_{Ch,30}$	$\alpha_{X,30}$
Particulate and gaseous components											
31	X_{c1}	--	Composites 1	$gCOD/m^3$	$\alpha_{C,31}$	$\alpha_{H,31}$	$\alpha_{O,31}$	$\alpha_{N,31}$	$\alpha_{P,31}$	$\alpha_{Ch,31}$	$\alpha_{X,31}$
32	X_{c2}	--	Composites 1	$gCOD/m^3$	$\alpha_{C,32}$	$\alpha_{H,32}$	$\alpha_{O,32}$	$\alpha_{N,32}$	$\alpha_{P,32}$	$\alpha_{Ch,32}$	$\alpha_{X,32}$
33	X_{ch}	$C_6H_{9.95}O_3P_{0.05}$	Carbohydrates	$gCOD/m^3$	0.4401	0.0608	0.489	---	0.01	---	---
34	X_{pr}	$(C_4H_{6.1}O_{1.2}N)_x$	Proteins	$gCOD/m^3$	0.5498	0.0699	0.2199	0.1604	---	---	---
35	X_{li}	$C_{51}H_{97.9}O_6P_{0.1}$	Lipids	$gCOD/m^3$	0.752	0.1201	0.118	---	0.01	---	---
36	X_h	$C_5H_{6.9}O_2NP_{0.1}$	Heterotrophic B.	$gCOD/m^3$	0.5155	0.0592	0.275	0.1203	0.03	---	---
37	X_{n1}	$C_5H_{6.9}O_2NP_{0.1}$	Nitrosomona B.	$gCOD/m^3$	0.5155	0.0592	0.275	0.1203	0.03	---	---
38	X_{n2}	$C_5H_{6.9}O_2NP_{0.1}$	Nitrobacter B.	$gCOD/m^3$	0.5155	0.0592	0.275	0.1203	0.03	---	---
39	X_{pao}	$C_5H_{6.9}O_2NP_{0.1}$	Phosphorous Acum. B.	$gCOD/m^3$	0.5155	0.0592	0.275	0.1203	0.03	---	---
40	X_{pha}	$C_4H_6O_2$	Cell internal storage	$gCOD/m^3$	0.2790	0.0698	0.3721	---	---	---	---
41	X_{pp}	$K_{0.33}Mg_{0.33}PO_3$	Poly-phosphate	gP/m^3	---	---	0.4793	---	0.3096	---	0.2110
42	X_{su}	$C_5H_{6.9}O_2NP_{0.1}$	Sugar degraders	$gCOD/m^3$	0.5155	0.0592	0.275	0.1203	0.03	---	---
43	X_{aa}	$C_5H_{6.9}O_2NP_{0.1}$	Aminoacid degraders	$gCOD/m^3$	0.5155	0.0592	0.275	0.1203	0.03	---	---
44	X_{fa}	$C_5H_{6.9}O_2NP_{0.1}$	LCFA degraders	$gCOD/m^3$	0.5155	0.0592	0.275	0.1203	0.03	---	---
45	X_{c4}	$C_5H_{6.9}O_2NP_{0.1}$	Valeric/Butyric degrad.	$gCOD/m^3$	0.5155	0.0592	0.275	0.1203	0.03	---	---
46	X_{pro}	$C_5H_{6.9}O_2NP_{0.1}$	Propionic degraders	$gCOD/m^3$	0.5155	0.0592	0.275	0.1203	0.03	---	---
47	X_{ac}	$C_5H_{6.9}O_2NP_{0.1}$	Acetid degraders	$gCOD/m^3$	0.5155	0.0592	0.275	0.1203	0.03	---	---
48	X_{h2}	$C_5H_{6.9}O_2NP_{0.1}$	Hydrogen degraders	$gCOD/m^3$	0.5155	0.0592	0.275	0.1203	0.03	---	---
49	X_{an}	$C_5H_{6.9}O_2NP_{0.1}$	Anammox degraders	$gCOD/m^3$	0.5155	0.0592	0.275	0.1203	0.03	---	---
50	X_I	--	Inert particulate material	$gCOD/m^3$	$\alpha_{C,50}$	$\alpha_{H,50}$	$\alpha_{O,50}$	$\alpha_{N,50}$	$\alpha_{P,50}$	$\alpha_{Ch,50}$	$\alpha_{X,50}$
51	X_P	--	Part. Decay	$gCOD/m^3$	$\alpha_{C,51}$	$\alpha_{H,51}$	$\alpha_{O,51}$	$\alpha_{N,51}$	$\alpha_{P,51}$	$\alpha_{Ch,51}$	$\alpha_{X,51}$
52	$X_{Me(oh)}$	$Fe(OH)_3$	Ferric hydroxide	g/m^3	---	0.0281	0.4492	---	---	---	0.5227
53	X_{MeP}	$FePO_4$	Ferric phosphate	g/m^3	---	---	0.4243	---	0.2055	---	0.3703
54	X_{II}	--	Inorganic Inert	g/m^3	---	---	---	---	---	---	1
55	G_{co2}	CO_2	Carbon dioxide gas	$gC/m^3_{(g)}$	0.2727	---	0.7273	---	---	---	---
56	G_{h2}	H_2	Hydrogen gas	$gCOD/m^3$	---	1	---	---	---	---	---
57	G_{ch4}	CH_4	Methane gas	$gCOD/m^3$	0.75	0.25	---	---	---	---	---
58	G_{nh3}	NH_3	Ammonia gas	$gN/m^3_{(g)}$	---	0.1765	---	0.8235	---	---	---
59	G_{n2}	N_2	Nitrogen gas	$gN/m^3_{(g)}$	---	---	---	1	---	---	---
60	G_{o2}	O_2	Oxygen gas	$gO_2/m^3_{(g)}$	---	---	1	---	---	---	---
61	G_{h2o}	H_2O	Water steam	$gH_2O/m^3_{(g)}$	---	0.1111	0.8889	---	---	---	---

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493 **Table 2.** *Relationship between Biological Processes and associated microorganism populations*

Biological Processes						Microorganism Populations											
						X_{an}	X_h	X_{n1}	X_{n2}	X_{pao}	X_{su}	X_{aa}	X_{fa}	X_{c4}	X_{pro}	X_{ac}	X_{h2}
Anammox				Anaerobic oxidation of $N\text{-}NH_4^+$		×											
AS-CNP	AS-CN Sharon	AS-C		Carbon oxidation			×										
			Nitrification	Nitritation				×									
				Nitratation					×								
			Denitrification	Denitrification on NO_3^-			×										
				Denitrification on NO_2^-			×										
			Bio-P storage and release							×							
	Anaerobic digestion	Ferm	Acidogenesis								×	×					
			Acetogenesis										×	×	×		
			Methanogenesis													×	×

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496 **Table 3.** *Expressions utilized in the kinetic equations*

Lumped variables used to simplify the kinetic equations description			
Valerate	$S_{VA} = S_{hva} + S_{va-}$	Readily degradable substrate	$S_S = S_{su} + S_{aa} + S_{fa} + S_{VA} + S_{BU} + S_{PRO} + S_{AC}$
Butyrate	$S_{BU} = S_{hbu} + S_{bu-}$	Inorganic carbon	$S_{IC} = S_{co2} + S_{hco3-}$
Propionate	$S_{PRO} = S_{hpro} + S_{pro-}$	Ammoniacal nitrogen	$S_{IN} = S_{nh4+} + S_{nh3}$
Acetate	$S_{AC} = S_{hac} + S_{ac-}$	Inorganic phosphorus	$S_{IP} = S_{hpo4=} + S_{h2po4-}$
Activation/Inhibition terms depending on the environmental conditions			
Oxygen activation	$A_{o2} = \frac{S_{o2}}{K_{A,o2} + S_{o2}}$	Oxygen inhibition	$I_{o2} = \frac{K_{A,o2}}{K_{A,o2} + S_{o2}}$
Nitrates activation	$A_{no3} = \frac{S_{no3-}}{K_{A,no3} + S_{no3-}}$	Nitrates/Nitrites inhibition	$I_{nox} = \frac{K_{A,nox}}{K_{A,nox} + (S_{no2-} + S_{no3-})}$
Nitrites activation	$A_{no2} = \frac{S_{no2-}}{K_{A,no2} + S_{no2-}}$		
Activation terms for source-sink components			
Inorganic nitrogen	$A_{IN} = \frac{S_{IN}}{K_{A,IN} + S_{IN}}$	Inorganic carbon	$A_{IC} = \frac{S_{IC}}{K_{A,IC} + S_{IC}}$
Inorganic phosphorous	$A_{IP} = \frac{S_{IP}}{K_{A,IP} + S_{IP}}$		
Activation/Inhibition terms depending on pH values			
pH inhibition of the acidogenesis and acetogenesis transformations	$I_{pH,aa} = \frac{K_{I,h,aa}^{2}}{K_{I,h,aa}^{2} + S_{h+}^{2}}$		
pH inhibition of the acetoclastic methanogenesis	$I_{pH,ac} = \frac{K_{I,h,ac}^{2}}{K_{I,h,ac}^{2} + S_{h+}^{2}}$		
pH inhibition of hidrogenotrophic methanogenesis	$I_{pH,h2} = \frac{K_{I,h,h2}^{2}}{K_{I,h,h2}^{2} + S_{h+}^{2}}$		
Inhibition terms caused by inhibiting components			
VFAs hydrogen inhibition during the acidogenesis	$I_{h2,fa} = \frac{K_{I,h2,fa}}{K_{I,h2,fa} + S_{h2}}$	Propionic hydrogen inhibition during the acetogenesis	$I_{h2,pro} = \frac{K_{I,h2,pro}}{K_{I,h2,pro} + S_{h2}}$
Valeric and Butyric hydrogen inhibition during the acetogenesis	$I_{h2,c4} = \frac{K_{I,h2,c4}}{K_{I,h2,c4} + S_{h2}}$	Ammonia inhibition	$I_{nh3} = \frac{K_{I,nh3}}{K_{I,nh3} + S_{nh3}}$

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498 **Table 4.** *Kinetic equations of the PTM transformations*

$$\rho_1 = k_{m,h} \cdot \frac{S_{su}}{K_{su\_h} + S_{su}} \cdot \frac{S_{su}}{S_S} \cdot \left[A_{o2} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_h$$

$$\rho_2 = k_{m,h} \cdot \frac{S_{aa}}{K_{aa\_h} + S_{aa}} \cdot \frac{S_{aa}}{S_S} \cdot \left[A_{o2} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_h$$

$$\rho_3 = k_{m,h} \cdot \frac{S_{fa}}{K_{fa\_h} + S_{fa}} \cdot \frac{S_{fa}}{S_S} \cdot \left[A_{o2} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_h$$

$$\rho_4 = k_{m,h} \cdot \frac{S_{VA}}{K_{VA\_h} + S_{VA}} \cdot \frac{S_{VA}}{S_S} \cdot \left[A_{o2} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_h$$

$$\rho_5 = k_{m,h} \cdot \frac{S_{BU}}{K_{BU\_h} + S_{BU}} \cdot \frac{S_{BU}}{S_S} \cdot \left[A_{o2} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_h$$

$$\rho_6 = k_{m,h} \cdot \frac{S_{PRO}}{K_{PRO\_h} + S_{PRO}} \cdot \frac{S_{PRO}}{S_S} \cdot \left[A_{o2} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_h$$

$$\rho_7 = k_{m,h} \cdot \frac{S_{AC}}{K_{AC\_h} + S_{AC}} \cdot \frac{S_{AC}}{S_S} \cdot \left[A_{o2} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_h$$

$$\rho_{33} = k_{m,su} \cdot \frac{S_{su}}{K_{S,su} + S_{su}} \cdot \left[I_{o2} \cdot I_{nox} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC} \cdot \cdot I_{pH,aa}\right] \cdot X_{su}$$

$$\rho_{34} = k_{m,aa} \cdot \frac{S_{aa}}{K_{S,aa} + S_{aa}} \cdot \left[I_{o2} \cdot I_{nox} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC} \cdot \cdot I_{pH,aa}\right] \cdot X_{aa}$$

$$\rho_{35} = k_{m,fa} \cdot \frac{S_{fa}}{K_{S,fa} + S_{fa}} \cdot \left[A_{IN} \cdot A_{IP} \cdot A_{IC} \cdot I_{o2} \cdot I_{nox} \cdot I_{h2,fa} \cdot I_{ph,aa}\right] \cdot X_{fa}$$

$$\rho_{36} = k_{m,c4} \cdot \frac{S_{VA}}{K_{S,c4} + S_{VA}} \cdot \frac{1}{1 + S_{BU}/S_{VA}} \cdot \left[A_{IN} \cdot A_{IP} \cdot A_{IC} \cdot I_{o2} \cdot I_{nox} \cdot I_{h2,c4} \cdot I_{ph,aa}\right] \cdot X_{c4}$$

$$\rho_{37} = k_{m,c4} \cdot \frac{S_{BU}}{K_{S,c4} + S_{BU}} \cdot \frac{1}{1 + S_{VA}/S_{BU}} \cdot \left[A_{IN} \cdot A_{IP} \cdot A_{IC} \cdot I_{o2} \cdot I_{nox} \cdot I_{h2,c4} \cdot I_{ph,aa}\right] \cdot X_{c4}$$

$$\rho_{38} = k_{m,pro} \cdot \frac{S_{PRO}}{K_{S,pro} + S_{PRO}} \cdot \left[A_{IN} \cdot A_{IP} \cdot A_{IC} \cdot I_{o2} \cdot I_{nox} \cdot I_{h2,pro} \cdot I_{ph,aa}\right] \cdot X_{pro}$$

$$\rho_{39} = k_{m,ac} \cdot \frac{S_{AC}}{K_{S,ac} + S_{AC}} \cdot \left[I_{o2} \cdot I_{nox} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC} \cdot I_{nh3} \cdot I_{ph,ac}\right] \cdot X_{ac}$$

$$\rho_{40} = k_{m,h2} \cdot \frac{S_{h2}}{K_{S,h2} + S_{h2}} \cdot \left[I_{o2} \cdot I_{nox} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC} \cdot I_{ph,h2}\right] \cdot X_{h2}$$

$$\rho_{84} = k_{d\_Aer} \cdot \left[A_{o2} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_{c2}$$

$$\rho_{88} = k_{d\_Anaer} \cdot \left[I_{nox} \cdot I_{o2} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_{c2}$$

$$\rho_{89} = k_{h\_Aer} \cdot \left[A_{o2} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_{ch}$$

$$\rho_{90} = k_{h\_Aer} \cdot \left[A_{o2} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_{pr}$$

$$\rho_{91} = k_{h\_Aer} \cdot \left[A_{o2} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_{li}$$

$$\rho_{95} = k_{h\_Anaer} \cdot \left[I_{o2} \cdot I_{nox} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_{ch}$$

$$\rho_{96} = k_{h\_Anaer} \cdot \left[I_{o2} \cdot I_{nox} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_{pr}$$

$$\rho_{97} = k_{h\_Anaer} \cdot \left[I_{o2} \cdot I_{nox} \cdot A_{IN} \cdot A_{IP} \cdot A_{IC}\right] \cdot X_{li}$$

$$\rho_{41} = k_{dec\_aer,xh} \cdot A_{o2} \cdot X_h$$

$$\rho_{45} = k_{dec\_aer,xsu} \cdot A_{o2} \cdot X_{su}$$

$$\rho_{46} = k_{dec\_aer,xaa} \cdot A_{o2} \cdot X_{aa}$$

$$\rho_{47} = k_{dec\_aer,xfa} \cdot A_{o2} \cdot X_{fa}$$

$$\rho_{48} = k_{dec\_aer,xc4} \cdot A_{o2} \cdot X_{c4}$$

$$\rho_{49} = k_{dec\_aer,xpro} \cdot A_{o2} \cdot X_{pro}$$

$$\rho_{50} = k_{dec\_aer,xac} \cdot A_{o2} \cdot X_{ac}$$

$$\rho_{51} = k_{dec\_aer,xh2} \cdot A_{o2} \cdot X_{h2}$$

$$\rho_{69} = k_{dec\_an,xh} \cdot I_{o2} \cdot I_{nox} \cdot X_h$$

$$\rho_{73} = k_{dec\_an,xsu} \cdot I_{o2} \cdot I_{nox} \cdot X_{su}$$

$$\rho_{74} = k_{dec\_an,xaa} \cdot I_{o2} \cdot I_{nox} \cdot X_{aa}$$

$$\rho_{75} = k_{dec\_an,xfa} \cdot I_{o2} \cdot I_{nox} \cdot X_{fa}$$

$$\rho_{76} = k_{dec\_an,xc4} \cdot I_{o2} \cdot I_{nox} \cdot X_{c4}$$

$$\rho_{77} = k_{dec\_an,xpro} \cdot I_{o2} \cdot I_{nox} \cdot X_{pro}$$

$$\rho_{78} = k_{dec\_an,xac} \cdot I_{o2} \cdot I_{nox} \cdot X_{ac}$$

$$\rho_{79} = k_{dec\_an,xh2} \cdot I_{o2} \cdot I_{nox} \cdot X_{h2}$$

$$\rho_{98} = k_{AB,H2O} \cdot \left(K_{a,H2O} - S_{oh-} \cdot S_{H+}\right)$$

$$\rho_{99} = k_{AB,IC} \cdot \left(K_{a,IC} \cdot S_{co2} - S_{hco3-} \cdot S_{h+}\right)$$

$$\rho_{100} = k_{AB,IN} \cdot \left(K_{a,IN} \cdot S_{nh4+} - S_{nh3} \cdot S_{h+}\right)$$

$$\rho_{101} = k_{AB,IP} \cdot \left(K_{a,IP} \cdot S_{h2po4-} - S_{hpo4=} \cdot S_{h+}\right)$$

$$\rho_{102} = k_{AB,VA} \cdot \left(K_{a,VA} \cdot S_{hva} - S_{va-} \cdot S_{h+}\right)$$

$$\rho_{103} = k_{AB,BU} \cdot \left(K_{a,BU} \cdot S_{hbu} - S_{bu-} \cdot S_{h+}\right)$$

$$\rho_{104} = k_{AB,PRO} \cdot \left(K_{a,PRO} \cdot S_{hpro} - S_{pro-} \cdot S_{h+}\right)$$

$$\rho_{105} = k_{AB,AC} \cdot \left(K_{a,AC} \cdot S_{hac} - S_{ac-} \cdot S_{h+}\right)$$

$$\rho_{106} = K_L a_{co2} \cdot \left(K_{H,co2} \cdot P_{gas,co2} - S_{co2}\right)$$

$$\rho_{107} = K_L a_{o2} \cdot \left(K_{H,o2} \cdot P_{gas,o2} - S_{o2}\right)$$

$$\rho_{108} = K_M a_{H2O} \cdot \left(P_{H2O}^{SAT} - P_{h2o}\right)$$

$$\rho_{109} = K_L a_{nh3} \cdot \left(K_{H,nh3} \cdot P_{gas,nh3} - S_{nh3}\right)$$

$$\rho_{110} = K_L a_{ch4} \cdot \left(K_{H,ch4} \cdot P_{gas,ch4} - S_{ch4}\right)$$

$$\rho_{112} = K_L a_{h2} \cdot \left(K_{H,h2} \cdot P_{gas,h2} - S_{h2}\right)$$

499
500

Table 5. *Stoichiometry of biochemical transformations*

Components i →		1	2	3	4	6	8	10	12	14	16	17	18	19	20	21	22	23	24	25	26	27	28	29
Transformations j ↓		S_{su}	S_{aa}	S_{fa}	S_{hva}	S_{hbu}	S_{hpro}	S_{hac}	S_{h2}	S_{ch4}	S_p	X_{ch}	X_{pr}	X_{li}	X_{c2}	X_p	X_{su}	X_{aa}	X_{fa}	X_{c4}	X_{pro}	X_{ac}	X_{h2}	X_h
1	Aerobic uptake of S_{su}	-1																						Y_h
2	Aerobic uptake of S_{aa}		-1																					Y_h
3	Aerobic uptake of S_{fa}			-1																				Y_h
4	Aerobic uptake of S_{VA}				-1																			Y_h
5	Aerobic uptake of S_{BU}					-1																		Y_h
6	Aerobic uptake of S_{PRO}						-1																	Y_h
7	Aerobic uptake of S_{AC}							-1																Y_h
33	Acidogenesis of S_{su}	-1				$f_{bu,su}\cdot(1-Y_{su})$	$f_{pro,su}\cdot(1-Y_{su})$	$f_{ac,su}\cdot(1-Y_{su})$	$f_{h2,su}\cdot(1-Y_{su})$								Y_{su}							
34	Acidogenesis of S_{aa}		-1		$f_{va,aa}\cdot(1-Y_{aa})$	$f_{bu,aa}\cdot(1-Y_{aa})$	$f_{pro,aa}\cdot(1-Y_{aa})$	$f_{ac,aa}\cdot(1-Y_{aa})$	$f_{h2,aa}\cdot(1-Y_{aa})$									Y_{aa}						
35	Acetogenesis of S_{fa}			-1				$f_{ac,fa}\cdot(1-Y_{fa})$	$f_{h2,fa}\cdot(1-Y_{fa})$										Y_{fa}					
36	Acetogenesis of S_{VA}				-1		$f_{pro,va}\cdot(1-Y_{c4})$	$f_{ac,va}\cdot(1-Y_{c4})$	$f_{h2,va}\cdot(1-Y_{c4})$											Y_{c4}				
37	Acetogenesis of S_{BU}					-1		$f_{ac,bu}\cdot(1-Y_{c4})$	$f_{h2,bu}\cdot(1-Y_{c4})$											Y_{c4}				
38	Acetogenesis of S_{PRO}						-1	$f_{ac,pro}\cdot(1-Y_{pro})$	$f_{h2,pro}\cdot(1-Y_{pro})$												Y_{pro}			
39	Acetoclast. Methanog.									$1-Y_{ac}$														
40	Hydrogen. Methanog.									$1-Y_{h2}$														
41, 69	Decay of X_h														1									-1
45, 73	Decay of X_{su}														1		-1							
46, 74	Decay of X_{aa}														1			-1						
47, 75	Decay of X_{fa}														1				-1					
48, 76	Decay of X_{c4}														1					-1				
49, 77	Decay of X_{pro}														1						-1			
50, 78	Decay of X_{ac}														1							-1		
51, 79	Decay of X_{h2}														1								-1	
84, 88	Disintegration of X_{c2}										$f_{sp,xc2}$	$f_{ch,xc2}$	$f_{pr,xc2}$	$f_{li,xc2}$	-1		$f_{xp,xc2}$							
89, 95	Hydrolysis X_{ch}	1										-1												
90, 96	Hydrolysis X_{pr}		1										-1											
91, 97	Hydrolysis X_{li}	$1-f_{fa,li}$		$f_{fa,li}$										-1										

Table 6. *Stoichiometry of acid-base and liquid-gas equilibriums*

Components i →	4	5	6	7	8	9	10	11	12	13	14	15	30	31	32	33	34	35	36	37	38	39	40	41	42	43
Transformations j ↓	S_{hva}	S_{va-}	S_{hbu}	S_{bu-}	S_{hpro}	S_{pro-}	S_{hac}	S_{ac-}	S_{h2}	G_{h2}	S_{ch4}	G_{ch4}	S_{hco3-}	G_{co2}	S_{co2}	S_{nh3}	G_{nh3}	S_{nh4+}	S_{h2po4-}	$S_{hpo4=}$	S_{oh-}	S_{h+}	G_{h2o}	S_{h2o}	G_{o2}	S_{o2}
98 Water equilibirum															$\nu_{Sco2,98}$			$\nu_{Snh4+,98}$		$\nu_{Shpo4-,98}$	1	$\nu_{Sh+,98}$		$\nu_{Sh2o,98}$		$\nu_{So2,98}$
99 Inorg. Carbon equilibrium													1		$\nu_{Sco2,99}$			$\nu_{Snh4+,99}$		$\nu_{Shpo4-,99}$		$\nu_{Sh+,99}$		$\nu_{Sh2o,99}$		$\nu_{So2,99}$
100 Inorg. Nitrogen equilibrium															$\nu_{Sco2,100}$	1		$\nu_{Snh4+,100}$		$\nu_{Shpo4-,100}$		$\nu_{Sh+,100}$		$\nu_{Sh2o,100}$		$\nu_{So2,100}$
101 Inorg. Phosphorous equilibrium															$\nu_{Sco2,101}$			$\nu_{Snh4+,101}$	−1	$\nu_{Shpo4-,101}$		$\nu_{Sh+,101}$		$\nu_{Sh2o,101}$		$\nu_{So2,101}$
102 Valerate equilibrium	−1	1													$\nu_{Sco2,102}$			$\nu_{Snh4+,102}$		$\nu_{Shpo4-,102}$		$\nu_{Sh+,102}$		$\nu_{Sh2o,102}$		$\nu_{So2,102}$
103 Butyrate equilibrium			−1	1											$\nu_{Sco2,103}$			$\nu_{Snh4+,103}$		$\nu_{Shpo4-,103}$		$\nu_{Sh+,103}$		$\nu_{Sh2o,103}$		$\nu_{So2,103}$
104 Propionate equilibrium					−1	1									$\nu_{Sco2,104}$			$\nu_{Snh4+,104}$		$\nu_{Shpo4-,104}$		$\nu_{Sh+,104}$		$\nu_{Sh2o,104}$		$\nu_{So2,104}$
105 Acetate equilibrium							−1	1							$\nu_{Sco2,105}$			$\nu_{Snh4+,105}$		$\nu_{Shpo4-,105}$		$\nu_{Sh+,105}$		$\nu_{Sh2o,105}$		$\nu_{So2,105}$
106 CO_2 dissolution														−1	$\nu_{Sco2,106}$			$\nu_{Snh4+,106}$		$\nu_{Shpo4-,106}$		$\nu_{Sh+,106}$		$\nu_{Sh2o,106}$		$\nu_{So2,106}$
107 O_2 dissolution															$\nu_{Sco2,107}$			$\nu_{Snh4+,107}$		$\nu_{Shpo4-,107}$		$\nu_{Sh+,107}$		$\nu_{Sh2o,107}$	−1	$\nu_{So2,107}$
108 H_2O evaporation															$\nu_{Sco2,108}$			$\nu_{Snh4+,108}$		$\nu_{Shpo4-,108}$		$\nu_{Sh+,108}$	1	$\nu_{Sh2o,108}$		$\nu_{So2,108}$
109 NH_3 dissolution															$\nu_{Sco2,109}$	1	−1	$\nu_{Snh4+,109}$		$\nu_{Shpo4-,109}$		$\nu_{Sh+,109}$		$\nu_{Sh2o,109}$		$\nu_{So2,109}$
110 CH_4 dissolution											1	−1			$\nu_{Sco2,110}$			$\nu_{Snh4+,110}$		$\nu_{Shpo4-,110}$		$\nu_{Sh+,110}$		$\nu_{Sh2o,110}$		$\nu_{So2,110}$
112 H_2 dissolution									1	−1					$\nu_{Sco2,112}$			$\nu_{Snh4+,112}$		$\nu_{Shpo4-,112}$		$\nu_{Sh+,112}$		$\nu_{Sh2o,112}$		$\nu_{So2,112}$

Table 7. *Stoichiometry of the Source-Sink components*

32	35	37	39	41	43
S_{co2}	S_{nh4+}	$S_{hpo4=}$	S_{h+}	S_{h2o}	S_{o2}
$\nu_{Sco2,j} = -\sum_{i=1}^{31}\left(\frac{\beta_{C,i}\cdot\nu_{ij}}{\beta_{C,Sco2}}\right)$	$\nu_{Snh4+,j} = -\sum_{i=1}^{34}\left(\frac{\beta_{N,i}\cdot\nu_{ij}}{\beta_{N,Snh4+}}\right)$	$\nu_{Shpo4=,j} = -\sum_{i=1}^{36}\left(\frac{\beta_{P,i}\cdot\nu_{ij}}{\beta_{P,Shpo4=}}\right)$	$\nu_{Sh+,j} = -\sum_{i=1}^{38}\left(\frac{\beta_{Ch,i}\cdot\nu_{ij}}{\beta_{Ch,Sh+}}\right)$	$\nu_{Sh2o,j} = -\sum_{i=1}^{40}\left(\frac{\beta_{H,i}\cdot\nu_{ij}}{\beta_{H,Sh2o}}\right)$	$\nu_{So2,j} = -\sum_{i=1}^{42}\left(\frac{\beta_{O,i}\cdot\nu_{ij}}{\beta_{O,So2}}\right)$
$\beta_{E,i}$: Mass of the element E per stoichiometric unit of the component *i* calculated from the *i* mass fractions					

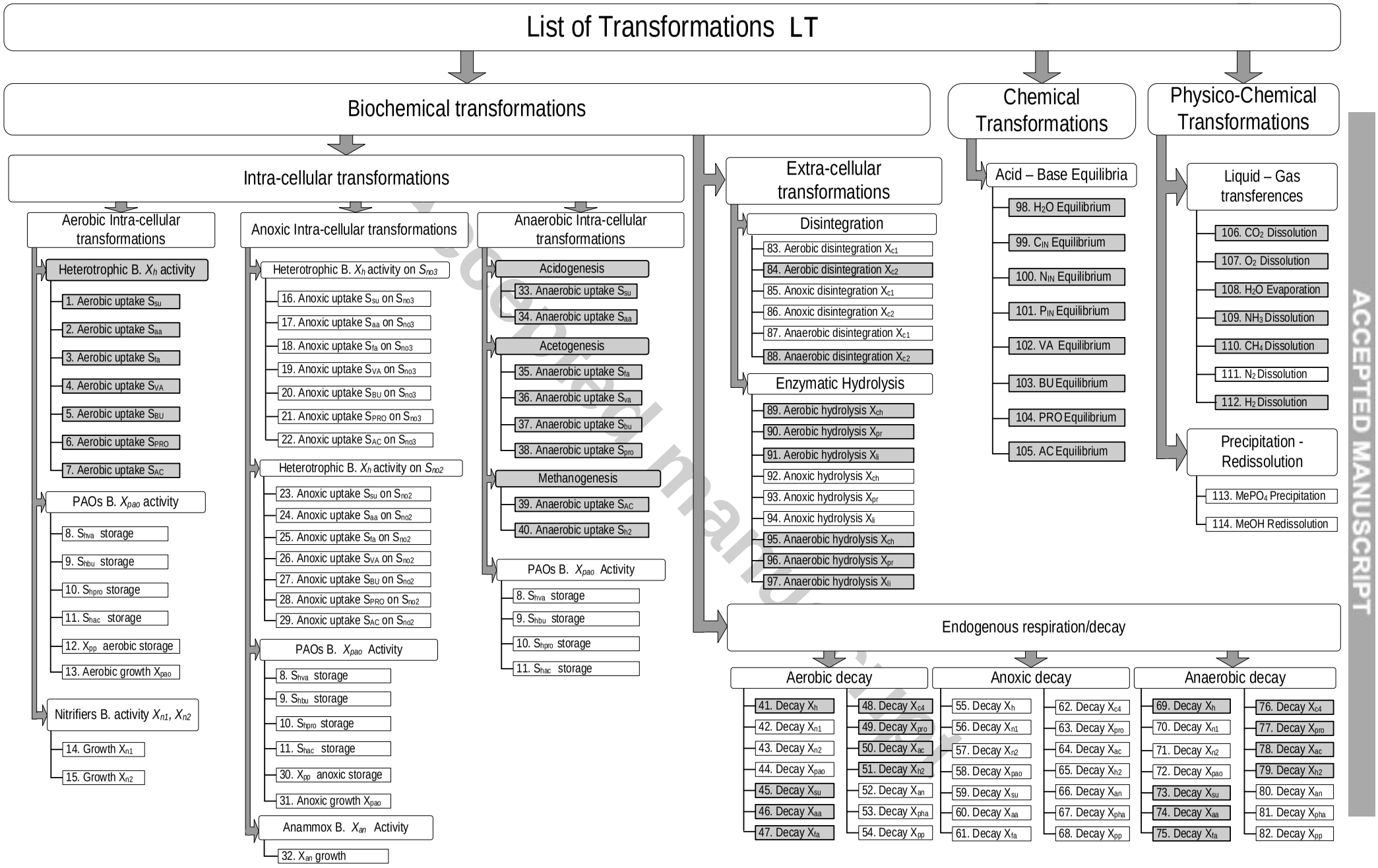

Figure 1. *List of Transformations proposed in this paper*

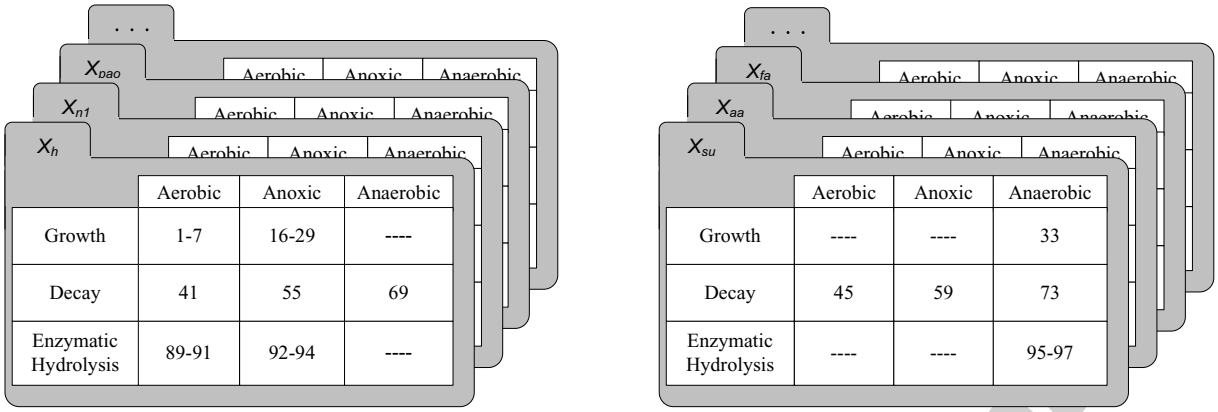

Figure 2. *Transformations related to X_h and X_{su} activity*

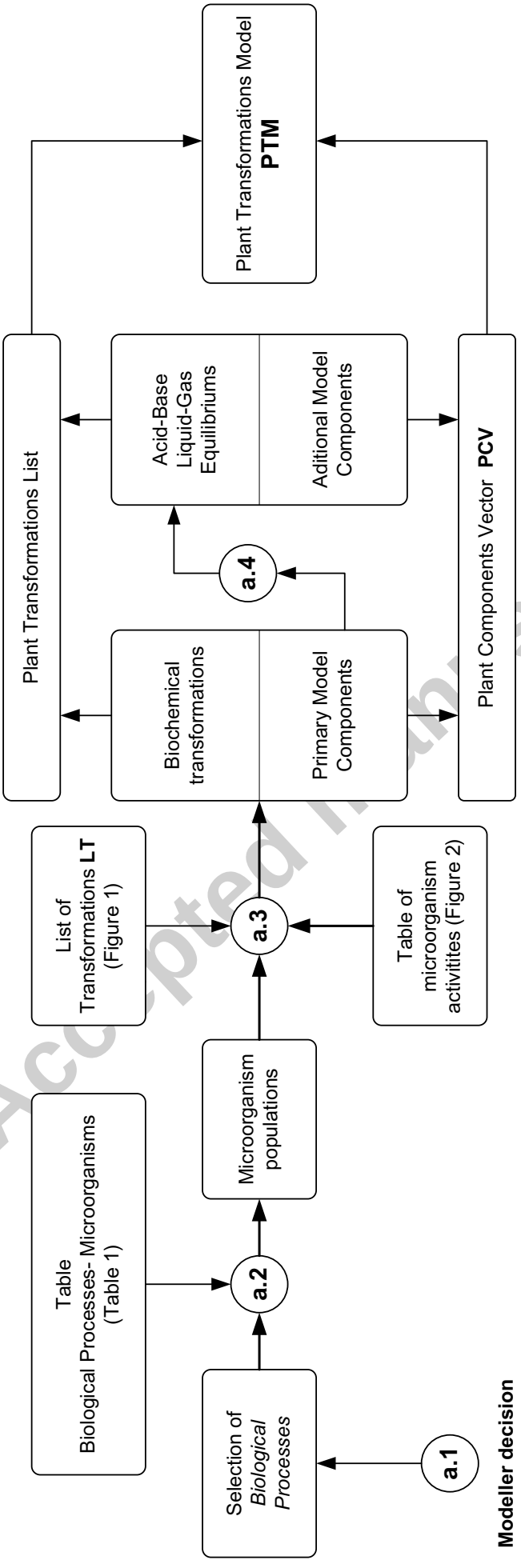

Figure 3. *Scheme of the procedure for PTM construction*

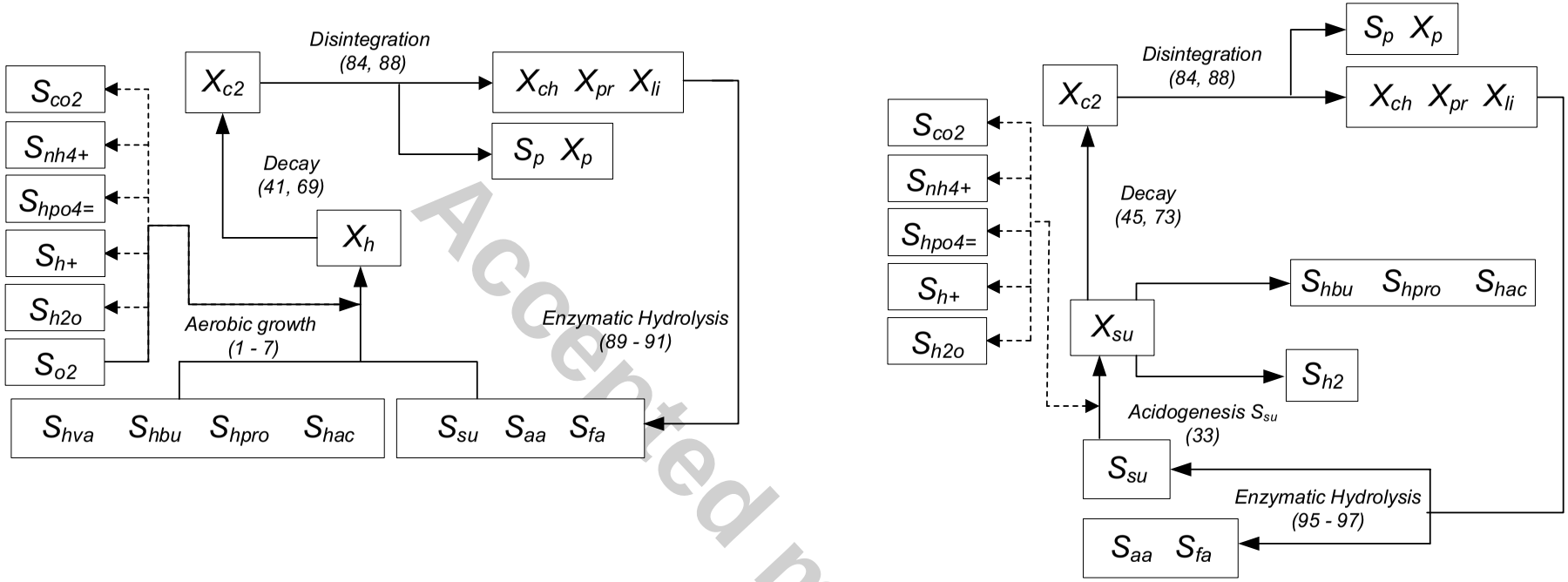

Figure 4. *Components and biochemical transformations involved in the X_h and X_{su} activity*

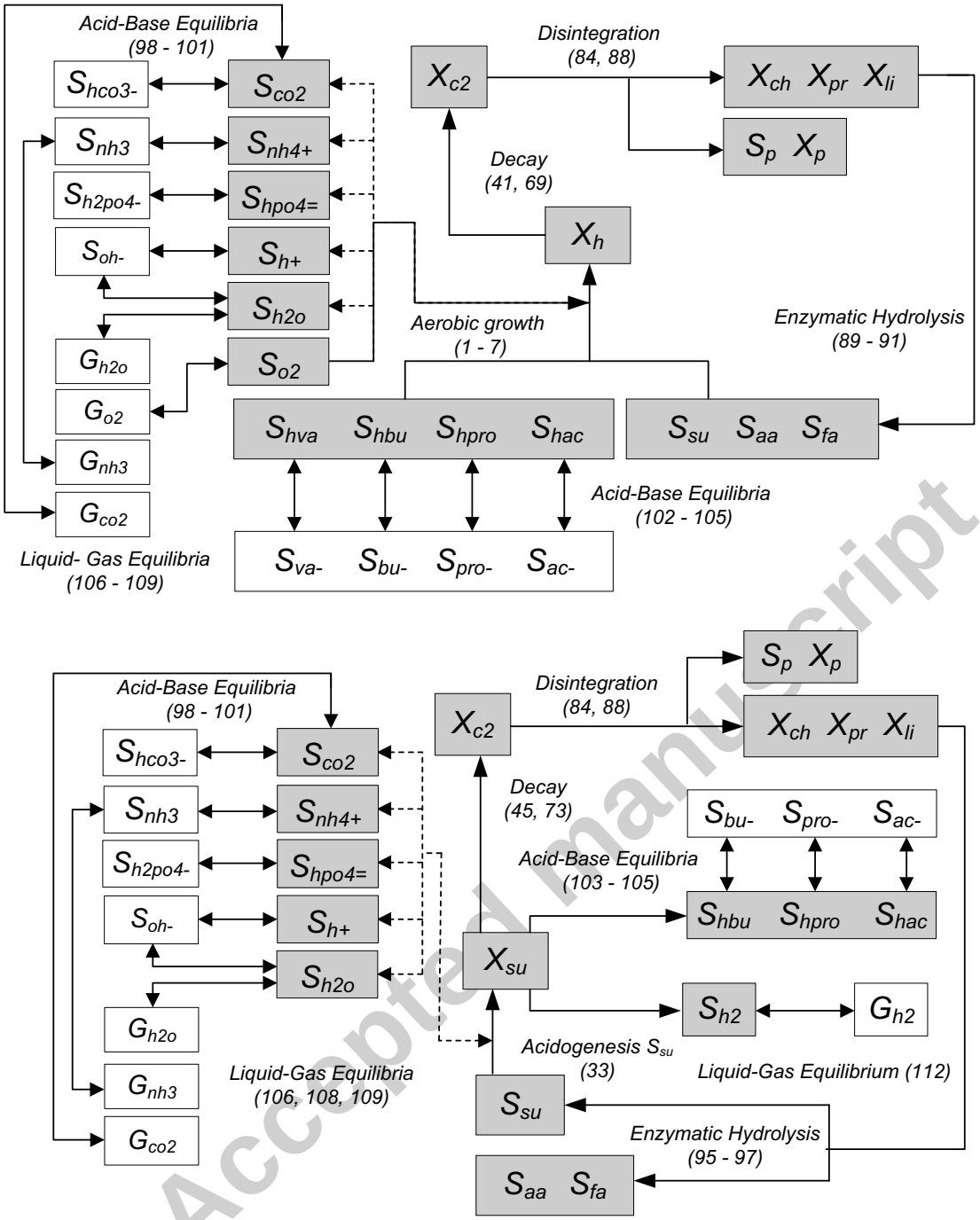

Figure 5. *Components and transformations incorporated in the X_h and X_{su} activity*