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# Development of an integrated approach for wastewater treatment plant optimization based on dynamic modelling and environmental assessment

Ana Barbara Bisinella de Faria

► **To cite this version:**

Ana Barbara Bisinella de Faria. Development of an integrated approach for wastewater treatment plant optimization based on dynamic modelling and environmental assessment. Chemical and Process Engineering. INSA de Toulouse, 2016. English. NNT : 2016ISAT0039 . tel-01652117

**HAL Id: tel-01652117**

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# THÈSE

En vue de l'obtention du

## DOCTORAT DE L'UNIVERSITÉ DE TOULOUSE

Délivré par :

Institut National des Sciences Appliquées de Toulouse (INSA de Toulouse)

---

**Présentée et soutenue par :**  
**Ana Barbara BISINELLA DE FARIA**

le mardi 18 octobre 2016

**Titre :**

Development of an integrated approach for wastewater treatment plant optimization based on dynamic modelling and environmental assessment

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**École doctorale et discipline ou spécialité :**

ED MEGEP : Génie des procédés et de l'Environnement

**Unité de recherche :**

Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (LISBP)

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## **English abstract**

Wastewater treatment plants are moving towards energy and nutrients recovery facilities. Simultaneously, they are submitted to stricter regulation with respect to environment and human health. Facing the great challenge of reducing operational costs along with the reduction of environmental impacts and the guaranty of plants robustness, tools might be developed in order to provide an integrated assessment. The goal of this work is to develop a reliable and predictive framework containing rigorous dynamic wide-plant modelling, extended boundaries life cycle assessment for scenarios evaluation and an efficient multi-objective optimization tool. The developed framework for environmental evaluation coupled to dynamic modelling was initially applied to several case studies including urine source separation, enhanced primary clarification and urine treatment by nitrification/ anaerobic ammonium oxidation, offering both performance results and environmental hotspots. Given the important benefits of the urine source separation provided by the previous results, a flexible and dynamic phenomenological influent generator was adapted in order to provide realistic dynamic data concerning urine and wastewater streams in different urine retention scenarios. Finally, as the complex combination of biological, chemical and physical processes leads to a computational expensive problem, a feasibility study (computational time and reliability) on the multi-objective optimization was conducted. Obtaining a set of solutions that avoids any prior discrimination among costs, environment and performance allowed thus the discussion of the involved trade-offs. Finally, the complete framework was applied to several case studies lightening on operational aspects of more sustainable options on wastewater management and treatment.

*Keywords: Wastewater; Modelling; Life Cycle Assessment; Multi-Objective Optimization; Urine Source Separation*



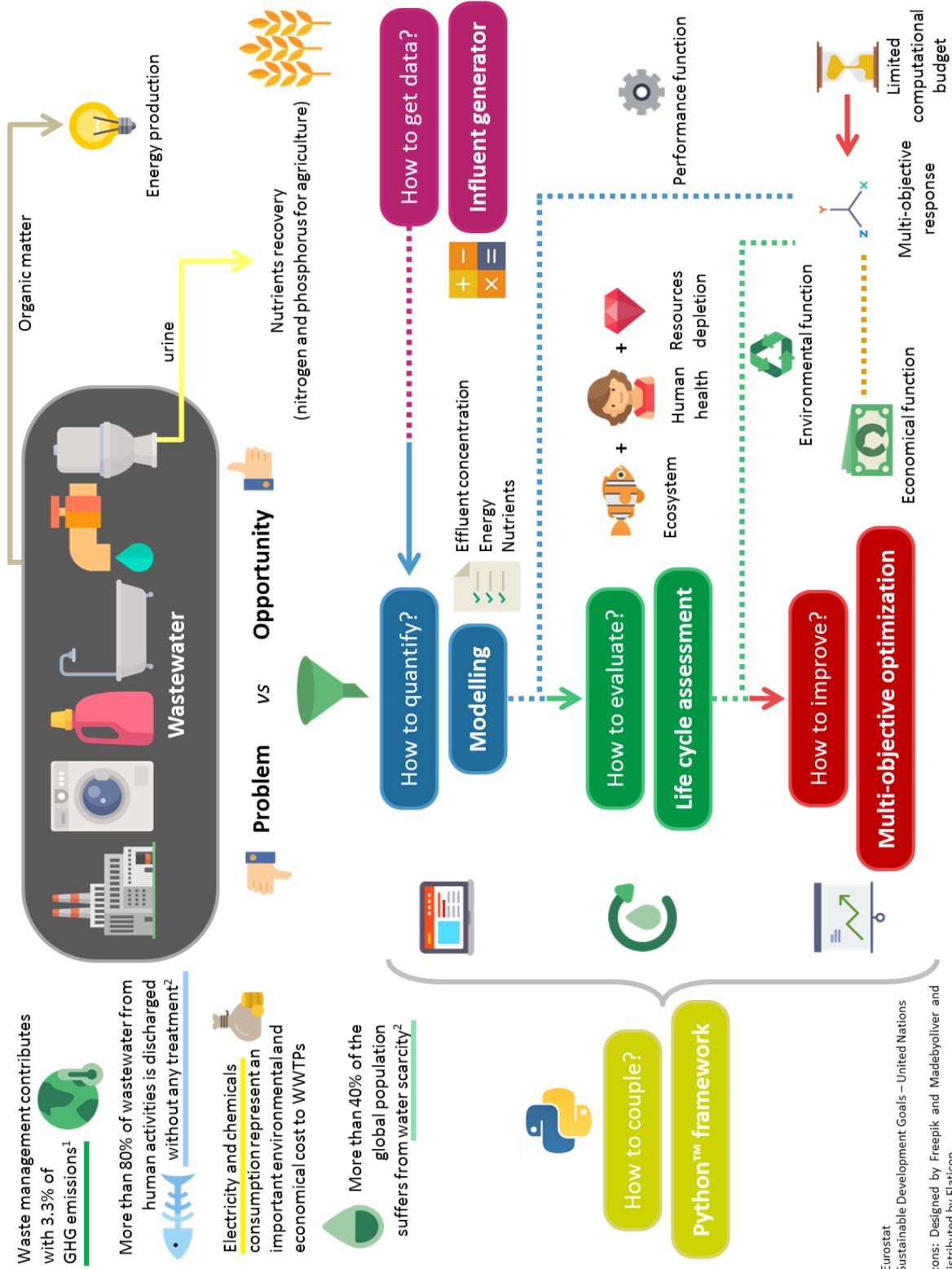
## Résumé en Français

Les stations d'épuration se tournent actuellement vers des installations de récupération d'énergie et des nutriments. Dans le même temps, elles sont soumises à une réglementation de plus en plus stricte en ce qui concerne l'environnement et la santé humaine. Face au défi ambitieux de réduire les coûts d'exploitation et les impacts environnementaux tout en garantissant la robustesse du procédé, il est nécessaire de développer des outils capables de fournir une évaluation intégrée du procédé. L'objectif de ce travail est de développer une plateforme réaliste et prédictive contenant trois aspects: la modélisation rigoureuse et dynamique de l'ensemble de la station d'épuration; l'analyse de cycle de vie aux frontières étendues pour l'évaluation des scénarios et enfin un outil d'optimisation multi-objectif efficace. La plateforme développée pour l'évaluation environnementale couplée à la modélisation dynamique a d'abord été appliquée à plusieurs cas d'étude. Ainsi des résultats de performance et d'impacts environnementaux ont été obtenus pour la séparation de l'urine à la source, la décantation primaire avancée et le traitement de l'urine par nitrification/ oxydation anaérobie de l'ammonium, et d'autres filières. Compte tenu des importants avantages de la séparation de l'urine établis par les résultats précédents, un générateur d'influents phénoménologique, flexible et dynamique a été adapté afin de fournir des données dynamiques réalistes concernant les flux d'urine et des eaux usées dans les différents scénarios de rétention d'urine. Enfin, comme la combinaison complexe de processus biologiques, chimiques et physiques conduit à un problème lourd en calcul, une étude de faisabilité (temps de calcul et fiabilité) a été réalisée sur l'optimisation multi-objectif. L'obtention d'un ensemble de solutions qui évite toute discrimination préalable entre les coûts, l'environnement et les performances ont permis la discussion des enjeux impliqués. Finalement, la plateforme complète a été appliquée à plusieurs cas d'étude et clarifie les aspects opérationnels des options plus durables en matière de gestion et de traitement des eaux usées.

*Mots-clés: Eaux usées; Modélisation; Analyse de Cycle de Vie; Optimisation Multi-Objectif; Separation de l'Urine à la Source*



# Graphical abstract





## **Scientific production**

### **Scientific papers published in international and peer reviewed journals**

Bisinella de Faria, A.B., Spérandio, M., Ahmadi, A., Tiruta-Barna, L., 2015. Evaluation of new alternatives in wastewater treatment plants based on dynamic modelling and life cycle assessment (DM-LCA). *Water Research*. 84, 99-111.

Bisinella de Faria, A.B., Ahmadi, A., Tiruta-Barna, L., Spérandio, M., 2016. Feasibility of rigorous multi-objective optimization of wastewater management and treatment plants. *Chemical Engineering Research and Design*. (accepted – under publication)

Bisinella de Faria, A.B., Besson, M., Ahmadi, A., Udert, K.M., Spérandio, M., 2016. A dynamic influent generator to account for alternative wastewater management: the case of urine source separation. (in preparation)

Bisinella de Faria, A.B., Ahmadi, A., Spérandio, M., Tiruta-Barna, L., 2016. LCA based multi-objective optimization of conventional and innovative wastewater management and treatment scenarios. (in preparation)

### **Conferences with full text and proceedings**

de Faria, A.B. B., Spérandio, M., Ahmadi, A., Tiruta-Barna, L., 2014. A dynamic modelling-LCA integrated approach to evaluate new alternatives in WWTPs. IWA Specialized Conference “Global Challenges: Sustainable Wastewater Treatment and Resource Recovery”, October 26th – 30th, 2014. Kathmandu – Nepal (Oral presentation).

Bisinella de Faria, A.B., Tiruta-Barna, L., Ahmadi, A., Spérandio, M., 2015. Life cycle analysis of scenarios coupling urine separation, struvite recovery and anammox process. IWA Specialized Conference “Nutrient Removal and Recovery. Moving Innovations into Practice”, May 18th – 21st, 2015. Gdańsk – Poland (Oral presentation).

## **Conferences with abstract**

Bisinella de Faria, A.B., Tiruta-Barna, L., Ahmadi, A., Spérandio, M., 2015. Efficient multi-objective optimization on some promising alternatives to conventional wastewater treatment plants. 10th European Congress of Chemical Engineering, September 27th – October 1st, 2015. Nice – France (Oral presentation).

Bisinella de Faria, A.B., Spérandio, M., Ahmadi, A., Tiruta-Barna, L., 2015. A dynamic modelling-life cycle assessment (DM-LCA) platform for the evaluation of alternative wastewater treatment plants. 7th International Conference on Life Cycle Management, August 30th – September 2nd, 2015. Bordeaux – France (Poster).

Bisinella de Faria, A.B., Tiruta-Barna, L., Ahmadi, A., Spérandio, M., 2015. Mass and energy recovery versus environmental evaluation in conventional and alternative WWTPs. International Conference Recycling 2015, March 16th – 18th, 2015. Metz – France (Poster).

## **Seminars**

Bisinella de Faria, A. B., Tiruta-Barna, L., Ahmadi, A., Spérandio, M., 2016. Efficient multi-objective optimization on some promising alternatives to conventional wastewater treatment plants. OASIS Intermediate Workshop. January, 2016. Luxembourg (Oral presentation)

## **Acknowledgments – Remerciements - Agradecimentos**

This PhD thesis is a result of three years of work and a good souvenir that I will always keep in my mind. To all of you that have contributed to this work: thank you! Without you, this would never have been possible (even if there is not enough space to list you all, be sure that you have a special place in my heart).

I would like to express my gratitude to the members of the reviewing committee: Mrs. Aurora Seco, Mr. Jean-Philippe Steyer, Mrs. H  l  ne Hauduc and Mr. Kai Udert. The time and the attention you have dedicated to read and comment this work significantly improve the quality of this PhD thesis. Also, a special acknowledgment to Dynamita team who helped me a lot, especially when starting with Sumo.

Un merci    mes trois directeurs de th  se : Mathieu Sp  randio, Aras Ahmadi et Ligia Tiruta-Barna. Cela a   t   un   norme plaisir de travailler avec vous. Merci de m'avoir guid   et de m'avoir aid      tisser les liens entre 3 sujets extr  mement riches : la mod  lisation, l'ACV et l'optimisation ! Je vous remercie aussi   norm  ment pour toutes les discussions pendant ces trois ann  es de th  se et principalement de m'avoir donn   l'exemple de l'  coute avec un   norme respect de l'autre. Ensemble vous vous   tes compl  t  s et je ne peux que vous remercier de m'avoir permis,    la fois, de m'  loigner de mon sujet « classique » vers une curiosit   scientifique (merci Mathieu !) tout en me rappelant, avec un grand sourire, aux points essentiels (merci Ligia !) et toujours avec une patiente et un sens critique indescriptibles (merci Aras !).

Je tiens    remercier aussi    tous mes coll  gues du LISBP. Un merci tout particulier    mes coll  gues doctorants : les histoires et les fous rires partag  s m'ont   norm  ment aid  e pendant ces trois ann  es et resteront toujours dans ma m  moire ! Un   norme merci    mes coll  gues du bureau B4, les melting potes : Claire, Mathias et Allan! En plus d'avoir partag   le bureau, avec vous j'ai aussi partag   des tr  s bons moments. Un merci sp  cial aussi    Mathilde pour tout ton aide qui m'a permis de finir ce travail.

Un obrigada muito especial    todos da minha familia que, de longe ou perto, estiveram torcendo pela realiza  o desse trabalho. Um obrigada especial aos meus pais, Elizete e Messias e    minha irm   Joana pelo carinho e a paci  ncia sempre! Um pensamento e um agradecimento muito especial tamb  m ao meu padrinho Silvar: as palavras que voc   me deixou antes de partir, ficaram e ficar  o sempre em minha mem  ria me lembrando carinhosamente que, mesmo quando as dificuldades aparecem, vale a pena correr atr  s dos sonhos. Obrigada e fique em paz!

Por fim, obrigada novamente Allan, por ter sido muito mais que um companheiro de bureau. Obrigada por toda a for  a e paci  ncia nos momentos onde o p  r-do-sol me lembrava dos prazos a serem cumpridos e qu  o dif  cil era essa etapa. Com voc   eu dividi esses   ltimos anos e    com voc   que eu quero continuar a dividir todos os novos desafios que vir  o.

Thank you all! Merci    tous! Obrigada    todos!



# Summary

<i>English abstract</i> .....	<i>i</i>
<i>Résumé en Français</i> .....	<i>iii</i>
<i>Graphical abstract</i> .....	<i>v</i>
<i>Scientific production</i> .....	<i>vii</i>
Scientific papers published in international and peer reviewed journals .....	<i>vii</i>
Conferences with full text and proceedings .....	<i>vii</i>
Conferences with abstract .....	<i>viii</i>
Seminars .....	<i>viii</i>
<i>Acknowledgments – Remerciements - Agradecimento</i> .....	<i>ix</i>
<i>List of figures</i> .....	<i>xv</i>
<i>List of tables</i> .....	<i>xvii</i>
<i>List of abbreviations</i> .....	<i>xix</i>
<b>Chapter I. General Introduction</b> .....	<b>1</b>
I.1. Wastewater as a pollution stream .....	4
I.2. Wastewater as a resource recovery opportunity .....	6
I.2.1. Extracting resources from wastewater.....	6
I.2.2. Urine source separation .....	8
I.3. Quantifying benefits: Wastewater treatment modelling and simulation .....	10
I.3.1. Obtaining data: Influent generation.....	11
I.4. Evaluating benefits: Life Cycle Assessment (LCA).....	12
I.5. Improving systems: Multi-objective optimization .....	14
I.6. Research objectives and tasks .....	16
I.6.1. Thesis outline .....	18
<b>Chapter II. Coupling Dynamic Modelling and LCA</b> .....	<b>21</b>
<i>Entitled of the paper: Evaluation of new alternatives in wastewater treatment plants based on Dynamic Modelling and Life Cycle Assessment (DM-LCA)</i> .....	27
Abstract .....	27
II.1. Introduction .....	28
II.2. Materials and methods.....	30
II.2.1. The integrated DM-LCA methodology .....	30
II.2.2. Plant layout and scenarios .....	32
II.2.3. LCA.....	35
II.2.3.1. Goal & scope .....	35
II.2.3.2. Life cycle inventory.....	37
II.2.3.3. LCIA.....	39
II.3. Results and discussion.....	39
II.3.1. Reference scenario .....	39
II.3.2. Results of alternative scenarios: nutrient recovery, efficiency and energy consumption .....	42

II.3.3.	Results of alternative scenarios: environmental impacts.....	46
II.3.3.1.	Endpoint impacts.....	46
II.3.3.2.	Midpoint results.....	48
II.4.	Conclusion.....	52
<b>Chapter III.</b>	<b>Influent Generator.....</b>	<b>55</b>
	<i>Entitled of the paper: A dynamic influent generator to account for alternative wastewater management: the case of urine source separation .....</i>	<i>59</i>
	Abstract .....	59
III.1.	Introduction .....	59
III.2.	General overview .....	62
III.3.	Flow generation.....	65
III.4.	Pollutants generation .....	68
III.4.1.	General aspects.....	68
III.4.2.	Composite variables .....	68
III.4.3.	Fractionation into state variables.....	69
III.5.	Noise addition.....	77
III.6.	Example of simulations obtained with the generated influent.....	78
III.7.	Discussion .....	79
III.7.1.	Average results .....	79
III.7.2.	Daily and weekly profiles.....	81
III.8.	Use of the generated influent for process simulation .....	83
III.8.1.	Comparison between different models .....	83
III.8.2.	Effect of urine retention levels .....	85
III.9.	Conclusions .....	87
<b>Chapter IV.</b>	<b>Feasibility of Multi-Objective Optimization .....</b>	<b>89</b>
	<i>Entitled of the paper: Feasibility of rigorous multi-objective optimization of wastewater management and treatment plants .....</i>	<i>93</i>
	Abstract .....	93
IV.1.	Introduction .....	94
IV.2.	Materials and methods.....	98
IV.2.1.	Dynamic Modelling (DM) approach.....	98
IV.2.2.	Life Cycle Assessment (LCA) approach.....	101
IV.2.3.	Efficient Multi-Objective Optimization (EMOO).....	102
IV.2.3.1.	Problem formulation: objective functions, constraints and range of decision variables	102
IV.2.3.2.	Expensive optimization algorithm and general settings.....	107
IV.2.4.	Integrated framework: DM-LCA-EMOO .....	108
IV.3.	Results and discussion.....	111
IV.3.1.	WWTP optimization and objectives' dependencies.....	111
IV.3.2.	Drivers for an optimal treatment .....	115
IV.3.3.	Problem formulation and computational feasibility of multi-objective optimization	118
IV.4.	Conclusion.....	120

<b>Chapter V. Case Studies on Multi-Objective Optimization .....</b>	<b>121</b>
<i>Entitled of the paper: LCA based multi-objective optimization of conventional and innovative wastewater management and treatment scenarios.....</i>	<i>125</i>
Abstract .....	125
V.1. Introduction .....	126
V.2. Materials and methods.....	131
V.2.1. Dynamic Modelling – Life Cycle Assessment – Efficient Multi-Objective Optimization (DM-LCA-EMOO) coupling approach.....	131
V.2.1.1. Dynamic modelling (DM) .....	132
V.2.1.2. Life Cycle Assessment (LCA).....	133
V.2.1.3. Efficient Multi-Objective Optimization (EMOO).....	134
V.2.2. WWTP scenarios (conventional vs. innovative) .....	135
V.2.3. Optimization problem formulation.....	137
V.2.3.1. Objective function .....	137
V.2.3.2. Decision variables and constraints handling .....	140
V.2.3.3. Recall on optimization problem formulation.....	141
V.3. Results and discussion.....	142
V.3.1. Reference scenario .....	142
V.3.1.1. General results .....	142
V.3.1.2. Analysis on decision variables .....	147
V.3.1.3. Steady state versus dynamic modelling approach .....	149
V.3.1.4. Total Endpoint versus Midpoint Global Warming Potential.....	151
V.3.2. Alternative scenario (ANA) .....	153
V.3.3. Consequences on energy autarky .....	155
V.3.4. Benefits achieved from REF and ANA scenarios .....	157
V.4. Conclusions .....	159
<b>Chapter VI. Conclusions and perspectives .....</b>	<b>161</b>
<b>Résumé long en français .....</b>	<b>169</b>
<b>References .....</b>	<b>185</b>
<b>Supplementary Information.....</b>	<b>193</b>
A. Supplementary Information for chapter II.....	195
A.1. Emissions calculation .....	195
A.2. Inventory .....	201
A.3. Energy parameters.....	209
A.4. Effluent and ambient temperature .....	216
A.5. Agricultural spreading.....	219
A.6. Other midpoint and endpoint results .....	220
A.6.1 Environmental impact results for steady state and dynamic results.....	220
A.6.2 Environmental impact results for alternative scenarios.....	235
A.6.3 Cumulative energy demand for reference and alternative scenarios .....	251
A.7. General information .....	252
A.7.1 Potable water avoidance.....	252
A.7.2 Gas emission calculations.....	252

A.7.3	Urine influent calculation .....	252
A.7.4	General tables .....	253
B.	Supplementary Information for chapter III .....	257
B.1	Adapted Influent Generator Matlab code .....	257
C.	Supplementary Information for chapters IV and V .....	274
C.1.	Adapted Sumo2 Gujer matrix.....	274

## List of figures

Figure I.1. General overview of original BSM2.....	11
Figure I.2. Simplified scheme of the combined platform DM-LCA-EMOO .....	17
Figure II.1. DM-LCA framework developed with connections between Dynamic Modelling, LCA and Python™ interface.....	32
Figure II.2. Plant configuration used in this study. ....	33
Figure II.3. Expanded system boundaries for LCA.....	36
Figure II.4. Comparisons between steady state and dynamic simulations .....	41
Figure II.5. Energy distribution by consumption item .....	46
Figure II.6. Endpoint impacts for studied scenarios.....	47
Figure II.7. Contribution analysis for climate change (GWP100) using ReCiPe Midpoint (H) .....	48
Figure II.8. Contribution of each species to greenhouse gases emitted .....	49
Figure II.9. Contribution analysis for marine (A) and freshwater (B) eutrophication using ReCiPe Midpoint (H) .....	50
Figure II.10. Contribution analysis for fossil fuel depletion using ReCiPe Midpoint (H) .....	52
Figure III.1. General overview of the urine source separation influent generator .....	64
Figure III.2. Profiles for US and WW streams. ....	67
Figure III.3. Detail of fractionation block (E) .....	72
Figure III.4. Sankey diagram for COD fractions in urine versus COD in total wastewater.....	74
Figure III.5. Sankey diagram for nitrogen fractions in urine versus nitrogen in total wastewater .....	75
Figure III.6. Sankey diagram for phosphorus fractions in urine versus phosphorus in total wastewater .....	76
Figure III.7. Reduction of WW input variables when considering 50% urine source separation .....	80
Figure III.8. Weekly profile of flowrate; Daily variation of $S_{VFA}$ and $S_{NHx}$ .....	82
Figure III.9. Performance (Effluent ammonia and effluent nitrate and nitrite) and operational (Air flowrate) results for Sumo1 and ASM1 models .....	84
Figure III.10. Comparison of different urine retention levels considering performance (Effluent ammonia; Effluent nitrate and nitrite) and operational (Air flowrate) results.....	86
Figure IV.1. WWTP configuration.....	100

Figure IV.2. Structure of AMOEA-MAP framework used in this WWTP problem optimization.....	108
Figure IV.3. Structure of the integrated framework (Dynamic Modelling - Life Cycle Assessment - Efficient Multi-Objective Optimization).....	110
Figure IV.4. Pareto optimal curves for constrained and unconstrained optimization of WWTP.....	113
Figure IV.5. Zoom on optimal zones with water quality beyond the legally-imposed limits .....	114
Figure IV.6. Level of methanol addition - driver for N treatment - for all solutions belonging to the Pareto optimal front.....	115
Figure IV.7. Level of iron chloride addition – driver for P removal – for all solutions in the Pareto optimal front.....	116
Figure IV.8. Correlation scatterplots for decision variables and objective functions .....	118
Figure IV.9. Optimization improvement based on hypervolume distance indicator ( $I_H$ ) calculations	119
Figure V.1. Simplified structure of the integrated framework (Dynamic Modelling - Life Cycle Assessment - Efficient Multi-Objective Optimization).....	132
Figure V.2. Simplified flowsheet for the two WWTP scenarios studied in the present work.....	136
Figure V.3. Detailed configuration of the proposed WWTP scenarios in SUMO .....	137
Figure V.4. Pareto-optimal curves for constrained and unconstrained optimization of the reference WWTP.....	143
Figure V.5. Box-and-whisker plots for total nitrogen, ammonium ion and total phosphorus concentrations in effluent for the optimized reference scenario (REF).....	145
Figure V.6. Box-and-whisker plots for the main cost contributors in Operational Cost Index (OCI) function for the optimized reference scenario (REF) .....	146
Figure V.7. Correlation scatterplots on decision variables and objective functions (optimized REF scenario) .....	150
Figure V.8: Pareto-optimal fronts resulting from steady state <i>versus</i> dynamic simulations (REF scenario) .....	151
Figure V.9. Pearson product-moment correlations between different impact categories in LCIA .....	152
Figure V.10: Comparative optimal Pareto fronts on the reference scenario (REF) <i>versus</i> the urine treatment by nitrification/ anaerobic deammonification (ANA) .....	155
Figure V.11. Box-and-whisker plots on total nitrogen, ammonium ion and total phosphorus concentrations in effluent of the optimized ANA scenario .....	155
Figure V.12: EROI (Energy return on investment) calculations for all solutions belonging to the optimal Pareto front (REF and ANA scenarios).....	156

## List of tables

Table II.1. Comparison of scenarios.....	35
Table II.2. Comparison between this study and the literature for BNR processes .....	40
Table II.3. Main simulation results for the reference (steady state and dynamic simulations) and the alternative scenarios (dynamic simulations) .....	43
Table III.1. Input and calculated values for composite variables (case study of 50% urine retention). 66	
Table III.2. Considered initial values for total urine stream (TUS), separated urine stream (US), total wastewater without urine retention (TWW) and wastewater with urine retention (WW) .....	71
Table III.3. Ionic species molar ratio to ammonium for total wastewater and total urine stream .....	77
Table III.4. Noise factors considered in this study.....	78
Table III.5. Adapted inputs for ASM1 simulation .....	79
Table IV.1. Average influent characteristics.....	101
Table IV.2. Proposed $\alpha$ values for OCI function.....	103
Table IV.3. Proposed $\beta$ values for EQI function.....	104
Table IV.4. Decision variables considered in this study .....	106
Table IV.5. Decision variables values for chosen optimal points .....	116
Table V.1. Influent characteristics .....	137
Table V.2. Proposed $\alpha$ values for OCI function .....	138
Table V.3. Proposed $\beta$ values for EQI function .....	139
Table V.4. Decision variables chosen for REF and ANA scenarios .....	140
Table V.5. List of comparative studies on different problem formulations and innovative scenarios in the field of WWTP optimization .....	141
Table V.6. Benefits derived from ANA scenario when compared with REF scenario .....	158



## List of abbreviations

ADM	Anaerobic Digestion Model
AMOEА	Archive-based Multi-Objective Evolutionary Algorithm
ANAMMOX	Anaerobic Ammonium Oxidation
AS	Activated Sludge
ASM	Activated Sludge Model
ASP	Activated Sludge Process
ASDM	Activated Sludge Digestion Model
BSM1	Benchmark Simulation Model N°1
BSM2	Benchmark Simulation Model N°2
CED	Cumulative Energy Demand
COD	Chemical Oxygen Demand
DM	Dynamic Modelling
DO	Dissolved Oxygen
EA	Evolutionary Algorithm
EMOO	Efficient Multi-Objective Optimization
EPC	Enhanced Primary Clarification
EQI	Effluent Quality Index
EROI	Energy Return On Investment
FU	Functional Unit
GHG	Greenhouse Gas
HFO	Hydrous Ferric Oxides
IAMO	Importance Adaptive Mutation Operator
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
ISS	Inorganic Suspended Solids
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
MAP	Memory-based Adaptive Partitioning of search space
MDG	Millennium Development Goals
MOO	Multi-Objective Optimization
NSGA	Non-Sorting Genetic Algorithm
OCI	Operational Cost Index

PE	Person equivalent
RER	Europe
SI	Supplementary Information
SRT	Sludge Retention Time
TKN	Total Kjeldahl nitrogen
TN	Total Nitrogen
TOC	Total Organic Carbon
TP	Total Phosphorus
TSS	Total Suspended Solids
USS	Urine Source Separation
VSS	Volatile Suspended Solids
WRRF	Water Resource Recovery Facility
WWTP	Wastewater Treatment Plant

# **Chapter I. General Introduction**



According to the United Nations, worldwide, 40% of people suffer from water scarcity and this number is projected to increase. In 2011, 41 countries experienced water stress and by 2050, it is expected that at least one in four people would be affected by recurring water shortages. Globally, still 2.4 billion people use unimproved sanitation facilities and at least 1.8 billion people use a source of drinking water that is fecally contaminated. As a consequence, approximately 1,000 children die each day due to water and sanitation-related diseases that might be prevented.

The Millennium Development Goals (MDGs) proposed in 2000 by the United Nations Development Program that comprised among the 8 main goals, the achievement of environmental sustainability arrived to its completion in 2015. As discussed in the final report of MDGs (United Nations, 2015), progress was achieved such as that 1.9 billion people have gained access to piped drinking water since 1990, 2.1 billion people have now access to improved sanitation and 98% of ozone-depleting substances have been eliminated since 1990.

However, much progress is still to be achieved and some gap points were left behind. As discussed in the final report, climate change and environmental degradation is worsening. Numbers concerning direct environmental impacts are alarming: Global emissions of carbon dioxide (CO<sub>2</sub>) have increased by over 50% since 1990 and the growth rate of emissions between 2000 and 2010 were more important than in each of the three previous decades; Emissions of methane (CH<sub>4</sub>) and dinitrogen monoxide (N<sub>2</sub>O), potent greenhouse gases, could rise by 50% and 25% respectively between 1990 and 2020 and the average global temperature increased by 0.85°C from 1880 to 2012; Further, the global average sea level rose by 19 cm from 1901 to 2010 and about 40% of the oceans are currently heavily affected by human activities; Finally, it is estimated that 90% of wastewater in developing countries is discharged into water bodies without treatment (United Nations, 2016).

Nonetheless, not only numbers are alarming. Changes in the worldwide context are becoming more and more evident when considering population growth together with the urbanization and the industrialisation, the increasing food demand, the changes in the land use and in the standards of living (UN-Water, 2015). Accordingly, with the increasing pressure on existing sewage collection and treatment systems, wastewater is being discharged without treatment and thus water quality is decreasing. This lack of treatment leads to direct impacts on the equilibrium of aquatic ecosystems and finishes by changing also anthropogenic activities, from urban development to food production and industry. As a consequence, environment is pressured and threatened and human health is also being degraded.

Therefore, it is becoming clearer that wastewater, as a pollution stream produced by anthropogenic activity that needs to use natural resources, has to return to the environment in a safe way. This is essential to cease the degradation generated by this non-ecological cycle which leads to all depletion

of essential resources, degradation of ecosystems and finally the exposition of the human health to an imminent danger. It is thus mandatory to find a more conscientious wastewater management and treatment to achieve higher levels of treatment together with robustness of the system in order to lead this ecosystem-human health-resources nexus to evolve together. In this sense, instead of being a source of problems, well-managed wastewater should play a positive role in the environment leading to improved food security, health and economy. However, it can only be done if wastewater management is considered as part of an integrated, full life cycle and ecosystem-based management system that comprises social, economic, environmental and geographical aspects (Corcoran et al., 2010).

### **I.1. Wastewater as a pollution stream**

As a result of a dynamic anthropogenic activity, wastewater is highly variable in function of more or less ecological lifestyle, geographical location, water availability, etc. Also, sewer collection system characteristics and the industry contribution in the municipal wastewater might influence the composition of the wastewater entering a wastewater treatment plant (WWTP). In this context, total wastewater, which is mainly of water, might contain a changeable composition that includes pathogens, organic compounds, synthetic chemicals (such as pharmaceutical and personal care products), nutrients (especially nitrogen and phosphorus), organic matter, heavy metals, etc. Those pollutants might be in solution, as particulate matter or as colloidal species. Also, biodegradable or inert species are present having sometimes cumulative, persistent and synergistic characteristics that might affect the ecosystem if not correctly managed (Henze and Comeau, 2003; Corcoran et al., 2010).

When output water quality after treatment is not acceptable, some impacts are well known to happen and efforts have to be done in order to avoid them. According to Corcoran et al. (2010), eutrophication is one of the most prevalent problems. It is defined as the process where water bodies (such as lakes, rivers, and coastal waters) become increasingly rich in plant biomass, as a result of the abundance of nutrients (mainly nitrogen and phosphorus) leading to toxic algal blooms, changes in biodiversity and consequently hypoxic events.

Another environmental impact that is gaining more interest last years is the climate change as, instead of only influencing ecosystems, it started influencing directly human health as it can have an impact on water scarcity, rainfalls and water quality. According to Corcoran et al. (2010), the relationship between wastewater and climate change can be seen from different perspectives. Considering human

activity, water usage practices are directly influenced by climate change as both volumes and quality of available water are changing. However, also technically, wastewater has to be managed differently and emitted greenhouse gases from wastewater treatment should be mitigated. This concerns particularly CO<sub>2</sub>, CH<sub>4</sub> (25-fold global warming potential of CO<sub>2</sub>; IPCC, 2006) and N<sub>2</sub>O (298-fold global warming potential of CO<sub>2</sub>; IPCC, 2006). Thus, there is a pressing need to investigate and implement alternatives to conventional wastewater treatment, which minimize the direct production of greenhouse gases and the indirect ones (for instance from power consumption).

A zoom in energy consumption shows that, for instance, water and wastewater treatment plants account for 3 to 4% of total electricity in United States and this energy consumption is in similar range for other developed countries. Therefore, reducing energy consumption for wastewater treatment might avoid environmental degradation linked to energy production. In this sense, the energy autarky of the wastewater treatment systems might, not only improve economics but also decrease air pollution and greenhouse gas emissions, enhance energy and water security and protect public health and environment (Gude, 2015).

Historically, wastewater has been treated by conventional Activated Sludge Process (ASP). In this system, organic matter and nutrients are treated by combining biological, chemical, physical and mechanical processes and this is done with a microbial biomass that is aerated and kept in suspension. Basically, an ASP consists of an aerated reactor where biological reactions take place. Following the biological reactor, a clarifier is responsible for retaining biomass in order to ensure a sludge retention time (SRT) that allows the efficiency of the treatment. Non recirculating biomass is purged to ensure stability. The flowsheet of ASPs might also contain a primary clarifier where particulate matter is retained, non aerated reactors where denitrification takes place, internal recycles to transport nitrate from the aerobic to the anoxic zone, anaerobic digestion of produced sludge and post-denitrification zone to achieve lower reject levels.

However, nowadays, ASPs have been identified as energy intensive and chemical consuming with also an excess sludge disposal issue (Gude, 2015; Lackner et al., 2014). In order to increase sustainability in wastewater treatment, several approaches have been described in the literature. One of the promising ones is the partial nitrification coupled to the anaerobic ammonium oxidation (Anammox). In this process, nitrite is firstly produced from ammonium by ammonia oxidizing bacteria (AOB); following, ammonium (as electron donor) and nitrite (as electron acceptor) are converted anaerobically into nitrogen gas and nitrate by anammox bacteria (Lackner et al., 2014). When applied to a full-scale installation, the process allows up to 70–90% of total nitrogen removal with a 65% reduction in aeration energy, a 100% reduction in carbon addition and approximately 50% reduction in alkalinity requirements when comparing to traditional processes (Gude, 2015; Jetten et al., 1997; Kartal et al., 2010)

## **I.2. Wastewater as a resource recovery opportunity**

### *I.2.1. Extracting resources from wastewater*

Wastewater has been described nowadays as both a resource and a problem by several authors. Since 2013, publications from Water Environment Federation (WEF) started using the term Water Resource Recovery Facility (WRRF) instead of WWTP, in order “to better focus on the products and benefits of treatment rather than the waste coming into such facilities” (WE&T, 2013).

In the past, the main idea behind wastewater treatment was the accomplishment of permitted reject limits. Nowadays, the goals are moving towards the maximization of recovery of valuable resources although water quality is maintained and robustness in process is achieved.

When conducting a balance across the potential energy that might be recovered from wastewater, Shizas and Bagley (2004) estimated that wastewater contains 9.3 times the energy required to treat it. However, this value might vary between 3.6 (when considering recoverable energy with recovery from organics and nutrients) and 13 (when including heat recovery) times higher than the energy required for treating it (Gude, 2015).

When considering nutrients, the most important part comes from urine. For instance, as discussed by Tidaker et al. (2007), the urine from Swedish population contains approximately 36 kilotons of nitrogen and 3.3 kilotons of phosphorus while 170 kilotons of nitrogen and 15 kilotons of phosphorus were consumed from mineral fertilizers in Sweden in 2001. Therefore, if nitrogen, phosphorus and even potassium in urine were utilised in substitution of synthetic fertilizers, the industrial production of those might be decreased and the discharge of those nutrients in water bodies would also be reduced (Johansson et al., 2000).

However, extracting resources from wastewater is not new. Some alternatives such as the production of fit-for-purpose water, the biosolids used in lands and the energy generation from anaerobic digestion are already common in WWTPs. Nowadays, new processes are starting to be studied in order to produce/recover specific compounds from wastewater such as precipitated struvite to be used as a slow-release fertilizer, the production of biologically-deriving polyhydroxyalkanoates from sludge and the use of digester gas to produce methanol or ammonia (WERF, 2011).

Also, the use of biosolids and the wastewater itself in farmlands is gaining more acceptances by population. While in developing countries the wastewater reuse is driven among others by the limited capacity to treat wastewater and the lack of other acceptable water sources for agriculture, in

developed countries water reuse and recycling are increasingly seen as a means to respond to physical water scarcity and water reallocations from agriculture to other uses. Also, nowadays, all the strict environmental standards lead to land application of wastewater and sludge to be unavoidable and economically feasible (Drechsel et al., 2010).

Anaerobic digestion nowadays is a currently valorisation process in several WWTPs. In this process, as the redox potential is low, microbial fermentation takes place and converts organic material to biogas (mainly  $\text{CH}_4$  and  $\text{CO}_2$ ) that can thus be used to produce energy in cogeneration systems. Another consequence of anaerobic digestion is the mineralisation of biodegradable organic compounds that leads to high concentration of  $\text{NH}_4^+$  and  $\text{PO}_4^{3-}$  in solution and the stabilisation of the sludge (van Lier et al., 2008). Several studies have been conducted in order to improve biogas production aiming to invert the energy balance and lead WWTPs to be in energy autarky (Schaubroeck et al., 2015; Aichinger et al., 2015). Considering that biogas production is fully dependent of volatile suspended solids (VSS) entering the digester that will be degraded, one possibility of increasing biogas production is forcing the input of more organic matter into the digester. This can be done by recovering the organic matter entering the WWTP by an enhanced primary clarification (with an addition of chemicals to achieve better flocculation), previously to its degradation in the water line by the microbial oxidation. Another advantage of recovering organic matter at this point is that less bacterial growth to treat carbon will take place in the aerated basins and thus less energy will be required to aerate the activated sludge (Flores-Alsina et al., 2014). More recent research have been also developed for high rate activated sludge process (HRAS) – Jimenez et al., 2015 - working at low SRT and also for partial nitrification and anammox process on the mainstream (Laureni et al., 2016). If the coupling of the two previously mentioned approaches succeeded, this innovative plant would allow minimising the aerobic degradation of organic matter and producing more fermentable sludge for AD (Xu et al., 2015).

One of the promising opportunities in the phosphorus recovery is the struvite precipitation from wastewaters. Struvite (ammonium magnesium phosphate hexahydrate -  $\text{MgNH}_4\text{PO}_4 \cdot 6 \text{H}_2\text{O}$ ) is a slow release fertilizer that might substitute conventional industrial fertilizers. The recovery of struvite from wastewater would allow not only a decrease in mineral fertilizers production and depletion of natural phosphorus resources but also a decrease in rejected phosphorus in water bodies together with the necessary production of crops to respond to population growth. However, in order to be feasible and present real advantages, struvite precipitation should be conducted in nutrient-rich wastewaters containing mainly phosphate and ammonium. Several studies have been conducted for the struvite precipitation using, among others, digester supernatant, landfill leachate and urine. However, as discussed by Maurer et al. (2006) without addition of phosphate, only 3% of nitrogen in urine might

be eliminated in struvite precipitation (with an efficient precipitation of 98% of phosphorus). Therefore, more research on new processes for nitrogen recovery is still necessary.

As discussed previously, several recovery opportunities are available and well applied in WWTPs. However, currently, one of the bottlenecks to fully benefit from resource recovery in wastewater is that, in municipal wastewater, nutrient-rich streams (e.g.: urine and faeces) should not be diluted (e.g.: by greywater) and thus, source-separation should be encouraged. At the same time, the choice of centralized or decentralized systems is not evident: Among others, the management approach depends on the area (urban or rural), the size and density of the population, the development level, the technical feasibility, the treatment quality required, the education and culture of the population, being necessary to evaluate case-by-case (Corcoran et al., 2010; Libralato et al., 2012).

Many aspects in centralized and decentralized systems have been discussed in literature. According to Libralato et al. (2012), when considering centralized systems, it should be highlighted the competitive costs of existing plants, the potential eutrophication phenomena and rainwater overload problems. In the other hand, decentralized systems may respond to diverse situations, diminishes or stop the reduction of water quality and allow treated wastewater recovery and reuse such as in the case of urine separation.

Also, some disadvantages have also been experienced in decentralized pilot systems such as precipitation with consequently clogging of pipes and odour as well as the difficulties when changes in centralized system are required and storage and transport have to be added to the new management structure (Maurer et al. 2006; Udert et al., 2003). Considering impacts, some studies showed greater impacts for acidification when analysing environmental footprint of source-separated systems. However, it has also been pointed out that, in contrast with conventional systems, that are already optimized, alternative systems has to be well assessed in order to achieve optimal results in terms of effluent quality and energy/chemicals consumption (Remy, 2010).

### *1.2.2. Urine source separation*

By the 1990s, various groups began working on the idea that separating urine at source could increase sustainability in wastewater treatment. Those approaches are based on urine composition which represents only 1% of the total volume in domestic influents and 14% of total organic carbon but is the main contributor of some nutrients with 85% of total N, 50% of the total P, and 55% of total K (Maurer et al., 2006; Larsen and Gujer, 1996).

Besides the recovery of substantial nutrients, urine separation also avoids advanced nitrogen removal (which is the most important energy consumer in a WWTP) and phosphorus elimination (which consumes important quantities of chemicals). Moreover, urine separation at source allows achieving robustness in the WWTP as ammonia peaks input are avoided or might be distributed along the time having immediate advantages in nitrification. Following consequences are thus the increased stability and reliability of the process and the reduction of the plant size (Rossi et al., 2009; Rauch et al., 2003).

Currently, a range of treatment possibilities (with/ without nutrients recovery) are available for the collected urine stream. As proposed by Maurer et al. (2006), the urine collected in source-separating toilets can be used for example for N-recovery (e.g. by ion-exchange, ammonia stripping or isobutylaldehyde-diurea precipitation), P-recovery (e.g. by struvite formation), nutrient removal (e.g. by anammox treatment) and micropollutants elimination. Also, as discussed by authors, nowadays it is not possible to find a process that answers to all nutrients recovery needs; thus a combination of processes is required. For instance, previous struvite precipitation triggered by magnesium that is able to precipitate most of the phosphorus might be followed by a biological treatment that is capable of eliminating organics and nitrogen. For complete urine valorisation the combination of a biological nitrification (in a biofilm system) and a vacuum evaporation has been proposed in the last years (Udert and Wächter, 2012). It allows converting half the ammonium into nitrate and then to produce a concentrated solution of ammonium-nitrate which can be used as a fertiliser. This is now technically feasible but the global environmental evaluation is still necessary to assess the global gain as, for instance, the energy demand is relatively high.

Finally, when urine is separated at source and aimed to be treated specifically, it is important to understand the complex composition of this fluid as well as the possible interactions between present substances. As showed by Udert et al. (2006), three main processes take place after urine collection: First, microbial hydrolysis of urea leads to ammonia and bicarbonate; Following, with the pH increase, one can notice the appearance of mineral precipitates such as struvite, hydroxyapatite ( $\text{Ca}_5(\text{PO}_4)_3\text{OH}$ ) and calcite ( $\text{CaCO}_3$ ); Additionally, with the pH increase, ammonia volatilisation takes place (Udert et al., 2006). Considering the previously described processes, a distinction between substance species has to be made between fresh and stored urine.

### **I.3. Quantifying benefits: Wastewater treatment modelling and simulation**

When one wants to understand and compare the functioning of both conventional and alternative wastewater management and treatment options, there is a need in obtaining realistic results. However, this is neither easy nor feasible when considering alternative scenarios that are currently only available at laboratory scale or unexplored experimentally. Modelling is thus an inexpensive and elegant way of comparing those alternative options.

Traditionally, simulation has been used to understand the interaction between the involved processes in a WWTP together with performance evaluation, control strategies, design and optimization. From this perspective, activated sludge systems, which are the most applied biological wastewater treatment method, are also consequently the most advanced considering modelling and simulation.

The simulation of activated sludge systems includes many processes and variables to guarantee the modelling of different steps of the treatment such as the carbon oxidation, nitrification and denitrification. These processes have to be mathematically tractable and representative of the reactions occurring in the reactors. Besides biological reactions, physical, chemical and mechanical reactions also take place. Moreover, when modelling a full plant (i.e. whole plant modelling), the set of state variables might not be the same for every part of the system (e.g. water line and sludge train). Two approaches are then available to handle this issue. The first one is the supermodel approach where all state variables are available for all units; the second one is the interface approach where relations between each compound should be established in the model when changing from one type of unit to another – e.g. between water and sludge line (Nopens et al., 2009).

Efforts have been made to achieve standardisation in WWTP modelling and simulation when one is willing to compare different strategies. Among them, the Benchmark Simulation Model no. 1 (BSM1) and no.2 (BSM2) should be mentioned, that are protocols for implementation and impact and performance evaluation of existing and new control strategies in WWTTPs. They comprise plant layout, simulation model, influent loads, test procedures and evaluation criteria (Alex et al., 2008; Jeppsson et al., 2007). The general overview of the original BSM2 flowsheet is given in figure I.1.

The main BSM2 flowsheet components are the primary clarification, the five activated sludge reactors for nitrogen removal that are modelled using ASM1, the secondary clarification, the gravity thickening, the anaerobic digestion (based on ADM1), the dewatering and the storage tank. It includes also, AD/AS model interfaces to deal with input and output of the anaerobic digester and dynamic influent characteristics from Gernaey et al. (2005). It has also to be noticed that respected reject limits for this benchmark are total nitrogen inferior to  $18 \text{ gN.m}^{-3}$ , COD inferior to  $100 \text{ gCOD.m}^{-3}$ ,

ammonium inferior to  $4 \text{ gN.m}^{-3}$ , TSS inferior to  $30 \text{ gTSS.m}^{-3}$  and  $\text{BOD}_5$  inferior to  $10 \text{ gBOD.m}^{-3}$ . Moreover, phosphorus elimination (and consequently its quantification) is not available in the original BSM2 configuration (Alex et al., 2008).

In the general protocol study of BSM2 proposed by Jepsso et al. (2007), some main points are highlighted such as the importance of integrating the full plant (water and sludge line) in order to lead the WWTP to be thought as one completely integrated system that accounts for all possible benefits and disadvantages. In this case, more reliable results would be achieved. Additionally, the control of all units and sub-process should be integrated. Accordingly, the extended evaluation period considers more realistic aspects such as seasonal variations (including temperature during the year) and the slow dynamics of anaerobic digestion processes (Jeppsson et al., 2006).

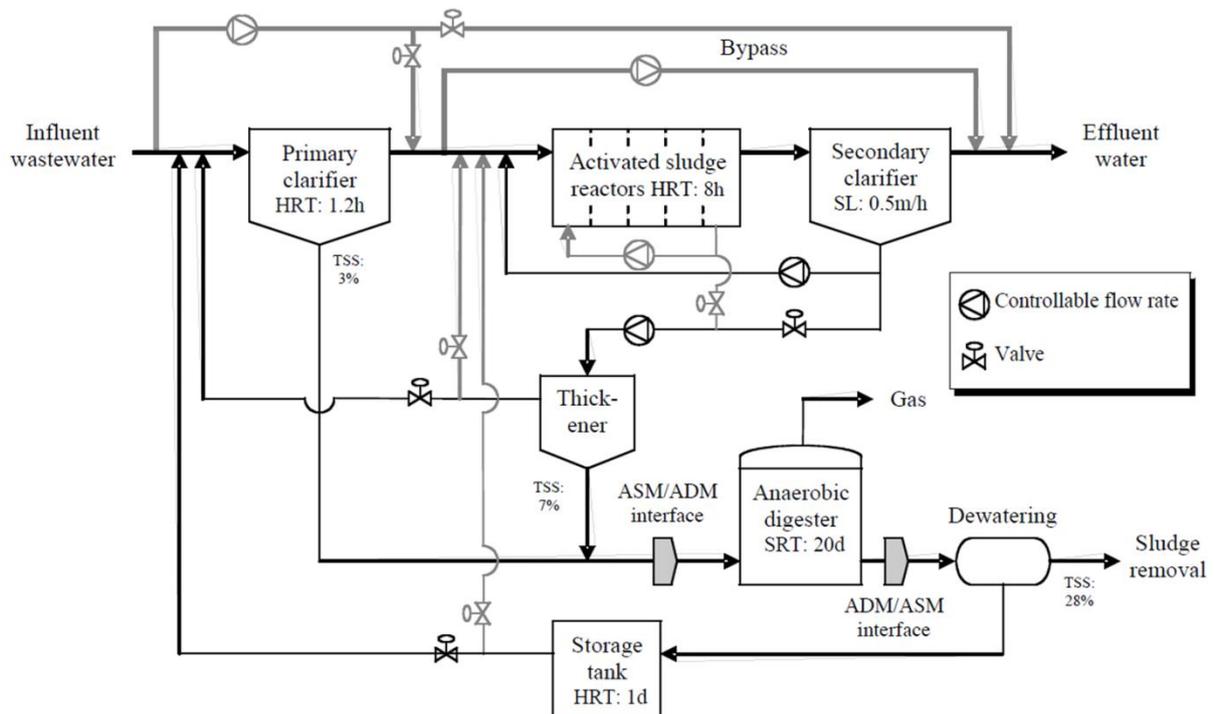


Figure I.1. General overview of original BSM2

(Alex et al., 2008)

### I.3.1. Obtaining data: Influent generation

As discussed previously, wastewater composition is highly variable according to human's life style. Therefore, when trying to understand the complex interaction between all the parameters involved in

the wastewater management and treatment systems, it is essential to consider this dynamic condition, as the system is not well represented by a steady state one.

Although, powerful and rigorous models are available for the simulation of systems, if a dynamic and realistic representation of influents is not provided, results might be misleading. For instance, when considering fluctuations in the WWTP influent, robustness in the plant might only be ensured if the system is capable of treating peaks of flows and nutrients (Alex et al., 2008).

The influent of a municipal WWTP is a mixture of several contributing streams such as domestic wastewater (including toilet, kitchen and bath/laundry wastewater), industrial wastewater, stormwater, sewer infiltration, etc (Henze and Comeau, 2003).

Martin and Vanrolleghem (2014) published a critical review on generating influent data for WWTPs. According to the authors, three different types of influent generators are described in the literature: i.) When one needs to complete data about quantity and quality of the wastewater; ii.) When composite variables need to be translated into state variables (ASM family ones, for instance); iii.) When one needs to know the uncertainty present in the influent data. Also, according to authors, one of the promising approaches in this field is the phenomenological generation of influents as it allows the user to adapt the model to obtain data for instance according to geographical location and catchment size.

#### **I.4. Evaluating benefits: Life Cycle Assessment (LCA)**

Even when having data to evaluate conventional and new technologies, one could claim that depending on the methodology used to assess the process, results would be different. There is thus a need for a standardized methodology to evaluate the whole process and its requirements. Currently, different assessment tools are available to evaluate the sustainability of systems such exergy analysis, economic analysis and Life Cycle Assessment (LCA) (Balkema et al., 2002).

Aiming to analyse environmental footprint of WWTPs, several studies have been suggesting the use of LCA. It is a methodological framework for assessing the environmental impacts attributable to the life cycle of a process or a product. The idea of using LCA in WWTPs is to account for all background process (e.g. energy consumption, chemicals production and transport utilization) besides the foreground process which has his own environmental emissions.

According to ISO 14044 (2006), LCA is defined as the “compilation and evaluation of the inputs, outputs and potential environmental impacts of a product system throughout its life cycle”. Considering this, when analysing conventional and alternative WWTPs for long-term environmental

sustainability, effluent quality discharge impact has to be considered (end-of-pipe approach) but also all the processes associated to the main treatment such as the sludge treatment and disposal, energy consumption and production of ancillary materials (background processes).

Also, the four main steps that are recommended by the ISO 14044 (2006) are to be followed: i.) the goal and scope definition; ii.) the inventory definition; iii) the impact assessment phase and iv.) the interpretation.

The first step, the goal and scope definition, allows the description of the system in terms of the system boundaries, function and functional unit (FU), and allocation methods. It is important as the correct definition of the FU allows the latter comparison between alternatives. The second step, the Life Cycle Inventory (LCI) is the compilation of all estimated consumption of resources from the environment and emitted substances to the environment during the process/product life cycle. By the end of this step, an inventory of the system is obtained based on a well-defined functional unit. Following, the third step, Life Cycle Impact Assessment (LCIA) provides the correlation between emitted substances and indicators of impacts on the environment. Finally, the last step, the life cycle interpretation occurs naturally as when conducting the LCA one wants to take decisions after comparing options (Rebitze et al., 2004) and identifying the hot spots of the system.

In the field of water and wastewater treatment, LCA has already been used in several studies to evaluate the environmental performances of proposed technologies. Different LCA applications have been published so far (Corominas et al., 2013a) for different WWTPs configurations as well as for sewage sludge management technologies (Yoshida et al., 2013) and for the full urban water system (Loubet et al., 2014). However, as results are usually obtained by site collected data, it can neither be used to automatically analyse general trends nor to process optimization. Therefore, the consideration of an LCA together with WWTP modelling and simulation tools is be a powerful approach to allow the modification of operational and design parameter when aiming to conceive more sustainable systems.

However, it has to be highlight that, in order to be realistic and to provide a fair comparison against studied scenarios, LCA have to be conducted considering the appropriate boundaries and the proper allocation methodology. For instance, when analysing WRRFs, the conventional WWTP Life Cycle Assessment has to be adapted to account for all avoided impacts generated by the production of by-products. Similarly, the new functions of the system have to be added as it will not deliver the same functional unit anymore.

Another important feature of the LCA that allows it to be applied to the quantification of impacts and the evaluation of scenarios in WWTPs considers the main emissions of the plant. Even if nowadays, life cycle impact assessment methodologies are not capable of integrating all substances leaving a

WWTP, such as personal care products and medicaments residues, the main burdens of the implementation of a wastewater treatment (for instance, the reject of non-treated pollutants, the greenhouse gases emitted and the high consumption of energy and chemicals) can be correctly quantified and evaluated by the currently available impact categories (for instance, marine and freshwater eutrophication, human toxicity, climate change and resources depletion).

## **I.5. Improving systems: Multi-objective optimization**

When a novel technology is able to be evaluated considering sustainability but also technical and economic aspects, an optimization can be conducted. Additionally, it may consider not only one optimal functioning point; it is possible to compromise between all trade-offs without any preliminary judgement.

As described by Deb (2011), multi-objective optimization (MOO) consists of optimizing more than one objective simultaneously. As opposed to the single objective optimization, the multi-objective optimization minimizes all usually conflicting objective functions simultaneously without using expressions of weight between objectives. Hence, a set of solutions, called Pareto-optimal solutions, is usually obtained by the end of a multi-objective optimization. The concept of domination is generally used in the context of multi-objective optimization to discriminate between solutions and to locate the globally non-dominated (minimum) solutions, while maintaining the diversity in a given Pareto-front (Deb, 2001). A further processing step, the decision making process, will be therefore required in order to comprise between the trade-offs and to find one optimal functioning point, when needed.

Additionally, as conflicting objectives are most often involved, none of the optimal solutions found can be improved without worsening at least one of the other objectives (Hakanen et al., 2011) and thus, solutions cannot be easily sorted only on their objective value.

There exist different ways to solve a multi-objective optimization problem among which evolutionary algorithms (EA), widely known due to their robustness. According to EAs, the optimization is carried out by using a population of solutions, usually created randomly and therefore robustness is ensured independently from the quality of initialization. Thereafter, the algorithm provides a generation-based (iterative) operation updating the current population to create new populations based on genetic operations such as genetic selection, crossover, mutation and migration. This generation-based operation is pursued until one or more pre-specified termination criteria are met (Deb, 2011).

From the application point of view, the optimization of WWTP design and operation has been applied since 1990s. However, commonly, the optimization strategies, described in the literature, are most often aggregation-based, which is to say that the optimization is conducted by aggregating several objectives into a unique objective function through weight factors representing the importance of each objective (Hakanen et al., 2011; 2013).

However, as described by Hreiz et al. (2015) in a review of ASPs optimization, several objectives have not the same units (and sometimes also contradictory) and cannot be instinctively combined in order to form a single objective function.

From a practical point of view, even if highly non-linear processes are present in a WWTP due, for instance, to the rigorous consideration of biochemical reactions, it is important to avoid the aggregation of objectives and preserve the intrinsically multi-objective structure of optimization problem. For instance, the quality of treated wastewater and the operational costs are two conflicting objectives as, reaching low organic matter, ammonium or phosphate concentrations in effluent leads to high consumption of energy and chemicals in the plant. Also, operating a plant with short SRT risks the stability of nitrification and may produce an excess of sludge; however, suspended solids quality and BOD is ensured (Hakanen et al., 2013) and thus only the operator expertise might compromise between different conflicting outcomes that are sometimes non quantifiable or highly dependent.

Multi-objective optimization is recognized to be more suitable to deal with WWTPs due to the conflicting nature of objectives taken into account. Additionally, the use of derivative-free algorithms such as EAs is favoured to avoid uncertainties due to the numerical approximation of gradients in highly-linear systems, and to ensure the robustness of the algorithm. Nevertheless, regarding the EAs, the main drawback is the considerable numerical budget required. However, the full WWTP case study is an example of an expensive optimization problem, where the resolution without an efficient optimization tool would be practically impossible.

Aiming to fix a computational budget that allows obtaining the optimal Pareto-front, Ahmadi et al. (2016) proposed a new Archive-based Multi-Objective Evolutionary Algorithm with Memory-based Adaptive Partitioning of search space (AMOEAMAP) to deal with expensive simulation-based problems and reduce the computational budget of the optimization to about 300 function evaluations. The adaptation relies mainly on the adaptive reticulation of the search space, to accelerate the search with no loss of accuracy and on a bi-population approach (Ahmadi et al., 2016).

## **I.6. Research objectives and tasks**

Envisaging novel and more sustainable wastewater management and treatment systems requires a multi-criteria decision support that is capable of considering all technical, economic and environmental aspects. Therefore, in order to perform alternative scenarios evaluation, decision making based on scenarios comparison, ecodesign or process optimization, it is necessary to have a tool capable of predicting in a reliable and interconnected way the benefits and drawbacks when applying a specific technology.

This thesis is in pursuit of a concluded thesis at “Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés” (LISBP) by Méry (2012). In this previous work, an integrated tool for process modelling and life cycle assessment applied to the environmental analysis of drinking water treatment plants was successfully developed. Moreover, the main focus of the previous cited work was to develop modelling and simulation of unit processes in steady state conditions (considered as satisfactory for this kind of processes) and on the application to an existing plant.

Following the idea of this former approach coupling process modelling and life cycle assessment studied by Méry (2012), it seemed evident that the same approach could be applied to other process fields such as a wastewater treatment plant. However, as the physico-chemical and biological processes involved in wastewater treatment are complex and highly dependent on wastewater inputs (composition, flow variation), it is extremely important to adopt a rigorous and dynamic modelling. Another interest sought in the present work is the building of perspective scenarios meaning that the tool should have a predictive aspect and eco-design capability. Multi-objective optimization approach should then be integrated to tackle the involved conflicting objectives.

**The major objective of this study is to obtain a platform coupling rigorous and wide-plant Dynamic Modelling (DM), extended boundaries Life Cycle Assessment (LCA) and an Efficient Multi-Objective Optimization (EMOO) tool.**

The developed platform, DM-LCA-EMOO, has to be flexible in order to allow different scenarios to be tested, as well as multi-criteria as different decision parameters might be present.

In order to achieve the objectives, the involved tools in the platform have to be interconnected with their process parameters and results. Initially, it is necessary to automatically control, run simulations and recover results from existing commercial WWTP simulators. When results are recovered, they have to be converted into the correct substances and modules for the LCA in order to allow the

consideration of foreground and background processes together with mass and energy balances. Examples of important recovered values are the violation of reject limits, the amount of energy produced on the amount of energy consumed (EROI), the average output concentrations, etc. By the end of the evaluation of a range of scenarios, general results about environmental impacts are to be obtained as well as a detailed contribution analysis in order to identify the most important hotspots of each scenario to be latter optimized. Finally, to allow the multi-objective optimization of scenarios, the platform has to be connected to an efficient multi-objective optimization algorithm that allows the optimization of WWTP as an expensive black-box problem. Figure I.2 presents in a simple way the main coupled tools in the combined platform together with its main expected outputs.

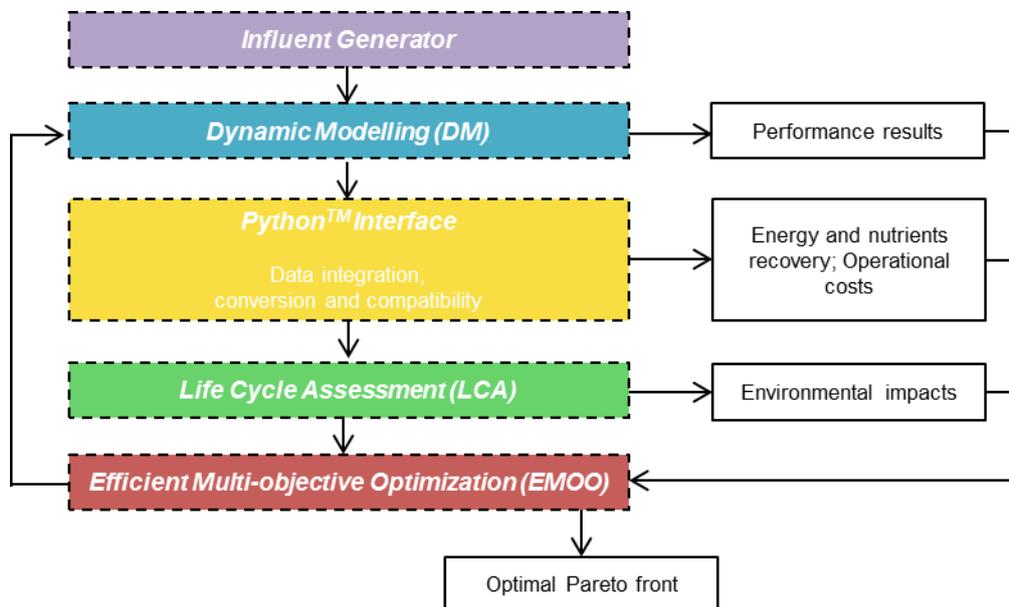


Figure I.2. Simplified scheme of the combined platform DM-LCA-EMOO

The developed platform should be able to evaluate and compare conventional and several alternative wastewater management and treatment options. Among the proposed alternatives, it is aimed to study the urine source separation with specific treatment (struvite production and nitritation/ anaerobic ammonium oxidation) and/or valorisation in agriculture and the enhanced primary clarification to increase biogas production in the plant and to achieve energy autarky.

The interest of such a combined and rigorous platform can be understood from two points of view. First, it is a tool for benchmark validation, which is to evaluate and compare conventional and alternative scenarios (DM-LCA approach – chapter 2). Secondly, when coupled to the expensive optimization tool, the platform is capable of optimizing both operational and design variables together (DM-LCA-EMOO approach - chapter 4 and 5), in the next phase, in order to validate a novel

configuration with an accurate readjustment of operation conditions due to the eventual modifications in the plant structure and operating conditions. Additionally, in order to fulfil the modelling and simulation objectives, a dynamic phenomenological influent generator must be adapted to take into account realistic inputs in the wastewater treatment plant and in the urine system treatment (chapter 3).

### *1.6.1. Thesis outline*

This thesis is structured in 6 chapters.

The previously presented chapter I introduces the thesis background and goals by presenting the main challenges to be addressed considering the existing approaches in the literature. In this context, the research objectives, the corresponding tasks and the relevant applications are defined.

Following, chapter II describes the initial development of the platform that couple dynamic modelling and life cycle assessment with extended boundaries. Moreover, the developed platform is used to evaluate conventional and alternative scenarios. Additionally, focusing on screening alternative scenarios for the future, attention was paid to the modelling and the analysis of hotspots of each scenario aiming to further optimize them.

Latter, chapter III presents the adaptation of a phenomenological and dynamic influent generator which is required to obtain more realistic influent data (and consequently simulation results) for scenarios having urine source separation together with the resulting wastewater stream.

Chapter IV is a preliminary study on the multi-objective optimization of WWTP that aims to understand the feasibility of such expensive optimization, from both computational and reliability points of view. Special attention is paid in this chapter to the problem formulation considering decisional variables, objective functions and constraints. The choice of an efficient optimization algorithm is also discussed and justified, while dealing with complex simulation-based optimization problems.

Succeeding, chapter V presents the application of the previous developed DM-LCA-EMOO approach to a reference and alternative WWTP scenarios. Also, different problem formulations are studied together with its impacts on Pareto front results.

Lastly, chapter VI presents the conclusion and the main findings of this work as well as perspectives following this thesis.

Additionally, several modifications and verifications over the original wide-plant modelling, which are not described along the following chapters, were conducted during this work. All the information

considering the adaptation and the corrections in the modelling are showed in the Supplementary Information document.

Note to the reader: The goal of this chapter is not to conduct a state-of-the-art on the thesis subject. As this thesis corresponds well to the contents proposed by either accepted or “in preparation” peer-reviewed articles, it was decided to structure this thesis report by including the original papers for each related chapter. Accordingly, the reader will find detailed literature information concerning each subject on the following chapters.



# **Chapter II. Coupling Dynamic Modelling and LCA**



*“Meeting the wastewater challenge is thus not a luxury but a prudent, practical and transformative act, able to boost public health, secure the sustainability of natural resources and trigger employment in better, more intelligent water management.” (Steiner and Tibajuka, in Corcoran et al., 2010)*

This chapter is published in *Water Research*, 84 (99-111), doi:10.1016/j.watres.2015.06.048. It is the result of the coupling of rigorous Dynamic Modelling (DM) and Life Cycle Assessment (LCA) with the corresponding application to several scenarios. The studied scenarios include i.) a reference scenario (REF: conventional influent input and plant layout); ii) an enhanced primary clarification scenario (EPC: addition of coagulant before primary clarification with 80% retention of total suspended solids); iii.) an urine source-separation scenario (USS: conventional plant layout receiving a modified influent without 50% of urine; yellow water treatment by precipitation with magnesium oxide to recover struvite and the residual nitrogen flow being reinjected in headworks); iv.) a scenario combining alternatives ii and iii (USS+EPC); v.) a scenario adapted from scenario iv where nitrogen rich stream from struvite precipitation is spread on farmland and valorised as fertilizer (USS+EPC+AGRI); vi.) an adapted scenario from iv where nitrogen rich stream is treated by nitrification/ deammonification together with the dewatering effluent from anaerobic digestion (USS+EPC+ANA).

The choice of scenarios reflects what was previously discussed in the introduction and is unavoidable nowadays: Wastewater treatment plants should move towards water resource recovery facilities in order to achieve more sustainable wastewater management and treatment systems. However, this eco-friendly perspective can only be achieved and well evaluated when having an integrated view on the whole process and considering the full pathway of wastewater, from the source generation to the treated water re-entrance into the environment and recovery of valuable products from wastewater. Accordingly, energy management, both consumption and production, has to move towards energy positive balances.

Several questions are to be answered when modelling those systems and concerning what has to be considered in order to be the most realistic as possible. In order to respond to this comparative approach that allows lightening on sustainable systems, the platform was developed considering the extended boundaries of the life cycle assessment, meaning that all direct and background emissions where considered as well as avoided emissions when nutrients and energy valorisations take place.

When considering the available studies on literature, it should be noted that they include mostly collected data and, therefore a specific site inventory is established. There are thus, two main consequences: Firstly, the study would logically be case specific and would not allow the consideration of more general scenarios; Secondly, as results are obtained from site inventories, they

would not allow analysing trends when changing parameters of the system and consequently optimization might not be feasible.

A review of LCA studies on wastewater is proposed by Corominas et al. (2013a). According to the authors, the integration of LCA in WWTPs has started since the 90s and up to now more than forty studies have been published in peer-reviewed journals. Moreover, the authors indicated that several works have found important benefits when considering source separation scenarios (including urine source separation) from both nutrients recovery and avoidance of pollutants points of view. In their review, different challenges were addressed such as the inclusion of new pollutants, different time horizons in the impact analysis and finally, the standardization of guidelines of LCA applied to wastewater. For instance, nowadays even though LCA is standardized by ISO 14000, different functional units, system boundaries, impact assessment methodologies and interpretation are still applied in the field of wastewater.

More globally, Loubet et al. (2014) proposed a review on life cycle assessment of urban water systems in order to complete the available review considering only parts of the system. Authors showed that when considering the contribution of drinking water production, drinking water distribution, wastewater collection and wastewater treatment, regardless the category, impacts came mainly from wastewater treatment representing for instance, on average, 44% of climate change impact, 78% of eutrophication impact and 39% of electricity consumption.

Considering the sewage sludge management, Yoshida et al. (2013) proposed a review of several studies and arrived to the conclusion that the most important challenges to be addressed are the quantification of fugitive gas emissions as well as the fate of emerging pollutants and the modelling of disposal practices in order to decrease uncertainty in LCA.

Foley et al. (2010) proposed an approach that is similar to the one developed in this study. Authors conducted a LCA from steady state modelling results of ten WWTP scenarios. The results showed that, in general, when a better water output quality is required (less nitrogen and phosphorus are to be rejected), infrastructure, operational energy, direct GHG emissions and chemical consumption impacts increase, which demonstrate the importance of background processes in a WWTP assessment. Authors also highlighted the importance of nutrient consideration, especially phosphorus recovery, to be further valorised as fertilizers.

Similarly, Corominas et al. (2013b) emphasized the inclusion of LCA in the decision-making of nutrient removal systems. Authors analysed nitrogen and phosphorus removal in several systems and showed that, for N&P and P-deficient scenarios, the strategies that are able to increase nutrient removal and/or energy savings present an environmental benefit. However, when considering N-

deficient scenarios, as more chemicals are required in the treatment, environmental benefits are not systematically provided.

Another remarkable study on WWTP modelling and LCA was proposed by Schaubroeck et al. (2015) considering the energy-positive WWTP in Strass, Austria. The study considered wastewater treatment as well as the supply chain and the utilization of the produced electricity from sludge digestion and the digestate (as fertilizer). Comparisons between the conventional scenario (using nitrification/denitrification) and a one-stage partial nitrification/anammox coupled to a codigestion showed a considerable benefit in natural resources depletion (by lowering the energy consumption and increasing the electricity production). Moreover, according to authors,  $N_2O$  emission still represent an important contribution to impacts and have thus to be optimized afterwards.

The present study aims to provide a coupled LCA-dynamic modelling platform capable of being properly adapted to several treatment benchmarks as well as providing comprehensive results on the performance and sustainability of each wastewater management and treatment scenario. Moreover, the developed platform is capable of identifying the main hotspots for a given configuration, which requires a rigorous modelling of the dynamic process. In this sense, important efforts have been made to operate with a full plant modelling despite the considerable requirements in computational time.

Modelling some emissions such as the dinitrogen monoxide, have not yet found a consensus between scientific and industrial communities. Therefore, regarding the  $N_2O$  emissions, a general approach was used by considering only an emission factor according to the ammonia uptake rate. The later can be subsequently integrated into the platform when a validated and widely-approved consensus is available in the literature, in order to achieve more realistic results (for instance to consider low dissolved oxygen concentration and high nitrite concentration in nitrification).



## **Entitled of the paper: Evaluation of new alternatives in wastewater treatment plants based on Dynamic Modelling and Life Cycle Assessment (DM-LCA)**

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### **Abstract**

With a view to quantifying the energy and environmental advantages of Urine Source-Separation (USS) combined with different treatment processes, five wastewater treatment plant (WWTP) scenarios were compared to a reference scenario using Dynamic Modelling (DM) and Life Cycle Assessment (LCA), and an integrated DM-LCA framework was thus developed. Dynamic simulations were carried out in BioWin® in order to obtain a realistic evaluation of the dynamic behaviour and performance of plants under perturbation. LCA calculations were performed within Umberto® using the Ecoinvent database. A Python™ interface was used to integrate and convert simulation data and to introduce them into Umberto® to achieve a complete LCA evaluation comprising foreground and background processes. Comparisons between steady-state and dynamic simulations revealed the importance of considering dynamic aspects such as nutrient and flow peaks. The results of the evaluation highlighted the potential of the USS scenario for nutrient recovery whereas the Enhanced Primary Clarification (EPC) scenario gave increased biogas production and also notably decreased aeration consumption, leading to a positive energy balance. Both USS and EPC scenarios also showed increased stability of plant operation, with smaller daily averages of total nitrogen and phosphorus. In this context, USS and EPC results demonstrated that the coupled USS+EPC scenario and its combinations with agricultural spreading of N-rich effluent and nitrification/anaerobic deammonification could present an energy-positive balance with respectively 27% and 33% lower energy requirements and an increase in biogas production of 23%, compared to the reference scenario. The coupled scenarios also presented lesser environmental impacts (reduction of 31% and 39% in total endpoint impacts) along with effluent quality well within the specified limits. The marked environmental performance (reduction of global warming) when nitrogen is used in agriculture shows

the importance of future research on sustainable solutions for nitrogen recovery. The contribution analysis of midpoint impacts also showed hotspots that it will be important to optimize further, such as plant infrastructure and direct N<sub>2</sub>O emissions.

*Keywords: WWTP; dynamic modelling; integrated LCA; urine separation; enhanced primary clarification; struvite.*

## **II.1. Introduction**

Nowadays, Wastewater Treatment Plants (WWTPs) are facing ever stricter regulations with respect to the environment and human health, and are also beginning to be considered as sources of material and/or energy, obtained by recovering nutrients such as nitrogen (N) and phosphorus (P), and through biogas production.

The collection of separate wastewater flows (e.g. urine, faeces, kitchen and bathroom wastewater) at their source could allow the recovery of nutrients thanks to the distinct composition of these flows. In this sense, there is a particular interest in urine, which represents less than 1% of the total volume and only 14% of total organic carbon (TOC) but 88% of total Kjeldahl nitrogen (TKN) and 57% of total phosphorus (Larsen and Gujer, 1996).

Urine can be treated with magnesium in order to form struvite ( $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$ ), a slow-release fertilizer (Maurer et al., 2006). In addition to the possibilities of recovery, urine separation can decrease the energy consumption in WWTPs through a reduction in the needs for N-removal besides the decrease in consumption of chemicals used for P-elimination. Another important feature of urine separation is the avoidance of ammonia peaks, which increases operating stability and allows plant size to be reduced (Rauch et al., 2003).

Additionally, if less organic matter is needed for denitrification, more organic matter can be dedicated to anaerobic digestion, which helps to turn the energy balance of WWTPs into a net positive energy (production of surplus of energy). Accordingly, Flores-Alsina et al. (2014) proposed the enhancement of total suspended solids (TSS) removal in the primary clarifier, which led to a higher chemical oxygen demand (COD) for the digestion and consequently more biogas production.

The negative feature of WWTPs is the generation of various (direct) forms of pollution through gas emissions, and effluent and sludge discharge into the environment. Moreover, the utilization of energy and chemicals by the plant is responsible for indirect environmental burdens due to the production of

these utilities. The environmental performance of different WWTP configurations can be evaluated by the Life Cycle Assessment (LCA) method (ISO 14040/44, 2006). While the Life Cycle Inventory (LCI) of background processes can be obtained from databases, the foreground process inventory is usually obtained by data collection at the plant. An alternative to data collection is modelling and simulation – a very useful tool when predictive results or ecodesign proposals are sought (Méry et al., 2013).

Numerous LCA applications have been published for different WWTP configurations and a state of the art has been drawn up by Corominas et al., (2013a). Yoshida et al. (2013) have published an LCA review of sewage sludge management and the environmental performance of WWTPs with nutrient recovery. However, the studies reviewed, mostly based on site data collection for LCI, cannot be used for outlining general trends or for process optimization, because of the great number of parameters, possible scenarios and treatment objectives.

Foley et al. (2010) used steady state simulation results obtained with Biowin<sup>®</sup> for a systematic evaluation of the life cycle inventories of ten scenarios in 6 WWTP configurations. The results showed that the quantity of infrastructure materials needed and the consumption of chemicals increased when lower N and P concentrations were imposed in the effluent, as did energy consumption and GHG emissions in N-limiting effluent scenarios. Flores-Alsina et al. (2014) used dynamic simulation applied to an extended version of BSM2 (Benchmark Simulation Model N<sup>o</sup>2) to calculate the greenhouse gases (GHGs) emitted on site and the amounts of energy and chemicals produced, with the aim of evaluating control/operating strategies. These authors also showed the importance of considering both water and sludge lines when analysing GHG emissions and pointed out the considerable environmental impact of N<sub>2</sub>O emission.

Rémy (2010) analysed eight impact categories when comparing alternative systems using pilot projects and literature data. The study showed that separation systems presented important benefits, although eutrophication and acidification were more increased by agricultural disposal of liquid fertilizers. The study also highlighted the importance of optimizing alternative treatment systems. Tillman et al. (1998) studied the impact of possible source separation systems in two regions in Sweden compared to existing conventional treatment systems. Their results showed that the urine separation scenario presented the lowest environmental impact (e.g. nitrogen emissions to surface water were reduced). Björklund et al. (2000) studied several treatment options and concluded that nutrient recycling could reduce the net impact, even though nutrient spreading could raise the acidification impact. They also highlighted the importance of ancillary systems for the environmental analysis.

To the best of our knowledge, none of these studies proposed an effective integration of process dynamic modelling and complete LCA. Such integration requires adapted modelling and evaluation tools, able to capture the influence of process parameters and dynamics in the impact calculation results. In this sense, some elaboration complexities and limitations involved are related to the fact that, as WWTPs are constantly subjected to flow and load perturbations, dynamic aspects should be taken into account in the aim of achieving relative robustness in operational conditions in any situation, ensuring stability and the correct operation of the plant. Also, as LCA is traditionally a non-dynamic methodology, an interface between dynamic modelling results and inventory flows in LCA is required, together with the conversion of specific inventory items (in order to obtain compatible units for inventory flows).

Lastly, considering the whole WWTP system means taking account not only of the benefits and drawbacks of coupled water and sludge lines but also of all background processes such as disposal of by-products, consumption of energy and chemicals, and transport.

Until now, the benefit of alternative wastewater management with urine separation has been estimated by a few studies with emphasis on the agricultural utilization of urine. However, a urine separation scenario has never been evaluated through whole plant modelling coupled with urine treatment (such as struvite precipitation and nitrification/deammonification with *Anammoxidans* bacteria) by a DM-LCA analysis.

So, the goal of the present study is to obtain reliable, predictive LCA results (mutually interconnected with the process parameters and dynamics) for reference and alternative scenarios in WWTPs. The alternative scenarios consider urine source-separation followed by urine treatment, and enhanced precipitation in the primary clarifier. This study also aims to identify possible benefits and drawbacks of alternative systems so that they can be further optimized as conventional systems have already been. To achieve this, a DM-LCA framework was developed for the predictive evaluation of global performances, coupling dynamic simulation results and environmental evaluation.

## **II.2. Materials and methods**

### *II.2.1. The integrated DM-LCA methodology*

As mentioned above, the integration of the dynamic modelling approach and LCA tools is a prerequisite when trying to analyse the total environmental footprint of a WWTP system.

The DM-LCA approach developed here used three different platforms, interconnected as shown in Figure II.1. WWTP scenarios were simulated with BioWin<sup>®</sup> v4.0.0.976, a Windows-based wastewater treatment process simulator that includes biological, chemical, and physical processes (Envirosim, 2014). The interface between WWTP dynamic modelling and LCA calculations were performed through Python<sup>™</sup> scripts.

To achieve the study objectives, model parameters were fixed initially and dynamic influent data was provided to the simulator (Fig. 1 data flow 1). Dynamic simulations were also designed to reach effluent quality limits (e.g. 10 g.m<sup>-3</sup> of total N, 1 g.m<sup>-3</sup> of total P, 35 g.m<sup>-3</sup> of total suspended solids, 100 g.m<sup>-3</sup> of total COD and 4 g.m<sup>-3</sup> of ammonium ion). As a result of the dynamic simulation, process inventories (Fig. 1 data flow 2) were generated with their own inputs and outputs. After the dynamic simulations, Python<sup>™</sup> scripts (Fig. 1 data flow 3) integrated the results over the simulation time. All parameter values and examples of calculations can be found in the Supplementary Information document (SI, Section 1).

The results were then converted to an Umberto<sup>®</sup>-compatible input file for foreground and background processes. Python<sup>™</sup> scripts also performed complementary calculations, based on the literature (e.g. calculation of cogeneration and energy requirements) and adjusted assignments between the output flows resulting from the BioWin<sup>®</sup> simulation and Umberto<sup>®</sup> input flows (Fig. 1 data flows 4, 5, 6 and 7).

LCA calculations were then performed with Umberto<sup>®</sup> (Fig. 1 data flow 8) using the Ecoinvent database (Fig. 1 data flows 9 and 12). This last step completed the LCI by adding the contribution of background processes to WWTP ones (inventory details in section 2.4.2), and calculated the LCI (Fig. 1 data flow 10) then the environmental impacts (Fig. 1 data flow 11). Three main types of results were generated: effluent concentrations and quality violations (Fig. 1 data flow A), energy parameters and nutrient recovery (Fig. 1 data flow B), and environmental impact results (Fig. 1 data flow C).

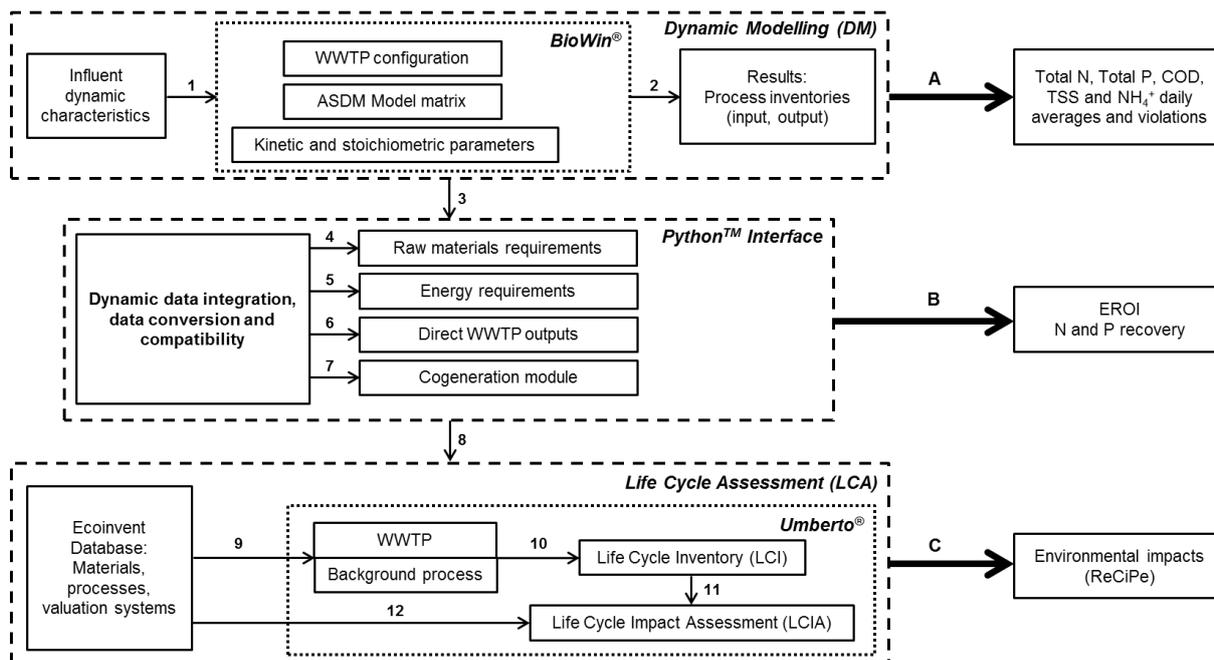


Figure II.1. DM-LCA framework developed with connections between Dynamic Modelling, LCA and Python™ interface

### II.2.2. Plant layout and scenarios

The reference WWTP scenario considered in this study was the biological nutrient treatment plant performing both nitrogen and phosphorus removal. The plant layout (Figure II.2) under study was similar to that proposed in BSM2 (Jeppsson et al., 2006). The kinetic model was a general full plant model (*BioWin*® ASDM - integrated activated sludge/anaerobic digestion model) coupling activated sludge processes and anaerobic digestion. A cogeneration unit based on the biogas produced was also considered to approach an energy self-sufficient system.

The system was simulated with an influent characteristic file generated by Gernaey et al. (2011) (dry and rainy periods were included). More details about considered influent can be found in SI (Section 7). Effluent and ambient temperature were modelled as proposed by the same authors using sinusoidal waves with characteristic bias, amplitude, frequency and phase for daily and seasonal aspects (Detailed correlations can be found in Section 4).

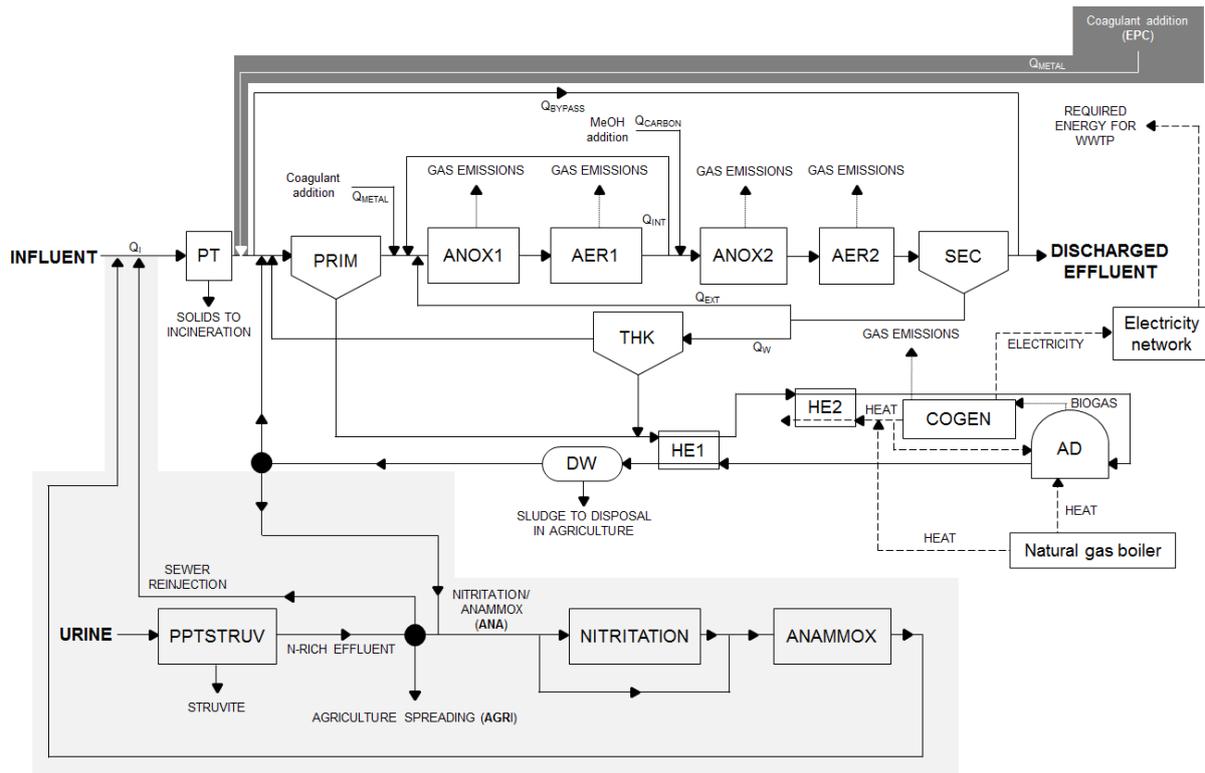


Figure II.2. Plant configuration used in this study.

Modifications due to urine source separation and enhanced primary clarification are shown in grey boxes. Solid lines: liquid and solid flows, dashed lines: energy flows, dotted lines: gas flows)

The WWTP is feed with a flow  $Q_I$ . The treatment comprised a pre-treatment (PT) unit for grit removal followed by a primary treatment unit (PRIM: volume =  $900 \text{ m}^3$ , height = 3 m,  $\eta_{\text{removal}} = 50\text{-}80\%$ ), 2 anoxic tanks (ANOX1: 2 successive tanks of  $1500 \text{ m}^3$  volume each) and 3 aerobic tanks (AER1: 3 successive tanks of  $3000 \text{ m}^3$  each, dissolved oxygen controlled at  $1.5\text{-}2.0\text{-}0.5 \text{ gO}_2 \cdot \text{m}^{-3}$ ). A post denitrification zone (ANOX2: volume =  $3000 \text{ m}^3$ , AER2: volume =  $500 \text{ m}^3$ , dissolved oxygen controlled at  $1 \text{ gO}_2 \cdot \text{m}^{-3}$  to release nitrogen bubbles) was also added to achieve acceptable effluent limits. Nitrate was recycled from the aerobic to the anoxic zone ( $Q_{\text{INT}}$ : 100-300% of  $Q_I$  to achieve denitrification in the first zone without external COD). The sludge was separated in a secondary clarifier (SEC: volume =  $6000 \text{ m}^3$  height = 4 m), which was also partly a wastage flow ( $Q_W$ : 300-400  $\text{m}^3 \cdot \text{d}^{-1}$ ) redirected to a thickener (THK:  $\eta_{\text{removal}} = 98\%$ ), and partly recycled in the anoxic zone ( $Q_{\text{EXT}}$ : 100% of  $Q_I$ ). The primary clarifier and thickener underflows were redirected to an anaerobic digester (AD: cylindrical tank with conical floor, total volume =  $3500 \text{ m}^3$ , liquid volume =  $3400 \text{ m}^3$ ; temperature =  $35^\circ\text{C}$ ) after being heated in heat exchangers (HE1 and HE2). Finally, biogas from anaerobic digestion was used in a cogeneration unit for electricity and heat production (COGEN:  $\eta_{\text{electrical}} = 35\%$ ;  $\eta_{\text{heating}} = 48.5\%$ ). The inlet flows of external carbon ( $Q_{\text{CARBOON}}$ : methanol) and coagulant

( $Q_{\text{METAL}}$ : iron chloride) were also dynamic and followed a constant daily profile. For the alternative scenarios, the flowsheet also comprised a struvite precipitation tank (PPTSTRUUV: volume = 5 m<sup>3</sup>), a nitrification tank (NITRITATION: volume = 500 m<sup>3</sup>; dissolved oxygen controlled at 1.0 gO<sub>2</sub>.m<sup>-3</sup>) and an anaerobic deammonification tank (ANAMMOX: volume = 1500 m<sup>3</sup>) with external alkalinity input. Finally, a bypass ( $Q_{\text{BYPASS}}$ ) was added in case of input flows higher than 60000 m<sup>3</sup>.d<sup>-1</sup>.

The evaluation period was extended (364 days) to take seasonal variations and the slow dynamics of anaerobic digestion processes into account (Jeppsson et al., 2006). It is important to consider dynamic influents when modelling WWTPs as they can reproduce the real inputs and their effects in effluent and sludge characteristics. The initial conditions for dynamic simulations were set after a steady state simulation.

For each scenario, operational parameters were adjusted in order to comply with the legal discharge requirements as followed: dosage of chemicals (iron, methanol) was imposed (in a steady state simulation) such that N and P in effluent were below the accepted limit. The set-points for dissolved oxygen in reactors were unchanged in all scenarios. Consequently the calculated air flow rate automatically adapted to the oxygen needs and organic load.

Six scenarios were compared in this study (Table II.1):

- 1) Reference case (REF) used the conventional influent input and plant layout as described above.
- 2) Enhanced primary clarification (EPC) was foreseen for the conventional influent input, the plant layout being slightly modified to add coagulant before primary clarification and thus achieve efficiencies of 80% of total suspended solids retention (Tchobanoglous et al., 2003).
- 3) The Urine Source-Separation (USS) scenario was supplied with an adapted influent (with reduction in TKN, total P and total COD). Urine was treated by precipitation with magnesium oxide (MgO) to recover P (and a small proportion of N) while producing struvite. In that scenario (scenario 3), the N-rich effluent resulting from precipitation returned to the WWTP to be treated. The residence time considered for urine in the storage tank was 14 days (after which time urea was considered to be fully hydrolysed). Urine separation efficiency was taken to be 50%. Also, during storage of urine, urea is hydrolysed to NH<sub>3</sub> but losses of NH<sub>3</sub> in pipes and storage are considered to be negligible.
- 4) The scenario combining both alternative treatments (USS+EPC), which used USS and EPC operational conditions.
- 5) Urine Source-Separation coupled with enhanced primary clarification and agricultural spreading (USS+EPC+AGRI) used the same parameters as the EPC and USS scenarios except for N-rich effluent, which was spread on farmland by a vacuum tanker.

6) Urine Source-Separation coupled with enhanced primary clarification and nitrification/deammonification of nitrogen-rich and dewatering effluents (USS+EPC+ANA).

Table II.1. Comparison of scenarios

No	Scenario name	Collection type	WWTP configuration	Urine post-treatment
1	REF	Conventional sewer	Conventional (AS+AD)	-
2	EPC	Conventional sewer	Enhanced primary clarification	-
3	USS	Urine Separated	Conventional (AS+AD)	Struvite precipitation + Reinjection
4	USS+EPC	Urine Separated	Enhanced primary clarification	Struvite precipitation + Reinjection
5	USS+EPC+AGRI	Urine Separated	Enhanced primary clarification	Struvite precipitation + Agricultural application
6	USS+EPC+ANA	Urine Separated	Enhanced primary clarification	Struvite precipitation + Nitrification/deammonification

### II.2.3. LCA

#### II.2.3.1. Goal & scope

On the DM-LCA platform developed in this study, LCA was aimed at evaluating the environmental performances of different treatment scenarios, so as to compare them and identify hot spots.

The boundaries of the system were taken to be as broad as possible (Figure II.3) and included process operation and infrastructure (when data were available). However, sewer construction, operation and maintenance were excluded as they were similar for all scenarios, and were not considered to be part of the treatment itself.

The functional unit used was “1m<sup>3</sup> of raw wastewater to be treated”. However, as different treatment types can deliver different efficiencies, limits for effluent discharge were also imposed as specified in section 2.1.

Boundaries expansion was considered to include the secondary function of fertilizers i.e. sludge, N-rich effluent and struvite (all used in agriculture) and the production of an excess of electricity when appropriate.

As sludge was not considered as a commercially valuable fertilizer, emissions connected with its spreading were allocated to the wastewater treatment process (Doka, 2009). In the case of struvite production from urine, even though it is a valuable product, emissions from its application were allocated to the wastewater treatment, as urine is a fraction of the wastewater and the chosen treatment must be responsible for all residues generated. For the N-rich effluent, as it was also a residue from the WWTP, the impacts and benefits of its agricultural application were considered. Avoidance of conventional fertilizers, i.e. triple super phosphate and ammonium nitrate (production and application) was taken into account when considering expanded boundaries, on the basis of the quantity of N and P that were bioavailable.

Plant was considered to be based on west European region. For the scenarios where an excess of electricity was produced, a conventional European electricity production grid was taken as the avoided process.

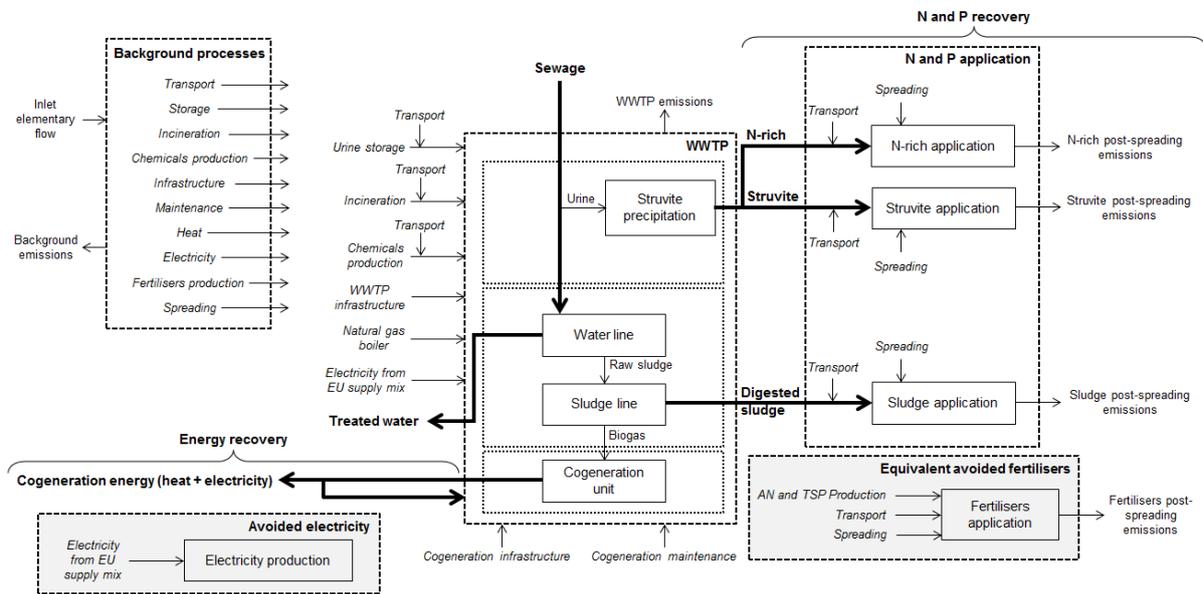


Figure II.3. Expanded system boundaries for LCA

Nowadays, there are also rising concerns about residues of drugs and personal care products but, as there is a lack of precise information in this area, these substances were not considered in the treatment simulations, nor in the inventory. As described by Udert et al. (2006), the majority of these substances

are present in urine and thus previous treatment may be necessary but, since available information is scarce, these treatments were not considered.

### *II.2.3.2. Life cycle inventory*

The inventory took account of all flow types proposed by the reference study included in the Ecoinvent 2.2. database (Doka, 2009) and also some others judged sensible in our case, such as a cogeneration system with electricity and heat production, external carbon source addition and production, fertilizer production from urine and its utilization.

For the direct gas emissions of carbon, it is important to emphasize that, in order to be consistent with IPCC (2006) guidelines, all organic carbon in sewage was considered to be biogenic. However, to achieve complete denitrification, it was necessary to use methanol (produced from natural gas) in some scenarios. Thus, there was a percentage of produced carbon dioxide (CO<sub>2</sub>) that originated from a fossil source. Emissions of N<sub>2</sub>O from WWTPs are considered to be 0.5% of ammonia nitrified flows in dynamic conditions (Czepiel et al., 1995). The volume and composition of offgas were calculated (from Biowin<sup>®</sup> software) based on gas/liquid transfer models. Calculations were based on transfer coefficients and concentration gradients with atmosphere. For anoxic reactors the volume of gas emitted was mainly related to the dinitrogen produced by denitrification which was calculated with the transfer surface. Heavy metal concentrations are not taken into account by Biowin as they are considered to be inert for biological processes. Their input concentrations in WWTPs were therefore taken from Doka (2009) and Henze and Ledin (2001) and allocated to effluent and sludge in specific quantities, using their specific transfer coefficients proposed by the same authors.

The amounts of chemicals consumed (FeCl<sub>3</sub> for P precipitation (coagulant), methanol, MgO, NaOH) that would consequently need to be produced in background processes were calculated according to simulation demands. The total amount of FeCl<sub>3</sub> required was calculated considering it to be used for both P precipitation and biogas purification (to avoid H<sub>2</sub>S formation). Grit removal in pre-treatment was also included in LCA, considering 31g of grit to be present in 1 m<sup>3</sup> of raw sewage (50% as plastics and 50% as paper to be disposed of in a municipal waste incinerator; Doka, 2009).

The electricity consumption was calculated by taking the sum of all electricity requirements (aeration of AER and NITRITATION tanks and THK, mechanical mixing of ANOX, ANAMMOX and AD tanks, pumping of main lines - influent input, dosing of chemicals, sludge outputs, recirculation lines, and effluent output - scrapping and dewatering unit) and subtracting the electricity produced in the cogeneration unit. Electricity that was produced was consumed by the WWTP itself and, when more

electricity was produced than consumed, it was considered to be injected into the network and the avoidance of electricity production was calculated. Heat production was calculated in a similar manner to electricity and it was used to heat sludge to be digested and to compensate for heat losses by AD walls. Process sludge was firstly preheated in countercurrent flow against digested sludge and the heat transfer was complemented by heat generated in the cogeneration unit (HE2). Details on the energy balance are given in SI Section 3.

Transports were based on Doka (2009) and were considered for grits collected (10 km by lorry), sludge to be disposed of (20 km by lorry), chemicals used (600 km by train and 50 km by lorry) and conventional fertilizers in extended boundaries (900 km by barge for N fertilizers, 400 km for P fertilizers, 100 km by lorry and 100 km by train). Transport of urine from houses to the WWTP (10 km by lorry) and struvite to the spreading site (20 km by lorry) were also considered.

Impacts of the agricultural application of sludge, struvite and classical fertilizers (from system expansion) took account of N gas-emissions in the form of  $\text{NH}_4$ ,  $\text{N}_2\text{O}$  and  $\text{NO}_x$ , P emissions to surface and ground water, and heavy metals to agricultural soil. The process of spreading sludge and N-rich effluent was considered by including a slurry spreading vacuum tank module and by a generic fertilizing process for other fertilizers and struvite. Detailed information about spreading is given in SI Section 5. In these calculations, a sludge bioavailability factor of 70% for P and 40% for N was applied (as recommended by Lundin et al., 2004). For the conventional fertilizers, struvite and N-rich effluent, 100% of N and P were considered to be bioavailable.

WWTP basic infrastructure (comprising a water line and a sludge line, see figure II.3) was included using a class 2 capacity data set from Ecoinvent (which includes dismantling). An annual sewage volume of approximately  $1.4 \times 10^7 \text{ m}^3$  was considered, and the plant lifetime was taken as 30 years. The basic infrastructure was the same for all scenarios and no modification of the size was considered (e.g. variation of reactor volumes). In scenarios with urine separation, urine flow was collected in storage tanks (fibreglass tanks) and later transported by truck to the treatment plant (no infrastructure changes were foreseen for the transportation of other flows). Struvite and nitrification/ANAMMOX infrastructure was not considered as tank volumes represented only a minor fraction of the WWTP.

The cogeneration unit was considered to have separate infrastructure (dataset from Ecoinvent) from the rest of the WWTP, which was calculated as a function of biogas input.

All inventory results are presented in SI Section 2 along with the Ecoinvent reference of each flow.

### II.2.3.3. LCIA

The environmental impacts were calculated in Umberto<sup>®</sup> v5.6 software using the LCA Ecoinvent database v2.2 and ReCiPe 2008 (Goedkoop et al., 2009) with endpoint (H,A) and midpoint (H) as in the LCIA method.

## II.3. Results and discussion

### II.3.1. Reference scenario

The simulation results obtained for the reference scenario were compared with available data from the literature (Table II.2), collected from both measurements on site and calculation approaches.

Energy requirements were similar to those reported in the literature, especially considering the reference LCA study in Ecoinvent. Biogas production was also in accordance with reference studies (Table II.2). Other parameters are difficult to compare given the variability of output effluent quality, process configuration and influent composition found in literature.

In terms of performance, the process was able to respect the limits (Section 2.1) on average. A number of violation days were observed during load peaks due to rain events, but these days corresponded to less than 9% of the simulation period for the reference scenario and less than 3% for other scenarios (Table II.3).

The LCA results were compared to literature studies. Although the WWTP configurations were not exactly identical, environmental impacts were expected to show similar trends. Considering the Ecoinvent process for WWTP (“treatment, sewage, to wastewater treatment, class 2, CH, [m<sup>3</sup>]”), infrastructure impacts were shown to make a contribution of approximately 30% to climate change, fossil fuel depletion and human toxicity. Ortiz et al. (2007) reported that approximately 43% of total impacts could be traced to the infrastructure for a conventional activated sludge plant.

Inventory for directly emitted substances can be found in SI (Section 2 – Effluent discharge, operation emissions and post-emissions). Considering the impacts generated by the direct emissions, comparisons with the Ecoinvent process (details in SI Section 7 Table II.2) presented similar results. Yoshida et al. (2014) also obtained a contribution of approximately 20% of direct gas emissions in the climate change impact category as well as a major contribution of effluent discharge to the marine

eutrophication impact category (data also presented by Renou et al. (2008)). Yoshida et al. (2014) also emphasize that background processes such as energy requirements and production from biogas have greater impacts than the foreground process (direct impacts) for all categories analysed, showing the importance of data collection. Finally, this study also agrees with previous ones that showed environmental burdens with the use of sludge in agricultural soil due to the presence of heavy metals (Foley et al. (2010); Lundin et al. (2004)), responsible for human toxicity impact.

Table II.2. Comparison between this study and the literature for BNR processes

<b>Parameter</b>	Unit	Ecoinvent 2.2 <sup>1</sup>	Tchobanoglous (2003) <sup>2</sup>	Corominas et al. (2013b) <sup>2</sup>	This study (Dynamic REF)
<b>Electricity consumed by the WWTP</b>	kWh.m <sup>-3</sup> sewage	0.28	0.39	0.18 – 0.24	0.31
<b>Biogas produced</b>	Nm <sup>3</sup> .m <sup>-3</sup> sewage	0.068	0.053	0.069 – 0.076	0.058

1 Results from site measurements

2 Results obtained by calculation/simulation

Globally, the results obtained for the reference scenario are in agreement with reported data, supporting the reliability of the DM-LCA approach and platform developed in this work.

The effect of dynamic versus steady state conditions on the simulation results are shown in Table II.3. Important underestimations are embedded in the steady state: violations of water quality limits do not exist and EROI is overestimated by 15%. Total effluent N is also shown in Figure II.4, together with total endpoint impacts and midpoint impacts for marine eutrophication, which is underestimated by 23% in the steady state. Results for all impact categories are shown in SI Section 6. The simulation results are strongly influenced by influent perturbations and the use of steady state results would lead to an underestimation of all impacts, which justifies the use of dynamic simulation in this study. These results also agree with those of Guo et al. (2012) where a large fluctuation of N<sub>2</sub>O emissions was observed between steady state and dynamic simulations (with steady state again being underestimated). N<sub>2</sub>O peaks are naturally observed during the daily nitrogen peaks in correlation with nitrification.

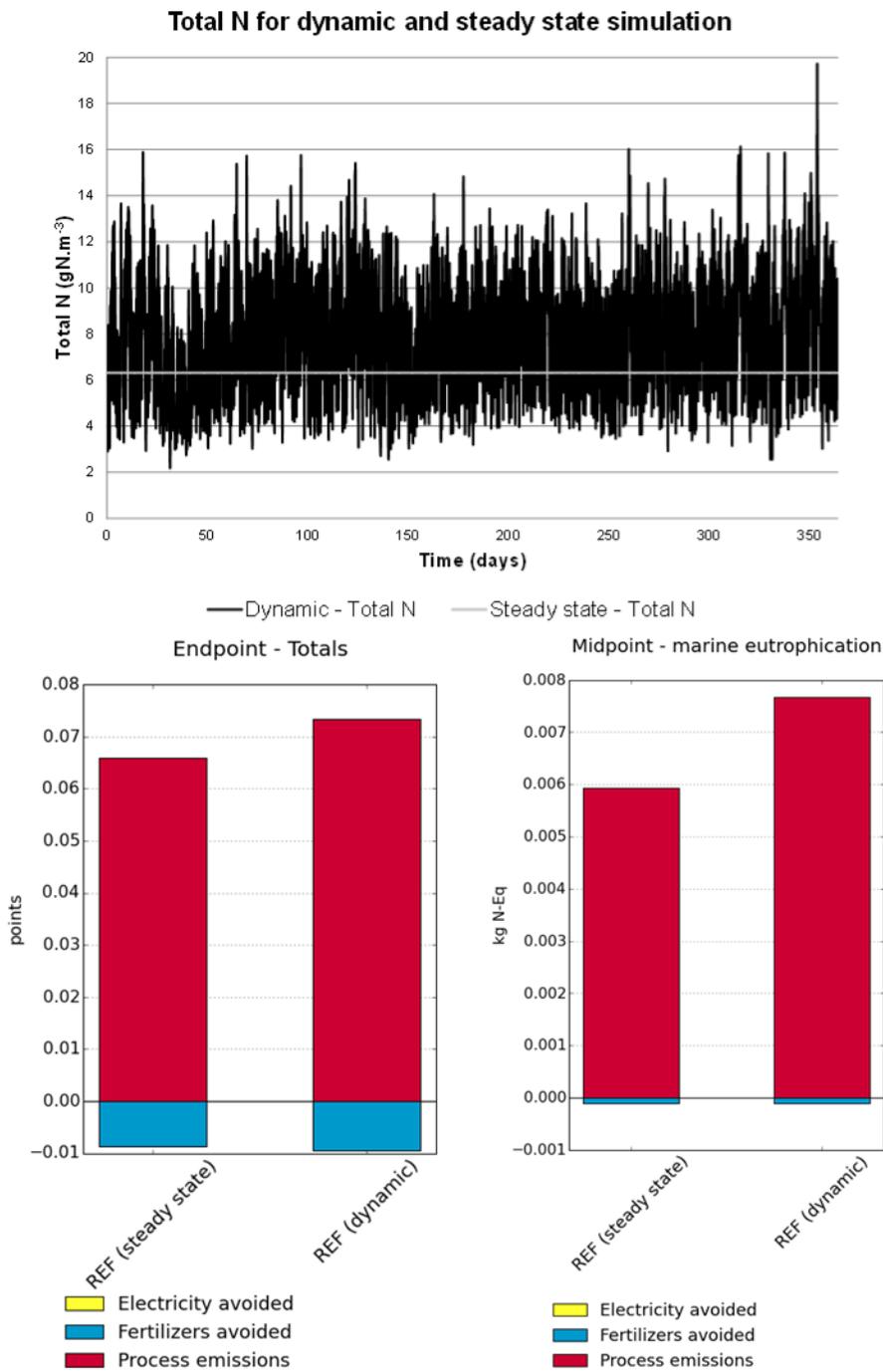


Figure II.4. Comparisons between steady state and dynamic simulations

(A) Effluent total N; (B) Endpoint total impact; (C) Midpoint marine eutrophication impact

*II.3.2. Results of alternative scenarios: nutrient recovery, efficiency and energy consumption*

Simulation results for alternative scenarios are shown in Table II.3. In comparison with the reference, alternative scenarios had a positive effect on the ability of the Activated Sludge Process (ASP) to match the nitrogen and phosphorus removal objectives. Enhanced primary clarification allowed the organic load entering into the ASP to be reduced, which reduced the oxygen needs and slightly facilitated the nitrification (lowering ammonia). On the other hand a little more methanol was necessary to maintain the denitrification efficiency. Urine separation reduced both phosphate and ammonia in the influent. As the P fraction from urine was crystallized into struvite, the  $\text{FeCl}_3$  needs were minimized in the USS scenario. In case of N removal from urine by either agricultural spreading or a deammonification process, the oxygen and methanol needs were also significantly reduced (scenarios USS+EPC+AGRI and USS+EPC+ANA).

Stability in effluent quality is also important when considering the long-term running of a WWTP. Regarding N limit violation, all alternative scenarios presented better results than the REF scenario. For USS+EPC+ANA, nitrogen removal was more stable due to less N entering WWTP (and lower ammonia peak load). However, slightly higher average nitrogen concentration was noticed. Concerning P limit violations, scenarios without enhanced primary clarification presented problems in stability since EPC allows direct removal of P from the water line (redirected to sludge). Total suspended solids and ammonia violations were also fewer in all alternative scenarios than in REF. COD results were not strongly influenced and were always within the regulation limits.

Table II.3. Main simulation results for the reference (steady state and dynamic simulations) and the alternative scenarios (dynamic simulations)

Scenarios	Effluent total N ( $\text{gN}\cdot\text{m}^{-3}$ )			Effluent total P ( $\text{gP}\cdot\text{m}^{-3}$ )			Effluent total COD ( $\text{gCOD}\cdot\text{m}^{-3}$ )		
	364 d- Average	Maximum daily average	Violations (days)	364 d- Average	Maximum daily average	Violations (days)	364 d- Average	Maximum daily average	Violations (days)
	Steady state REF	6.31			0.56			39.1	
REF	8.13	14.64	30	0.64	1.62	15	40.8	68.7	
EPC	6.39	13.10	5	0.41	1.14	2	44.1	71.1	
USS	6.93	11.82	9	0.55	1.36	7	41.5	67.1	
USS+EPC	6.51	11.96	5	0.35	0.99	0	43.5	70.6	
USS+EPC+AGRI	6.59	10.38	2	0.36	1.003	1	37.7	64.5	
USS+EPC+ANA	7.23	10.32	2	0.47	1.18	6	40.4	66.2	

Scenarios	Effluent total $\text{NH}_4$ ( $\text{gN}\cdot\text{m}^{-3}$ )			Effluent total suspended solids ( $\text{gTSS}\cdot\text{m}^{-3}$ )			Methanol dosage ( $\text{m}^3\cdot\text{d}^{-1}$ )	$\text{FeCl}_3$ dosage ( $\text{m}^3\cdot\text{d}^{-1}$ )
	364 d- Average	Maximum daily average	Violations (days)	364 d- Average	Maximum daily average	Violations (days)		
	Steady state REF	0.20			15.02			
REF	0.84	4.06	1	16.85	47.67	9	3.0 – 6.0	2.0 – 4.0
EPC	0.41	2.80	0	14.50	41.42	3	3.5 – 7.0	1.7 – 3.4
USS	0.56	2.93	0	16.12	45.09	6	3.0 – 6.0	1.6 – 3.2
USS+EPC	0.30	1.82	0	13.97	41.04	3	3.0 – 6.0	1.4 – 2.8
USS+EPC+AGRI	0.65	2.42	0	13.52	40.26	3	1.1 – 2.2	1.5 – 3.0
USS+EPC+ANA	1.00	2.25	0	13.33	39.67	2	-	1.3 – 2.6

Scenarios	Biogas (m <sup>3</sup> .h <sup>-1</sup> )	% Methane	Electricity from cogeneration (kWh.m <sup>-3</sup> )	Electricity requirement (kWh.m <sup>-3</sup> )	EROI <sup>1</sup> for electricity	Net energy requirement for entire life cycle	EROI <sub>Lc</sub> <sup>2</sup> for the entire life cycle
Steady state REF	76.29	71.8	0.222	0.297	0.75	-	-
REF	68.22	76.4	0.203	0.311	0.65	1.80	0.11
EPC	93.12	71.0	0.257	0.260	0.99	1.50	0.17
USS	68.96	75.9	0.210	0.311	0.67	1.72	0.12
USS+EPC	93.95	70.5	0.266	0.258	1.03	1.33	0.20
USS+EPC+AGRI	90.22	70.9	0.256	0.215	1.19	0.66	0.39
USS+EPC+ANA	90.87	70.3	0.256	0.234	1.10	0.80	0.32

Scenarios	Nutrients from sludge <sup>3</sup>			Nutrients from struvite			Nutrients from N-rich effluent			Total nutrients recovered		
	N (kg N.m <sup>-3</sup> )	P (kg P <sub>2</sub> O <sub>5</sub> .m <sup>-3</sup> )	P (kg P <sub>2</sub> O <sub>5</sub> .m <sup>-3</sup> )	N (kg N.m <sup>-3</sup> )	P (kg P <sub>2</sub> O <sub>5</sub> .m <sup>-3</sup> )	P (kg P <sub>2</sub> O <sub>5</sub> .m <sup>-3</sup> )	N (kg N.m <sup>-3</sup> )	P (kg P <sub>2</sub> O <sub>5</sub> .m <sup>-3</sup> )	N (kg N.m <sup>-3</sup> )	P (kg P <sub>2</sub> O <sub>5</sub> .m <sup>-3</sup> )	N (kg N.m <sup>-3</sup> )	P (kg P <sub>2</sub> O <sub>5</sub> .m <sup>-3</sup> )
Steady state REF	4.49E-03	1.55E-02	0	0	0	0	0	0	4.49E-03	1.55E-02	4.49E-03	1.55E-02
REF	4.57E-03	1.77E-02	0	0	0	0	0	0	4.57E-03	1.77E-02	4.57E-03	1.77E-02
EPC	5.89E-03	1.82E-02	0	0	0	0	0	0	5.89E-03	1.82E-02	5.89E-03	1.82E-02
USS	4.71E-03	1.62E-02	6.53E-04	6.53E-04	3.31E-03	3.31E-03	0	0	5.36E-03	1.95E-02	5.36E-03	1.95E-02
USS+EPC	5.94E-03	1.66E-02	6.53E-04	6.53E-04	3.31E-03	3.31E-03	0	0	6.59E-03	2.00E-02	6.59E-03	2.00E-02
USS+EPC+AGRI	5.58E-03	1.66E-02	6.53E-04	6.53E-04	3.31E-03	3.31E-03	1.44E-02	7.73E-05	2.06E-02	2.00E-02	2.06E-02	2.00E-02
USS+EPC+ANA	5.34E-03	1.52E-02	6.53E-04	6.53E-04	3.31E-03	3.31E-03	0	0	6.00E-03	1.85E-02	6.00E-03	1.85E-02

<sup>1</sup> EROI: Energy return on investment = electricity produced/electricity consumed at plant

<sup>2</sup> EROI<sub>Lc</sub>: Energy return on investment on the life cycle of WWTP = electricity produced/energy consumed on the plant life cycle

<sup>3</sup> Considering bioavailability

Concerning energy, scenarios with enhanced primary clarification produced more energy by cogeneration. Urine source-separation helped to decrease energy consumption at plants, thus giving a positive energy balance in coupled scenarios (represented by EROI values above 1). This made scenarios USS+EPC+AGRI and USS+EPC+ANA the most interesting from the energy balance standpoint (with EROIs of 1.19 and 1.10 respectively). Total energy consumption over the life cycle of the plant was estimated through Cumulative Energy Demand (CED) indicator. The main energy resources used by the life cycle system are fossil and nuclear ones (results are presented in SI Section 6.3).  $EROI_{LC}$  (defined as the electricity produced at plant divided by CED) of the six scenarios presented the same profile as EROI.

Regarding the energy consumption, aeration was the most important requirement, varying between 40% (in USS+EPC+ANA) and 55% (in REF) of total consumption, which is in agreement with full-scale studies (Tchobanoglous et al., 2003). The EPC and USS scenarios reduced aeration energy requirements by 26% in USS+EPC, 46% in USS+EPC+ANA and 48% in USS+EPC+AGRI, while the reduction in total electricity consumption varied from 20% to 33%. The second consumption requirement was represented by the mixing of different devices (figure II.5).

Compared to the reference scenario, biogas production was increased by 27% with the implementation of enhanced primary clarification (USS+EPC) in the plant.

Considering material recovery, USS scenarios allowed the source separation of valuable nutrients N and P. The greatest recovery of N was related to scenario USS+EPC+AGRI, where all remaining nitrogen, after struvite precipitation, could still be used in agriculture by means of direct liquid spreading. However, this method of N valorisation is still debatable because of its poor acceptance by the general public, the infrastructure modifications it requires, and high volatilization emissions depending on the spreading method. Regarding P recovery, USS+EPC and USS+EPC+AGRI scenarios showed the highest performance. In all scenarios, P was precipitated in sludge or as struvite, and losses of P only occurred with the effluent outputs. In this sense, USS+EPC and USS+EPC+AGRI scenarios not only presented the highest P recovery, but were also the most stable in P effluent, with respectively zero and one violation day during a period of one year.

Finally, external carbon addition (methanol) could be avoided in the nitrification/Anammox scenario and decreased significantly in the AGRI scenario. In both cases, less N had to be treated by activated sludge. Moreover, the dewatering effluent was also treated by nitrification/deammonification instead of the traditional treatment.

$FeCl_3$  consumption was strongly influenced by the coupled treatments, a smaller quantity being used in USS+EPC+ANA. However, the stability of P concentration in the effluent was ensured, with only 6 days of violations in one year and a maximum daily average of P not far from  $1 \text{ g}\cdot\text{m}^{-3}$ .

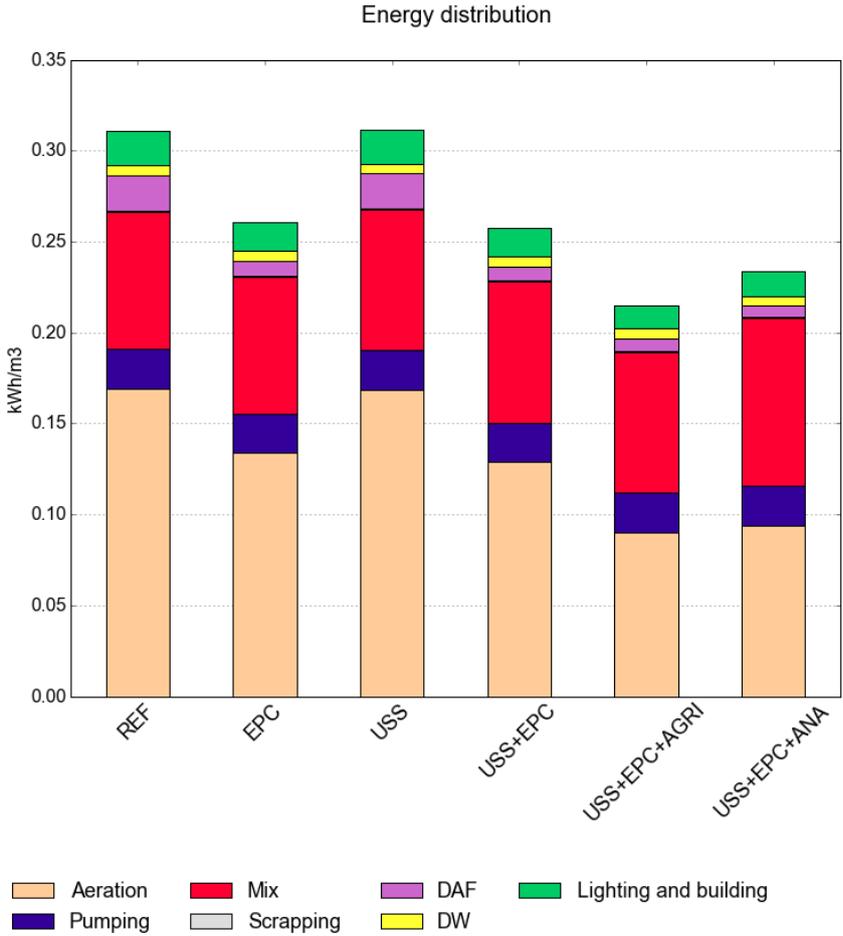


Figure II.5. Energy distribution by consumption item

II.3.3. Results of alternative scenarios: environmental impacts

II.3.3.1. Endpoint impacts

Figure II.6 synthesizes the ReCiPe endpoint results for all categories (ecosystem quality, human health, resources and total impacts, including the impacts generated and avoided) and as a percentage of impacts compared to REF (100%). Following these criteria, the performance of the scenarios decreases in the order USS+EPC+AGRI > USS+EPC+ANA > USS+EPC > EPC > USS > REF (i.e. REF has the highest impact score expressed in points). However, considering socio-cultural aspects and feasibility, USS+EPC+ANA and USS+EPC are the most conceivable as discussed previously. As shown in Figure II.6, implementation of USS or EPC strategies decreased all impact scores compared to the reference scenario. However, significant decreases in endpoint scores were only observed for the coupled scenarios, in particular when N-rich effluent was treated by nitritation/Anammox or

recycled in agriculture, achieving a reduction in resource depletion of 62.6%. Overall, the results agree with previous studies in the literature (Björklund et al., 2000; Rémy, 2010; Tillman et al., 1998) where separation systems also show a potential for more sustainable systems with less impact on the environment. Additionally, our study clearly shows that urine separation would bring the greatest advantages when a dedicated strategy was proposed for nitrogen removal or recovery, whereas only limited benefits would be obtained if only phosphorus was recovered.

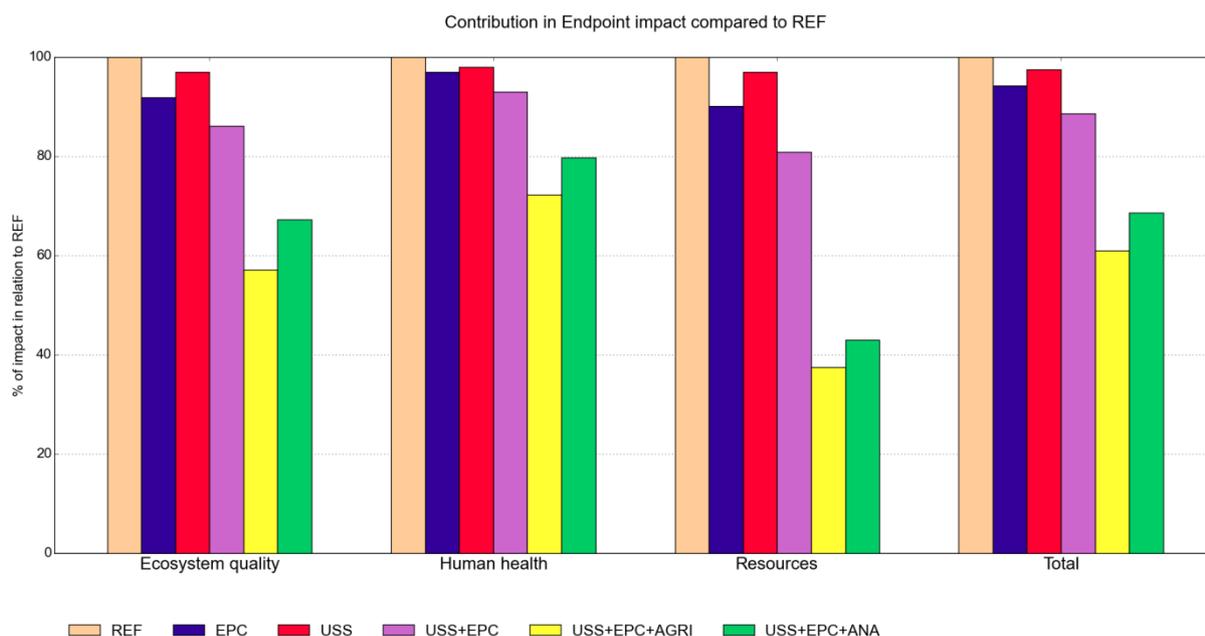


Figure II.6. Endpoint impacts for studied scenarios

In the ecosystem quality group, the main contribution was observed for both generated and avoided impacts on climate change. Climate change was also the main contributor in the human health group. However, in this case, particulate matter formation and human toxicity also became significant. As previously discussed for the reference scenario, for alternative scenarios, direct emissions of heavy metals in water and soil (sludge spreading) were responsible for human toxicity. For resources, metal depletion was negligible relative to fossil fuel consumption. We emphasize that scenarios with USS allow P to be recovered in the form of struvite (which is 100% bioavailable for plants) and so avoid natural resource consumption. However, the P resource is not considered in ReCiPe, despite its importance and scarcity. Complementary evaluation with other LCIA methods gave similar results (see SI Section 6).

II.3.3.2. Midpoint results

The analysis results for contributions to climate change, freshwater and marine eutrophication, and fossil fuel depletion are discussed below, since WWTPs are known to affect these categories (Figures II.7-II.10). Results for other categories are given in SI Section 6.

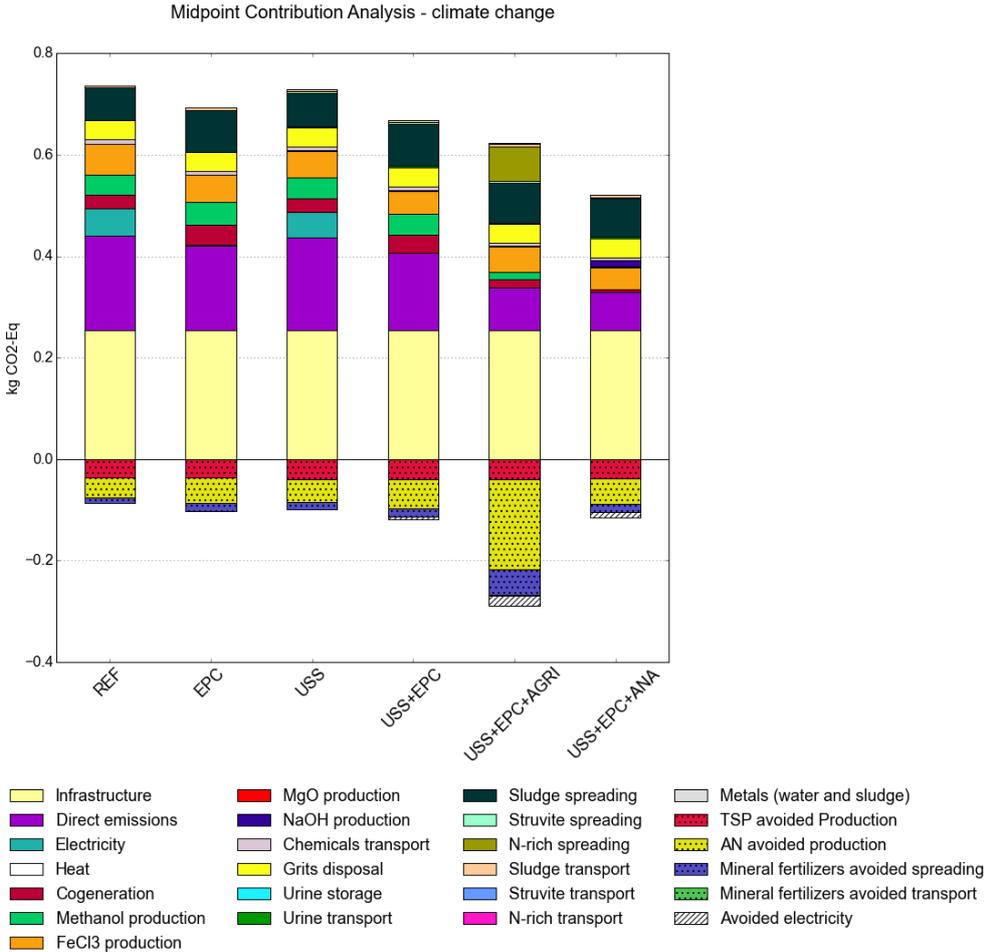


Figure II.7. Contribution analysis for climate change (GWP100) using ReCiPe Midpoint (H)

Considering the midpoint analysis of climate change, direct emissions decreased strongly with alternative scenarios because the emissions of N<sub>2</sub>O decrease when less N enters WWTP to be conventionally nitrified and denitrified. For nitrification/Anammox scenarios, all emitted CO<sub>2</sub> was biogenic as no methanol was added (cogeneration emissions were also not significant as CO<sub>2</sub> is biogenic). Details of WWTP gas emissions for each substance are given in Figure II.8. N<sub>2</sub>O was the main contributor for all scenarios, emphasizing the importance of decreasing its emission with

alternative strategies. The infrastructure still made the highest contribution to global warming potential (GWP) in all scenarios. Spreading of by-products (sludge, struvite and N-rich effluent) were also responsible for a large fraction of GWP, especially because of N<sub>2</sub>O post spreading and CO<sub>2</sub> emitted in the spreading process itself. Finally, GWP due to electricity consumption was also noticeable in the scenarios that were not self-sufficient. Considerable avoidance of conventional electricity production is to be noted in USS+EPC+AGRI and USS+EPC+ANA (on negative axis).

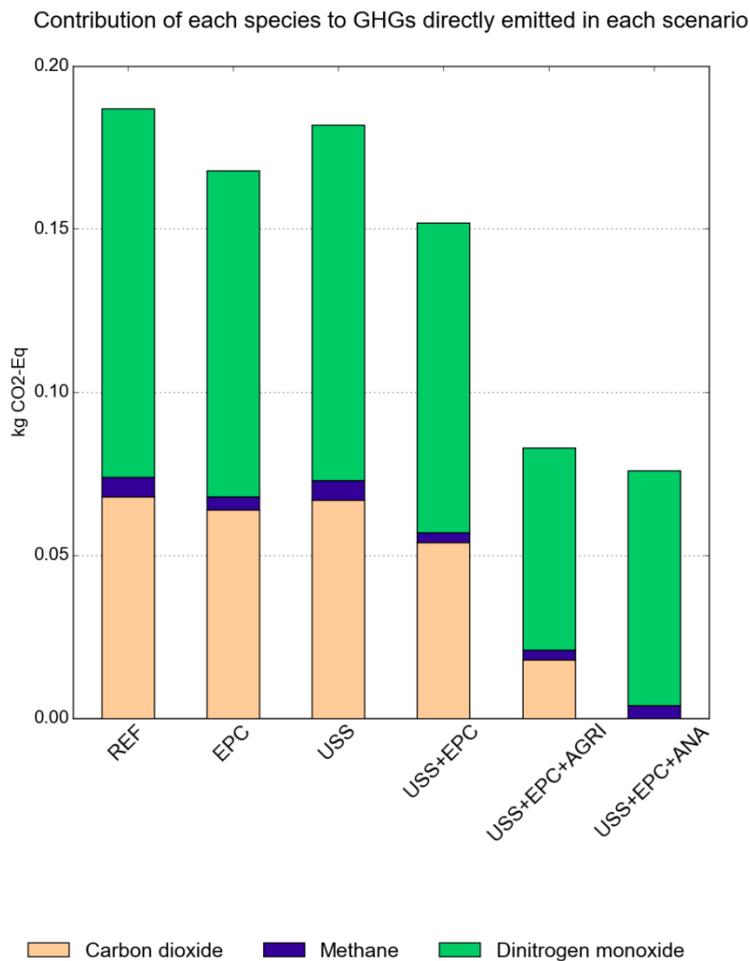


Figure II.8. Contribution of each species to greenhouse gases emitted



Freshwater eutrophication (linked only to P emissions in ReCiPe) depended mainly on the direct emissions of phosphorus, which varied slightly for the different scenarios. All alternative scenarios had a lower impact than the reference because the amounts of P discharged were lower. Scenarios containing enhanced primary clarification presented the most efficient phosphorus removal (effluent P concentration was also more stable in these scenarios). Also, there was a remarkable avoidance of freshwater eutrophication linked to P fertilizer production. Emissions in sludge and struvite spreading were linked to phosphate leaching to ground water and the run-off of P to surface water. (For details, see SI Section 5.) For marine eutrophication (for which only N emissions are considered in ReCiPe), direct emissions were the most impacting contribution, as was expected a priori.

For fossil fuel depletion (reduction of resources containing hydrocarbons), infrastructure and methanol production were the biggest contributors, leading to low impacts for USS+EPC+ANA (which did not use external carbon addition) and USS+EPC+AGRI (where a lower flow of methanol was used). Large impacts were also linked to energy production by the supply mix for non-self-sufficient scenarios and coagulant production. Marked impacts were also avoided when all N was recovered for agriculture (USS+EPC+AGRI).

Finally, regarding particulate matter formation, sludge spreading showed large impacts in all scenarios (due to  $\text{NH}_3$  volatilization). However, the impacts of N-rich spreading were compensated by the amount of conventional fertilizer spreading avoided. The same profile was also observed for photochemical oxidant formation and terrestrial acidification. However, unlike the available literature, this study did not show increases in acidification potential due to urine separation as urine was incorporated directly into the soil and low  $\text{NH}_3$  emissions were expected (Rodhe et al., 2004). Impacts of ionizing radiation were much influenced by  $\text{FeCl}_3$  production and electricity provision by the conventional European mix, so all scenarios containing EPC were less impacting for this category. Natural land transformation impacts were strongly influenced by avoidance of conventional N fertilizers (production), which gave the USS+EPC+AGRI scenario a low score (results can be found in SI Section 6).

The results presented above clearly show the importance of nitrogen recovery on the overall performance. This supports the idea that recent research on alternative economical solutions for N recovery, such as nitrification followed by distillation, electrolysis of urine and low-cost precipitation of struvite, proposed by several authors (Etter et al., 2011; Hug et al., 2013; Maurer et al., 2006; Udert and Wächter, 2012) should be included in future evaluations. Furthermore, coupled scenarios would also lead to a more sustainable design for WWTPs and the opportunity to recover nitrogen as well as phosphorus in sewage in order to avoid conventional fertilizer production and  $\text{N}_2\text{O}$  emissions when N is treated in the plant.

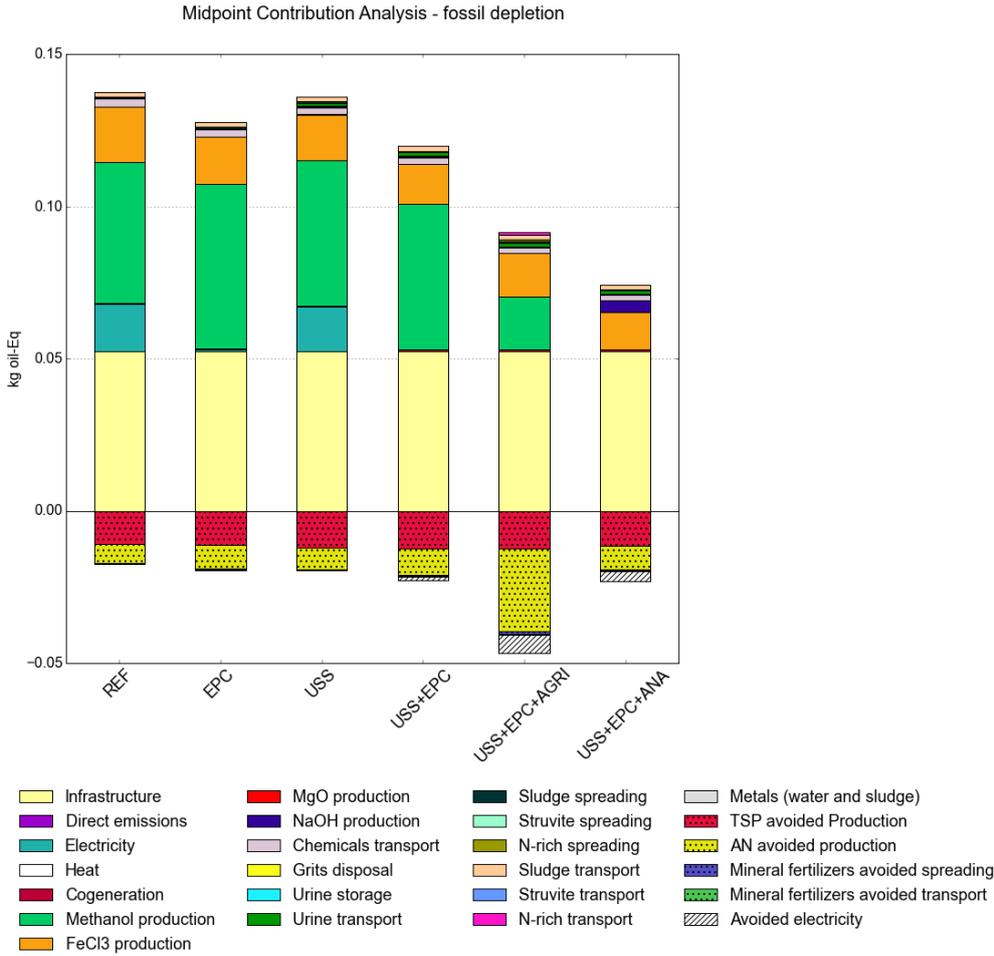


Figure II.10. Contribution analysis for fossil fuel depletion using ReCiPe Midpoint (H)

**II.4. Conclusion**

Decision making when evaluating WWTP scenarios is a difficult task as there are several interconnected parameters and variables that influence results at different levels. Environmental assessment would help in the ecodesign of these processes when low impacts are sought for specific impact categories.

In this context, a modelling platform was developed by combining dynamic modelling of wastewater treatment and LCA, in the aim of evaluating the environmental performances of different treatment scenarios. In this work, the approach was applied to six WWTP scenarios.

A major original aspect of this study was the use of dynamic simulations coupled with LCA calculations to build up the system’s life cycle inventory and provide complete impact evaluations, which gave more realistic information than steady state assessments when the system was perturbed.

Alternative scenarios not so far evaluated by LCA, such as nitrification/deammonification were also studied.

Concerning scenario analysis, urine source-separation (USS) was shown to have a positive effect on the effluent quality and to decrease the energy consumption in WWTP. On the other hand, enhanced primary clarification (EPC) led to important energy savings, as more energy was recovered in the sludge line and also less energy was consumed in the WWTP. When these two options are combined, WWTP can achieve a positive energy balance while respecting effluent quality limits more easily. For urine treatments after source-separation, agricultural spreading proved to be the scenario with the least environmental impact for most categories. However, the socio-cultural acceptability and feasibility of this type of scenario should be further analysed, including different technical methods for nitrogen recovery. Among the different scenarios, nitrification coupled with Anammox for nitrogen removal from urine proved to be an interesting option from the environmental, energy and feasibility points of view.

Finally, contribution analysis identified hot spots needing further optimization, such as infrastructure (which could be optimized in alternative treatments with, for instance, decrease in the anoxic zone or even skipping the post-denitrification zone), N<sub>2</sub>O direct emissions, which could be decreased by diminishing N input in WWTPs, and heavy metals in sludge, which could lead to toxicity problems (and possible avoidance of these problems when using source-separated flow products – such as struvite and N-rich effluents - in agricultural soil).



# **Chapter III. Influent Generator**



*“Show me your wastewater and I will tell you who you are” (Henze and Comeau, 2003)*

Nowadays, one might cite an important quantity of problems linked to environmental and human health that comes directly from water and wastewater management (or from the lack of it). It is essential thus to tackle the problem from two different points of view: Firstly, it is important to understand and work on the immediate consequences; however, having a view on the long term is essential as rapid global changes are taking place and communities will have to plan wastewater management against future scenarios. Moreover, solutions for smart wastewater management must be socially and culturally appropriate, as well as economically and environmentally viable into the future. Also, population education is essential when considering both wastewater management solutions and the reduction of wastewater produced (volumes and fate). Further, it is necessary to change populations mind in the sense of considering separation systems as not only provisional alternatives (Corcoran et al., 2010).

In this sense and when considering smarter and more sustainable ways of managing wastewater, urine source separation appears as one of the most promising alternatives. The interest is mainly focused on the important concentration of nutrients which are present in urine. These nutrients might be used to close the nitrogen and phosphorus cycles: from food production which needs fertilizers, to the human waste production. According to Larsen and Gujer (1996), urine represents a contribution of 88% of total nitrogen and 57% of total phosphorus in a small volume. Also, a wide range of processes for urine treatment are available nowadays (Maurer et al., 2006) including stabilisation (e.g.: by acidification or nitrification), phosphorus recovery (e.g.: by struvite formation), nitrogen recovery (e.g.: by ammonia stripping) and nutrient removal (e.g.: by anammox).

The recovery of nutrients, especially nitrogen and phosphorus, might be thus envisaged if yellow water is recovered separately and non-diluted. However, nutrient recovery presents a difference when considering nitrogen and phosphorus. Nitrogen is abundant in the atmosphere even if, to be obtained, N fertilizers require energy intense processes. Further, given the human interferences in nitrogen cycle, several environmental impacts might occur such as eutrophication, effects on human health and consequences from greenhouse gas emissions. However, when considering phosphorus, artificial fertilisers are obtained by mined phosphorus and the lifetime of economic reserves of phosphate rock is nowadays estimated to deplete between the next 30 to 370 years (Balkema, 2003).

Regarding experiences on urine source separation, several pilot studies or even ecological villages have been implemented nowadays. However, not many modelling and simulation studies have been found on the literature considering urine source separation. To the authors' knowledge, it is mainly due to the fact that urine has a highly variable concentration and its generation is not constant as it

depends on human behaviour and thus it is difficult to dynamically characterize urine in a realistic way. Accordingly, the mixture of the other streams from households will change as well as the influent in the WWTP. Therefore, it is essential to have a tool to generate realistic, dynamic and standardized urine stream as well as the other wastewater streams.

As discussed in a review proposed by Martin and Vanrolleghem (2014) on completion, analysis and generation of influents, several approaches are nowadays available to tackle the lack of information on influents. However, there is still an important need in implementing more realistic and case study influent generators in order to consequently obtain more predictive plant simulation results.

Accordingly, the objective of this study is to propose a flexible, dynamic and phenomenological influent generator to consider both yellow water and wastewater streams. This chapter is in preparation for submission in partnership with the Eawag institute in order to ensure realistic aspects in urine generation. The influent generator hereafter described was adapted from the dynamic and phenomenological influent generator from Gernaey et al. (2011). Urine and wastewater composition data was obtained from a literature compilation to respect real data; however, the model is flexible and allows the simulation of specific case studies (when the user wants to consider, for instance, other source separation systems, other generation dynamics or other geographical/catchment conditions) as well as the utilization of generated influents in different modelling platforms (ASM family models and wide plant model results are showed).

## **Entitled of the paper: A dynamic influent generator to account for alternative wastewater management: the case of urine source separation**

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### **Abstract**

The simulation of wastewater treatment plants allows obtaining predictive results when one needs to understand, evaluate, optimize or design a plant. However, one of the bottlenecks of the simulation feasibility is to obtain reliable and dynamic influent data. This difficulty is even more important when alternative scenarios are considered, such as source separated streams. The present paper offers an influent generator for the case where urine is separated at source and at a user-specified level of retention. The proposed tool contains several blocks to include different contribution and, due to its flexibility, allows the easily modification of parameters by the user in order to fit other case studies. The tool showed to be able to generate dynamic, long-term and predictive data for both urine and wastewater streams. Also, the extensive set of state variables allowed the generation of influents for different modelling platforms.

*Keywords: Urine source-separation; Influent generator; Phenomenological model; Dynamic influent*

### **III.1. Introduction**

Wastewater treatment plants (WWTPs) are a complex combination of biological, chemical and physical processes that shall be able to removal pollutants from wastewaters. Given the complexity of the system and the interaction between a large set of parameters, modelling and simulation allows, together with the understanding of involved processes, the performance evaluation and test of control strategies, the design verification of new treatment approaches and the optimization. However, a predictive and robust model might offer not realistic results if input data is not complete or if it is inaccurate.

In this sense, one of the limitations when considering the use of modelling is the scarce datasets available as it is a costly and a laborious task to obtain experimental data for long-term dynamic influent entering WWTPs (Martin and Vanrolleghem, 2014; Rieger et al., 2010). This difficulty is mostly present when measuring only flowrate is not enough: if pollutants data are required as dynamic, reliable and long-term inputs, on-line measurements might be necessary for instance (Gernaey et al., 2011). Therefore, if an influent generator is available and able to generate predictive data, hypothetical situations such as temperature changes, population growth in a catchment area, storm events, unconventional wastewater management options and so forth might be easily and reliably simulated.

Further, wastewater generation is by nature, a dynamic problem and thus WWTPs will be influenced by all daily, weekly and seasonally perturbations. Therefore, when considering simulation of dynamic WWTPs, there is an increasing need in reliability of influent data as considering steady state influent may lead to underestimated results considering real world effluent concentration and chemicals and energy consumption in plants.

Several model-based approaches for dynamic influent generation are available in the literature. An extensive review is proposed by Martin and Vanrolleghem (2014) and three main situations where influent shall be generated were identified by the authors: i) the available dataset is not complete and should be better characterized with expected wastewater quality and quantities; ii) one already has the main characteristics of the influent but efforts should be made in order to characterize flows into state variables (such as ASM family components); iii) the dataset has to be characterized considering uncertainty in order to be used later in the generation of other derived datasets.

To respond to the first situation, three approaches are proposed. The first one consists in the construction of databases based on experimental data that is used to complete or generate similar influent pollutant loads and flows. The second approach consists of using harmonic functions to describe the dynamic profile of wastewater streams. Following this idea, Langergraber et al. (2008) used a 2<sup>nd</sup> order Fourier series to propose realistic pattern for flow and composite variables (COD, TKN and TP) based on the sum of the main wastewater streams (infiltration water, urine with flush water and domestic wastewater without urine). The influent generated was compared to measured data and parameter set for model tuning was provided.

The third approach is based on phenomenological modelling and, as showed by Martin and Vanrolleghem (2014), is a promising research area as they can integrate knowledge about generating mechanisms and they should be improved in order to take into account both catchment area information and stochastic influence on inputs. Gernaey et al. (2011) proposed a dynamic influent

generator considering such an approach and taking into account all flow rate generation model, pollutants generation model, temperature generation model, first flush and transport in sewer model.

Following the actual switch from the conventional WWTPs (where pollutants are only treated) to recovery facilities (where wastewater is regarded as a resource) and from the centralized management and treatment option to the decentralized one, influent generation tools has also to be adapted in order to consider, for instance, source separation in households, vacuum toilets, usage of rainwater, etc.

Between the non-conventional wastewater management strategies that are nowadays gaining more interest as they may lead to a more sustainable approach one can cite urine source separation. The high interest is due to urine's high concentration in nitrogen and phosphorus. In average, 80% of nitrogen and 50% of phosphorus entering domestic WWTPs come from urine (Larsen and Gujer, 1996). When not separated at the source, these pollutants need to be treated in the plant and thus are responsible for important consumption of energy (for nitrification) and chemicals (coagulants for chemical precipitation of phosphorus and COD addition for denitrification).

The effect of combining urine separation and waste design was presented by Rauch et al. (2003). Authors provided a stochastic model that was applied to a virtual case study in order to understand the gains on WWTP load with peak shaving and in the aquatic environment with the reduction of combined sewer overflow. As presented by the authors, an interesting approach when urine is separated and stored is to release it into the sewer following an integrated strategy in order to adjust the pollutants input into the WWTP. The advantages of the application of this strategy would be not only the control of nitrogen level into the plant but also the avoidance of sewer overflow with urine which might have a harmful effect on water bodies. Also, as WWTPs are usually designed to deal with ammonia peak loads, shaving peaks would increase nitrogen treatment stability of existing plant and allow the reduction of new designed plants.

Stored urine might also be treated and several options are available on literature. Maurer et al. (2006) proposed a review on these methods showing that there are mainly purposes in treating urine: hygienisation, volume reduction, stabilization, recovery of N and P, nutrient removal and treatment of micropollutants.

However, when evaluating any of these treatment options it is necessary to well characterize this flow in order to correctly assess benefits and drawbacks of the innovative technology. Once again, one might consider data collection; however, important sources of noise and variation are present in the system varying from source separated toilet operation and efficiency to dietary of toilet users and thus recovery of these data can contain several assumptive conditions.

Moreover, urine is a complex fluid composed of several substances presenting a high variance and several spontaneous processes might occur during storage and transport. During storage, all urea is degraded and almost all nitrogen is available as ammonia, the pH rapidly increases, almost all calcium and magnesium are precipitated and there is an important concentration of biodegradable organic in urine that can be used by microorganisms during storage, even if most of them will not resist to storage (Udert et al., 2006).

The present paper aims to propose a dynamic influent generator (based on Gernaey et al., 2005; 2011) that takes into account urine source separation in households with a urine retention percentage that is easily modifiable by the user. The model generation allows obtaining two different flows: (i) the urine dynamically produced in households and (ii) the mainstream influent for WWTPs that is directly influenced by urine separation according to a more or less important urine retention. The proposed influent generator also aims to obtain not only composite variables, but also a detailed characterization of the flows into several state variables.

The remaining of this paper will be organized as follows: First, each model block (flowrate and pollutants) will be presented with its inputs and hypothesis as well as the fractionation model adopted. Following, results covering flowrate and variables for a fixed retention percentage (50%) will be presented and discussed. Latter, considered dynamics of the two obtained streams as well as noise addition will be showed and discussed. Finally, two types of comparisons are provided: (i) the case of using the generated dynamic influent data to fulfil a simulator which uses a plant-wide model versus the use of an interface approach model; (ii) the simulation of different urine retention percentages (from no retention to 100% retention).

## **III.2. General overview**

As discussed previously, this study is based on the original phenomenological influent generator from Gernaey et al. (1005; 2011). This influent generator has the advantage of being a flexible tool that can be easily modified and that it is implemented as open-source freely available. The tool was developed using the Matlab<sup>®</sup> 7.0 Simulink toolbox and model blocks that has not been changed in this modified version will not be detailed here. Moreover, the proposed modifications in the code keeps the flexibility idea originally proposed in order to fit other case studies.

Figure III.1 presents a general overview of the modified influent generator. Four main streams have to be defined here: (i) TWW stream corresponds to the total wastewater stream (household and other contributors) without any urine separation; (ii) TUS stream consists of total urine produced by the

specified population (the same as a retention of 100% of non-diluted urine); (iii) US stream corresponds to the user-specified separated urine and diluted in the new specified flush; (iv) WW stream represents the influent entering the wastewater treatment plant (contribution from industry, rainfall, infiltration and the household) without the urine retained (previously specified). This last stream (WW) is basically created from the difference of a conventional total wastewater stream (TWW) that is well defined in the literature and the separated urine stream (US).

As showed in figure III.1, the influent generator is structured in three main sections: The general settings (user input), the WW Generator and the US Generator. First, the user has to set the general parameters in order to fit his/her case study. Between those settings, the most important are the urine retention percentage and the size of the catchment. Other parameters (Old and new flushwater volumes, TWW and TUS composite variables and TWW and TUS fractionation) are pre-calibrated by the authors using the available literature and only have to be changed in very specific scenarios.

The WW generation is composed of five main parts: (i) Flowrate generation in households (without retained part of urine), flowrate generation in industries, seasonal infiltration (due to changes in groundwater level during the year) and rain generation (block A in figure III.1); (ii) Pollutants generation in households (without retained part of urine) and industries (block C in figure III.1); (iii) WW influent fractionation into a complete set of state variables (comprising also temperature profile generation) (block E in figure III.1); (iv) Application of a first flush effect in sewer (surface runoff following a storm event) (block G in figure III.1) and (v) Transport in sewers (responsible for smoothing concentration peaks depending on the size of the sewer) (block H in figure III.1).

On the other hand, the US generation is composed of only three main parts: (i) Urine flowrate generation (block B in figure III.1); (ii) Urine pollutants generation (block D in figure III.1) and (iii) Urine fractionation into a complete set of state variables (block F in figure III.1). First flush and transport in sewer blocks are not present in urine generation section as it is considered to be stored after generation and transported by trucks.

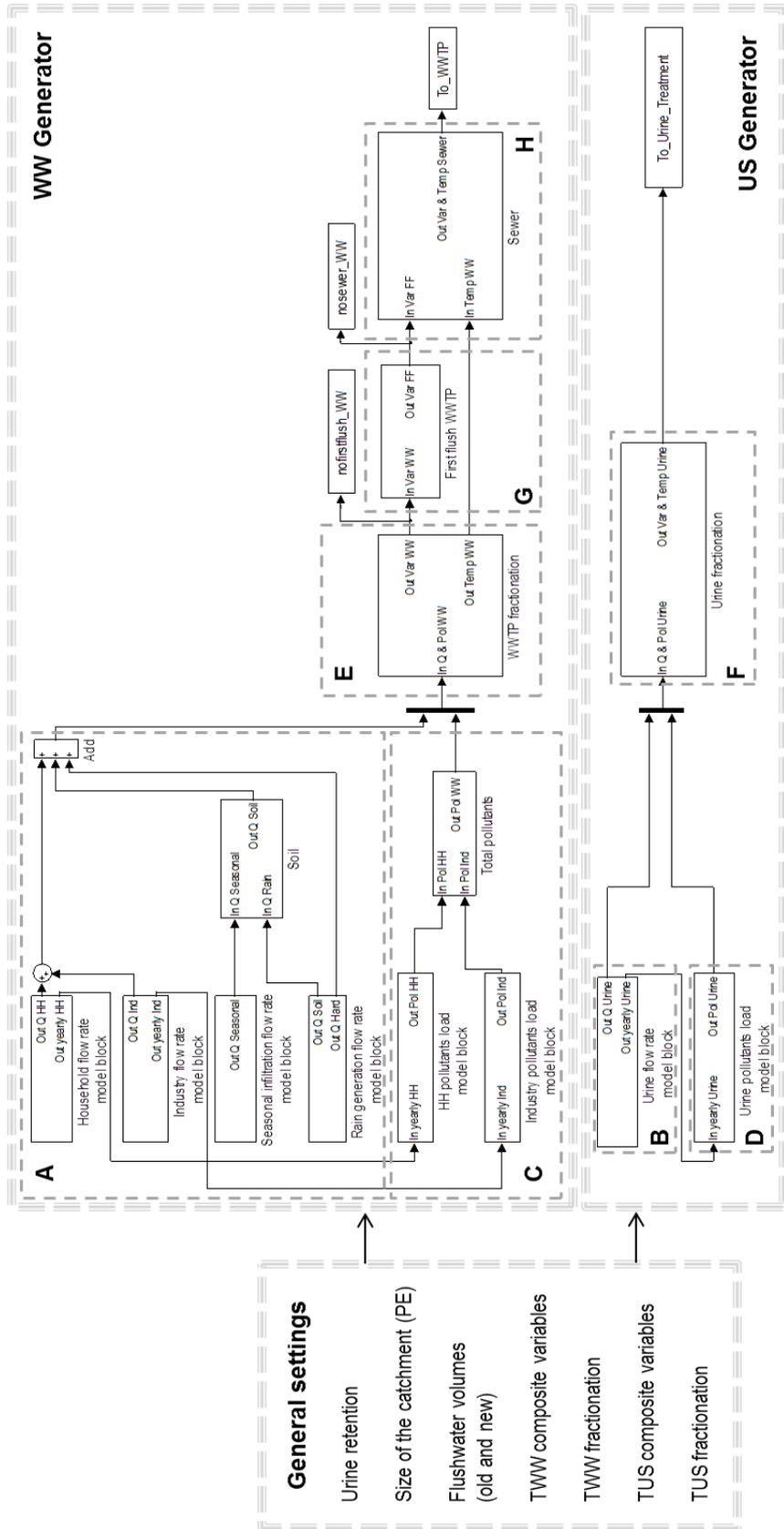


Figure III.1. General overview of the urine source separation influent generator

Details of each block will be given in the subsections below together with its main hypothesis. Blocks after fractionation (first flush effect and sewer transport) will not be discussed as they were not modified from the original version. Temperature for urine generated was considered to be the same as for conventional influent generated as a relatively long period of storage (and transport to the WWTP) is proposed. Finally, in order to easily explain the calculations done by the influent generator, a case study will be applied as an example in this study with the following characteristics: Urine is retained at a percentage of 50% and the catchment size is of 80,000 person equivalent (PE) for domestic contribution and industry represents approximately the contribution of 20,000 PE without urine retention. However, as discussed previously, the flexibility of the generator is preserved by using specific user setting parameters.

### **III.3. Flow generation**

Dynamics in flow generation considers all daily, weekly and yearly profiles. The chosen normalized profiles for flows generated in households are showed in figure III.2A for both wastewater and urine retained. This choice of using similar flowrate profiles for the US and WW is similar to the approach of Langergraber et al. (2008) that used a profile from a Fourier series for both domestic influent without urine and for the urine flow.

As showed in figure III.2A, both US and WW profiles followed a similar profile with comparable maximum and minimum values. However, a slightly delay is present in WW stream compared to US as normally flow peaks for the non-urine flowrates will arrive after pollutants (and consequently after urine generation) in a household. It has also to be noticed that the peaks arrives by the human activity hours (morning peak by 7-8am and afternoon peak by 4-6pm).

Considering weekly and holiday effects, those were considered to be the same for WW and US streams as they represent the “non-generation” of total wastewater in the household during these periods (reduction of 8% on Saturdays, 12% on Sundays and from 12-25% on holidays).

The considered total flowrate (TWW) from households is  $150 \text{ l.PE}^{-1}.\text{d}^{-1}$ . The urine flowrate is considered to be  $1.36 \text{ l.PE}^{-1}.\text{d}^{-1}$  according to a review on the published literature realized by authors (data not published). Moreover, in conventional toilets (without urine separation), the volume of water used per flush was considered to be of 5 l and of 0.15 l in urine diverting toilets per flush. Further, it is considered that each PE flushes toilet after urinating 5 times a day (STOWA, 2002). A summary of

input and calculated values for average flowrates are given in table III.1 with the proposed case study as example.

Finally, as showed in figure III.1, the total flow entering the wastewater treatment plant is composed not only of the household and the industry contributions; rain and seasonal variation of groundwater level are also comprised. The total flowrate entering the WWTP (WW) is thus obtained by the sum of previously described contributors and urine flowrate is obtained directly from urine model block. In average, household flowrate is supposed to represent 62% of the total flowrate entering the WWTP.

Table III.1. Input and calculated values for composite variables (case study of 50% urine retention)

Variables	Description	Units	Initialization		Calculated values based on the specified retention of 50%	
			TWW	TUS	WW	US
Q*	Flowrate	l.PE <sup>-1</sup> .d <sup>-1</sup>	150	1.36	136.82	1.055
CODsol	Soluble COD load	gCOD.PE <sup>-1</sup> .d <sup>-1</sup>	42	10.4	36.8	5.2
CODpart	Particulate COD load	gCOD.PE <sup>-1</sup> .d <sup>-1</sup>	78	0.78	77.61	0.39
TKN	Total Kjeldahl nitrogen load	gN.PE <sup>-1</sup> .d <sup>-1</sup>	13.33	9.78	8.44	4.89
SNH	Ammonium load	gN.PE <sup>-1</sup> .d <sup>-1</sup>	10	8.8	5.6	4.4
TP	Total phosphorus load	gP.PE <sup>-1</sup> .d <sup>-1</sup>	2.22	0.74	1.85	0.37
SPO4	Orthophosphate load	gP.PE <sup>-1</sup> .d <sup>-1</sup>	1.2	0.7	0.85	0.35
SNOx	Nitrite and nitrate load	gN.PE <sup>-1</sup> .d <sup>-1</sup>	-	-	-	-

\* The flowrate for TUS comprises only pure urine (without flush water) while the other streams already include flush water (a bigger flowrate that is present in TWW and is thus subtracted in WW; a small one that is added for US).

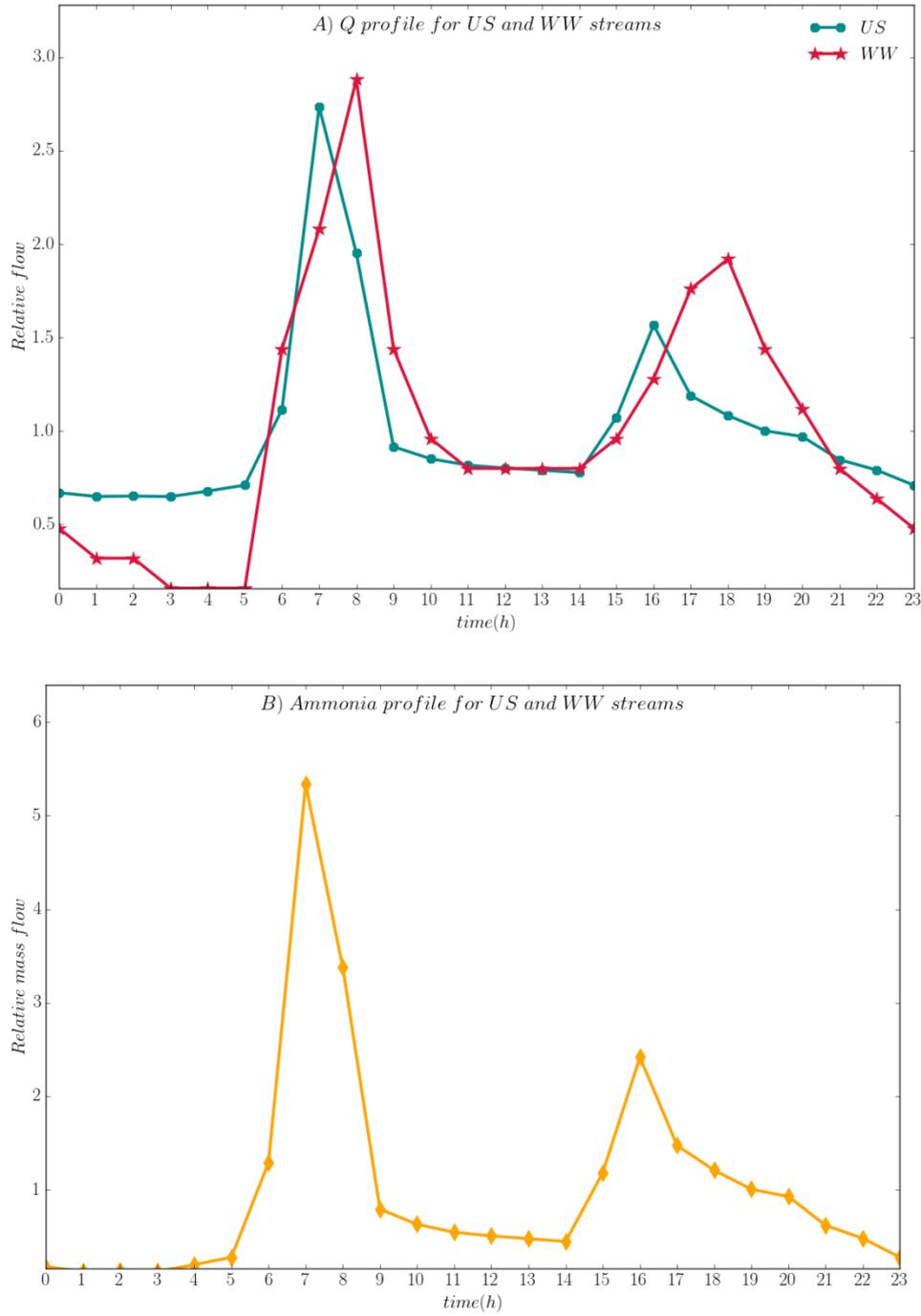


Figure III.2. Profiles for US and WW streams.

A) Daily flow rate profile; B) Daily ammonia mass flow profile

### **III.4. Pollutants generation**

#### *III.4.1. General aspects*

When considering the urine source separation in households, the most reliable way to determine the resulting load of pollutants present in each stream is to consider the total quantity of pollutants produced per PE (including urine and other contributors) as the average (non-dynamic) value is well characterized in literature as well as the values for pure urine. Therefore, the generation of pollutants followed some main steps: First, composite variables were specified for the total wastewater (TWW stream) and for the total urine stream (TUS) considering the total load of pollutants contained in the produced urine (retention of 100%). Following, according to the specified urine retention, new loads (of composite variables) are calculated for the domestic wastewater without urine – WW - and for the urine retained – US (Figure III.1, blocks C and D). Finally, fractionation was applied to final streams (WW and US, Figure III.1, blocks E and F) considering the total well known ratios for the fractionation of TWW and TUS in the recalculation of the new fractionation. However, considering that urine is only diluted when retained at source, fractionation values of TUS and US are the same; the same assumption is not valid for TWW and WW.

Finally, industry contribution is not extensively described as only slight modifications were done considering the original influent generator (pollutants are still calculated on a 20,000 PE basis; however it considers now the new values of pollutants per PE and profiles for phosphorus were also added).

#### *III.4.2. Composite variables*

The considered initial composite variables (soluble COD (CODsol), particulate COD (CODpart), TKN, Ammonium (SNHx), TP and Phosphate (SPO4)) are predefined in the generator from the literature being therefore adaptable for other case studies.

Considering the total wastewater without any urine retention, TWW, it was decided to base all calculations on the load of total COD, which was fixed to  $120 \text{ gCOD.PE}^{-1}.\text{d}^{-1}$ . This value is variable considering geographical location and more or less ecological lifestyles; however, this value is in the proposed range of 25-200 (Henze and Comeau, 2003). Further, ratios that are well known in the literature (Pons et al., 2004; Tchobanoglous et al., 2004; Henze and Comeau, 2003) were applied:

Total nitrogen/Total phosphorus = 6, Total COD/Total nitrogen = 9 and consequently Total COD/Total phosphorus = 54. Furthermore, other ratios were defined such 35% of soluble COD from the total COD, 75% of ammonium nitrogen in TKN, 54% of soluble phosphate in total phosphorus and no presence of nitrite and nitrate.

Accordingly, for a separation of 100% of urine, values were compiled from the literature and the model was fulfilled directly with loads per PE per day as, unlike TWW, TUS seemed to be less sensible to total loads than to ratios between variables.

Latter, composite variables were calculated for the specified urine retention as described previously. A summary of input values as well as calculated ones for a 50% urine retention are given in table III.1.

Considering dynamics, pollutants profile followed similar assumptions of flowrate profile variation. As the most important part of human pollutants generation are expected to happen more or less by the same time of morning and afternoon urine peaks, the same profile for WW and US in the generation of pollutants was applied. Accordingly, weekend effect and holiday effect were considered (reduction of 12% on Saturdays, 16% on Sundays and from 12-25% on holidays).

Figure III.2B shows the profile for ammonium flux profile. Dynamic profiles for other pollutants (composite variables) followed a similar profile and can be found in Supplementary Information. Finally, profiles for total phosphorus and phosphate (that are not originally used on ASM1 influent generator) were generated following the same profile of TKN and ammonium respectively.

After all, it has also to be noticed that urine has the exactly profile for flowrate and ammonium flux (peaks are superposed). This choice is mainly linked to the fact that urine is well represented by ammonium flux and that, as it is a human pollutant stream, it is expected to have variable flows with a more constant concentration in pollutants.

#### *III.4.3. Fractionation into state variables*

Figure III.3 details the fractionation block which is fulfilled with composite variables and generate state variables. As discussed previously, the modified version of the influent generator considers an extensive list of state variables: in general, variables are considered to be divided into soluble (S), colloidal (C) and particulate (X); also, biodegradable (subscript B) and unbiodegradable (subscript U) conditions are distinguished. A complete list of considered state variables is given in table III.2 together with its description, origin from composite variable and initialization values for the total

streams (TWW and TUS) and the specific urine retention case (50% retention – represented by WW and US) that will be discussed below.

In this study it was chosen to use a refined fractionation in order to achieve flexibility between the several platforms and models available nowadays. Following, a complete list is provided by the end and, in the case of a simulation using simpler state variables (such as when using ASM family models), state variables only have to be regrouped by the user in function of the model variables. Also, as it can be noticed in Table III.2, ions are also taken into account into the fractionation. This is especially important when source separation is considered as urine can be treated by several physicochemical processes and adding ionic species might add a realistic aspect to the process modelling.

The fractionation values for the total wastewater (TWW) and total urine (TUS) are illustrated in the Sankey graphics in figures III.4 (for COD), III.5 (for nitrogen) and III.6 (for phosphorus). For instance, starting from a total value of 100, variables are divided considering its chemical state (organic or mineral), physical state (soluble, colloidal or particulate) and biological state (biodegradable or inert). As previously discussed, fractionation values are established for total wastewater (TWW) and total urine (TUS) from the available literature and thus calculated for the two output streams (WW and US).

For instance, considering the COD fractionation, the composite variables already considered total soluble and particulate COD. Accordingly, in order to start the fractionation, a total inert part was defined and a colloidal part. Following, for the particulate part, ratios were applied to  $X_{OHO}$ ,  $X_E$  and  $X_U$ . Thus,  $X_B$  can be calculated by difference between the total particulate COD and the previously calculated particular species. Similarly, for the soluble and colloidal part, well defined ratios were applied to  $S_{VFA}$ ,  $S_{MEOL}$ ,  $C_B$  and  $C_U$ . Following, considering the total inert part in total COD previously described,  $S_U$  was obtained by difference with  $X_U$  and  $C_U$  (previously calculated). Finally,  $S_B$  is calculated by the different to the total soluble COD.

Similar assumptions were done for nitrogen and phosphorus ( $S_{NU}$  and  $S_{PU}$  were obtained by difference of inert N and P;  $S_{NB}$  and  $S_{PB}$  by difference of total organic N and P respectively).

Table III.2. Considered initial values for total urine stream (TUS), separated urine stream (US), total wastewater without urine retention (TWW) and wastewater with urine retention (WW)

Variable	Description	Unit	TWW	TUS	50% urine retention		
					WW	US	
Total COD	CODsol	S <sub>VFA</sub> Volatile fatty acids	gCOD.m <sup>-3</sup>	32.8	4359	22.1	2810
		S <sub>B</sub> Readily biodegradable substrate	gCOD.m <sup>-3</sup>	63.2	2630	59.2	1696
		S <sub>U</sub> Soluble unbiodegradable substrate	gCOD.m <sup>-3</sup>	30.0	657.8	29.8	424.0
	CODpart	C <sub>B</sub> Colloidal biodegradable substrate	gCOD.m <sup>-3</sup>	96.2	122.7	101.2	79.1
		X <sub>B</sub> Particulate biodegradable substrate	gCOD.m <sup>-3</sup>	288.0	368.7	302.9	237.7
		C <sub>U</sub> Colloidal unbiodegradable substrate	gCOD.m <sup>-3</sup>	19.2	20.6	20.2	13.3
		X <sub>U</sub> Particulate unbiodegradable substrate	gCOD.m <sup>-3</sup>	58.8	61.4	61.9	39.6
		X <sub>OH0</sub> Ordinary heterotrophs	gCOD.m <sup>-3</sup>	11.9	-	12.5	-
TKN	1	S <sub>NHx</sub> Total ammonia	gN.m <sup>-3</sup>	50.0	6471	34.2	4171
	Organic N	S <sub>NB</sub> Soluble biodegradable organic N	gN.m <sup>-3</sup>	7.0	504.9	5.9	325.4
		C <sub>NB</sub> Colloidal biodegradable organic N	gN.m <sup>-3</sup>	2.0	36.0	2.0	23.2
		X <sub>NB</sub> Particulate biodegradable organic N	gN.m <sup>-3</sup>	6.0	107.9	6.1	69.5
		S <sub>NU</sub> Soluble unbiodegradable organic N	gN.m <sup>-3</sup>	1.3	71.9	1.2	46.4
		C <sub>NU</sub> Colloidal unbiodegradable organic N	gN.m <sup>-3</sup>	0.1	-	0.1	-
		X <sub>NU</sub> Particulate unbiodegradable organic N	gN.m <sup>-3</sup>	0.2	-	0.2	-
TP	2	S <sub>PO4</sub> Orthophosphate	gP.m <sup>-3</sup>	6.0	514.7	4.9	331.8
	Organic P	S <sub>PB</sub> Soluble biodegradable organic P	gP.m <sup>-3</sup>	2.5	23.4	2.6	15.1
		C <sub>PB</sub> Colloidal biodegradable organic P	gP.m <sup>-3</sup>	0.6	1.4	0.7	0.9
		X <sub>PB</sub> Particulate biodegradable organic P	gP.m <sup>-3</sup>	1.9	4.1	2.0	2.6
		S <sub>PU</sub> Soluble unbiodegradable organic P	gP.m <sup>-3</sup>	0.1	0.5	0.1	0.4
		C <sub>PU</sub> Colloidal unbiodegradable organic P	gP.m <sup>-3</sup>	0.004	-	0.005	-
		X <sub>PU</sub> Particulate unbiodegradable organic P	gP.m <sup>-3</sup>	0.01	-	0.01	-
Ionic species	S <sub>CO2</sub> Total inorganic carbon	gCO <sub>2</sub> .m <sub>3</sub>	210.0	1.016 <sup>E+4</sup>	192.5	6548	
	S <sub>Ca</sub> Calcium	gCa.m <sub>3</sub>	47.5	168.2	49.7	108.4	
	S <sub>Mg</sub> Magnesium	gMg.m <sub>3</sub>	11.5	142.4	11.7	91.8	
	S <sub>Na</sub> Sodium (strong cations)	gNa.m <sub>3</sub>	86.5	2536	84.0	1635	
	S <sub>Cl</sub> Chloride (strong anion)	gCl.m <sub>3</sub>	180.0	3656	179.5	2356	

1: Ammonium

2: Soluble phosphate

Variables having a zero value were not included in the table (Endogenous products, other biomasses, nitrate and nitrite)

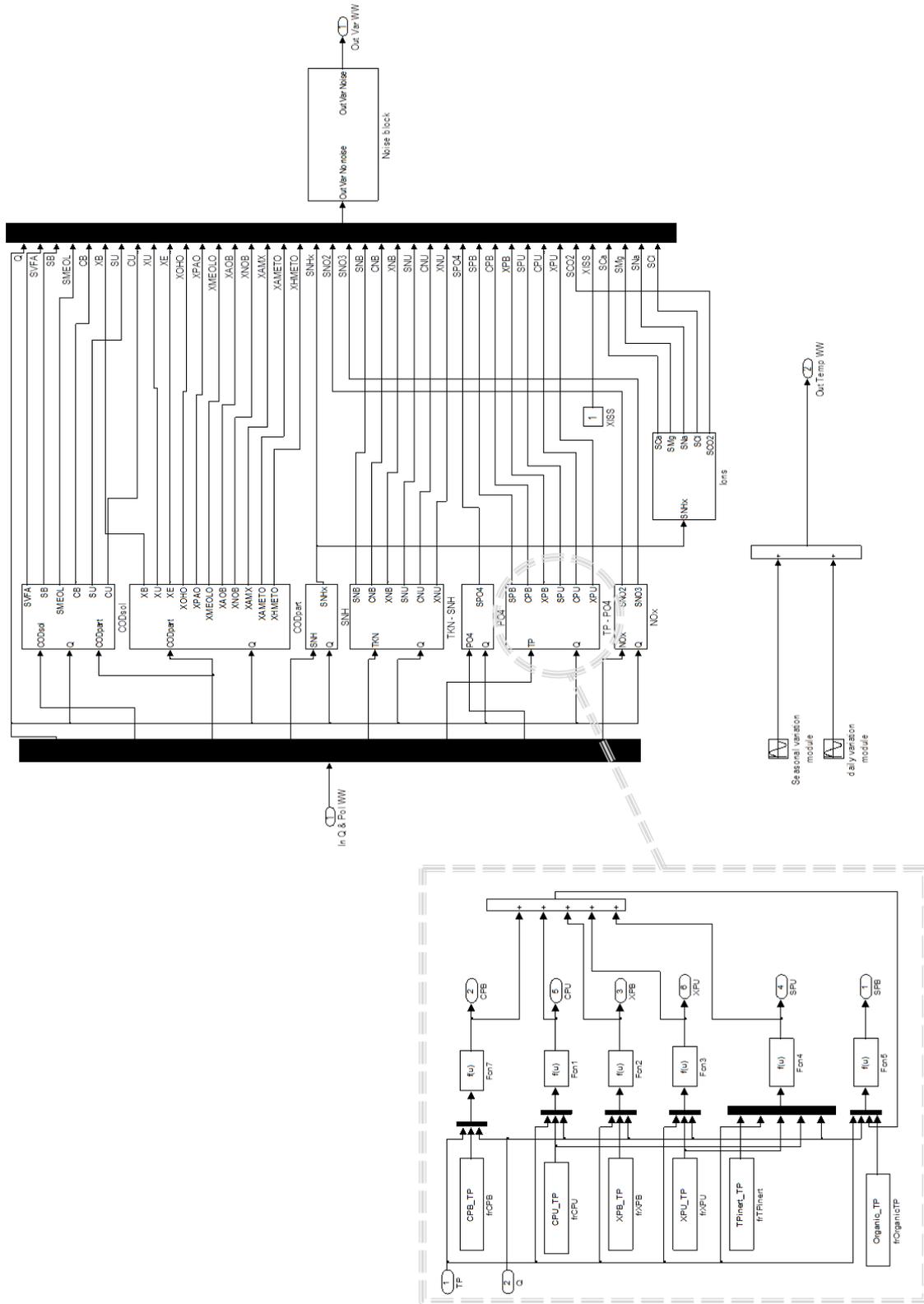


Figure III.3. Detail of fractionation block (E)

In order to define the fractionation values (especially for urine), some hypothesis were made based on literature and are listed as follows:

For urine 7% of the total COD is particulate (and colloidal) and thus 93% is considered to be soluble (Udert et al., 2013);

57% of soluble COD in urine is considered as VFAs (Udert et al., 2013) as urine is considered to be stored;

85% of COD in urine is considered to be easily biodegradable (Udert et al., 2006); An inert fraction of 9% is considered;

The ratio between particulate in colloidal and particulate is 75% and the hypothesis of 85% of biodegradable is applied to colloidal and particulate for both urine stream and wastewater.

Ammonium in urine is considered to be 90% of total nitrogen which is in accordance with values proposed by Udert et al. (2006) and STOWA (2002);

Soluble phosphate is considered to be 95% of total phosphorus in urine (Udert et al., 2006) ;

A fraction of 80% of soluble was applied to organic nitrogen and phosphorus for the urine stream;

Colloidal and particulate inert nitrogen and phosphorus are negligible in urine and thus not considered;

Even if stored urine is considered, precipitation was not included as it will be considered separately with its corresponding kinetics in a simulator when using the influent generated.

Regarding ionic variables, total inorganic carbon, calcium, magnesium, strong cations and strong anions (represented respectively by  $S_{CO_2}$ ,  $S_{Ca}$ ,  $S_{Mg}$ ,  $S_{Na}$ ,  $S_{Cl}$  as showed in table III.2) were considered following a ratio to  $S_{NH_4}$  (table III.3) and latter checked by electro neutrality in a simulator to verify if pH and alkalinity were consistent to real world values (US: pH=9.16, Alkalinity=0.289 eq.L<sup>-1</sup>; WW: pH=7.65, Alkalinity=0.0045 eq.L<sup>-1</sup>). The choice of using ammonium ion concentration profile in order to determine alkalinity and ions concentration profiles comes mainly from the fact that in the case of urine, bicarbonate will be generated by urea hydrolysis (that will also generate  $S_{NH_4}$ ). It has to be noticed that even if in some models ionic species will not be used, it is important to calculate them as the most part of urine treatment techniques are dependent of pH or specific ionic species.

Other general setting parameters consider the assumption from BSM2 that total suspended solids (TSS) are equal to 75% of the particulate COD and the conventional ratios between COD and Volatile Suspended Solids (VSS) for biomass (1.42), for  $X_B$  (1.8) and for  $X_U$  (1.3). Following the last assumptions, inorganic suspended solids (ISS) can be calculated (in the end, after sewer), by the difference between TSS and VSS.

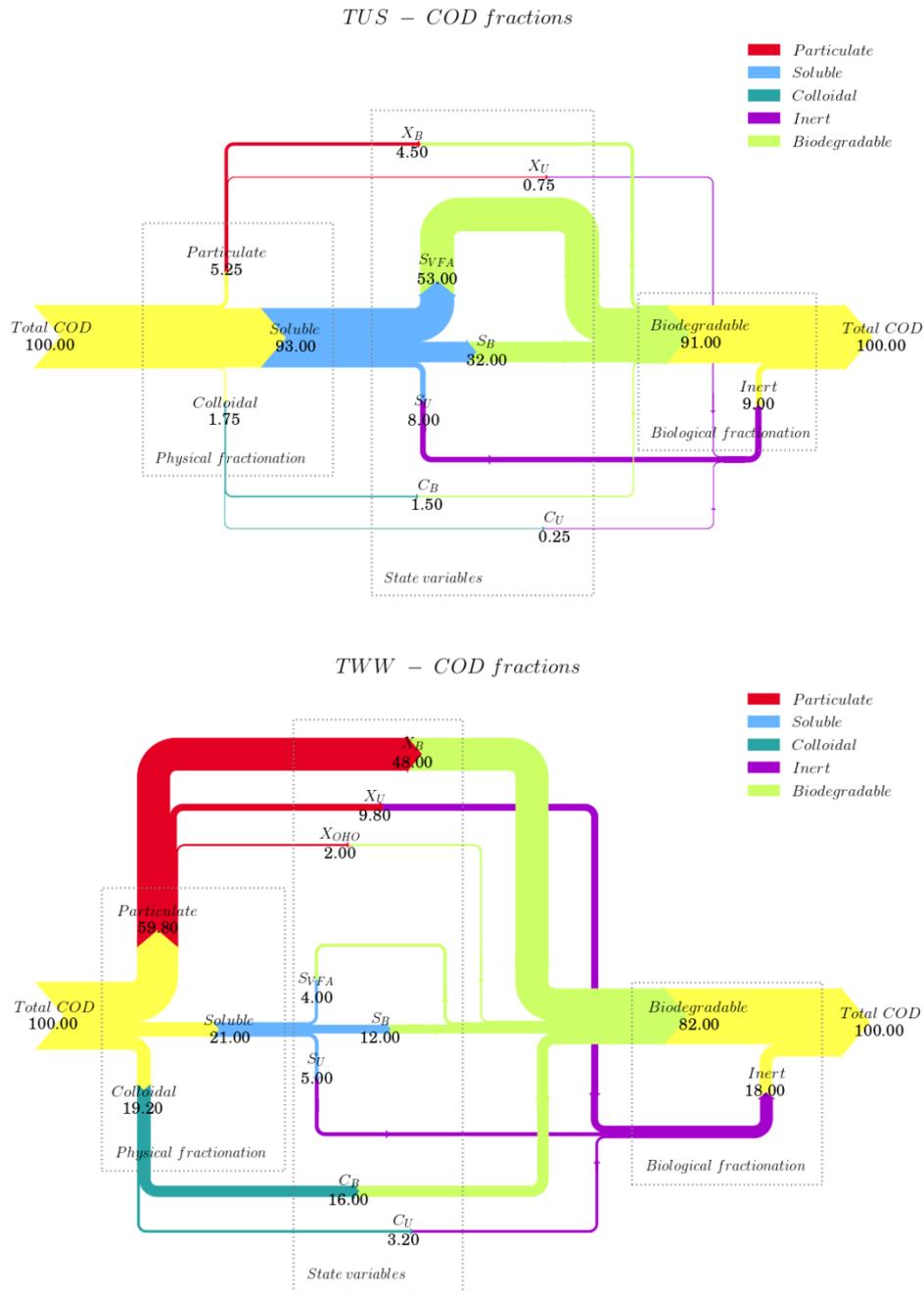


Figure III.4. Sankey diagram for COD fractions in urine versus COD in total wastewater

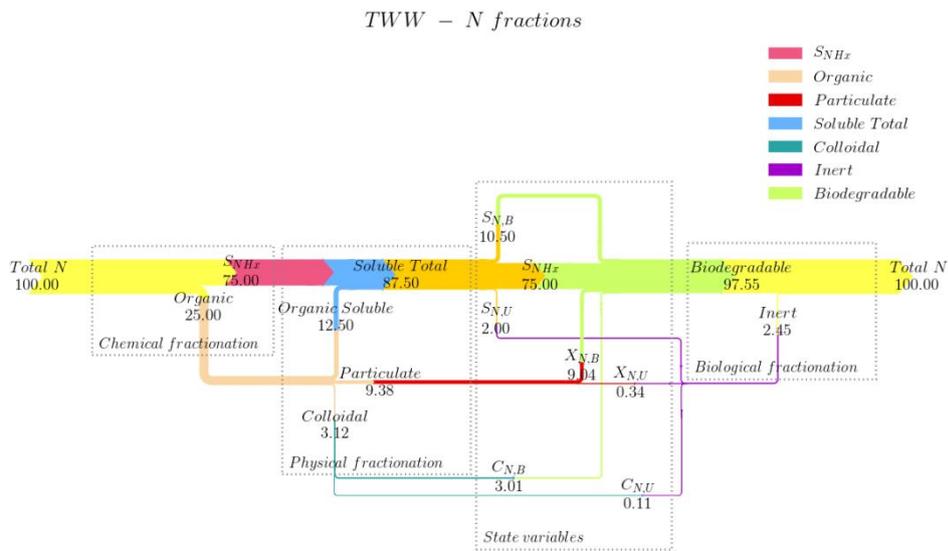
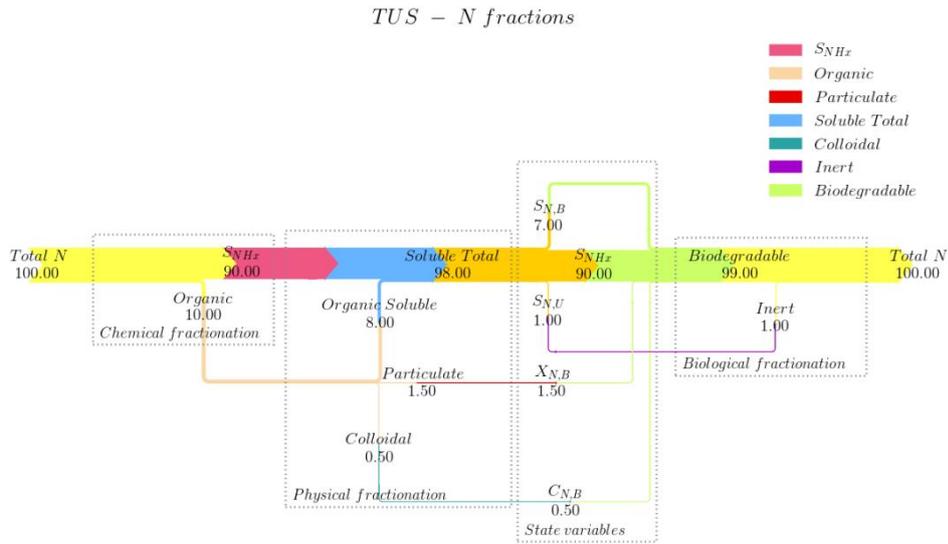


Figure III.5. Sankey diagram for nitrogen fractions in urine versus nitrogen in total wastewater

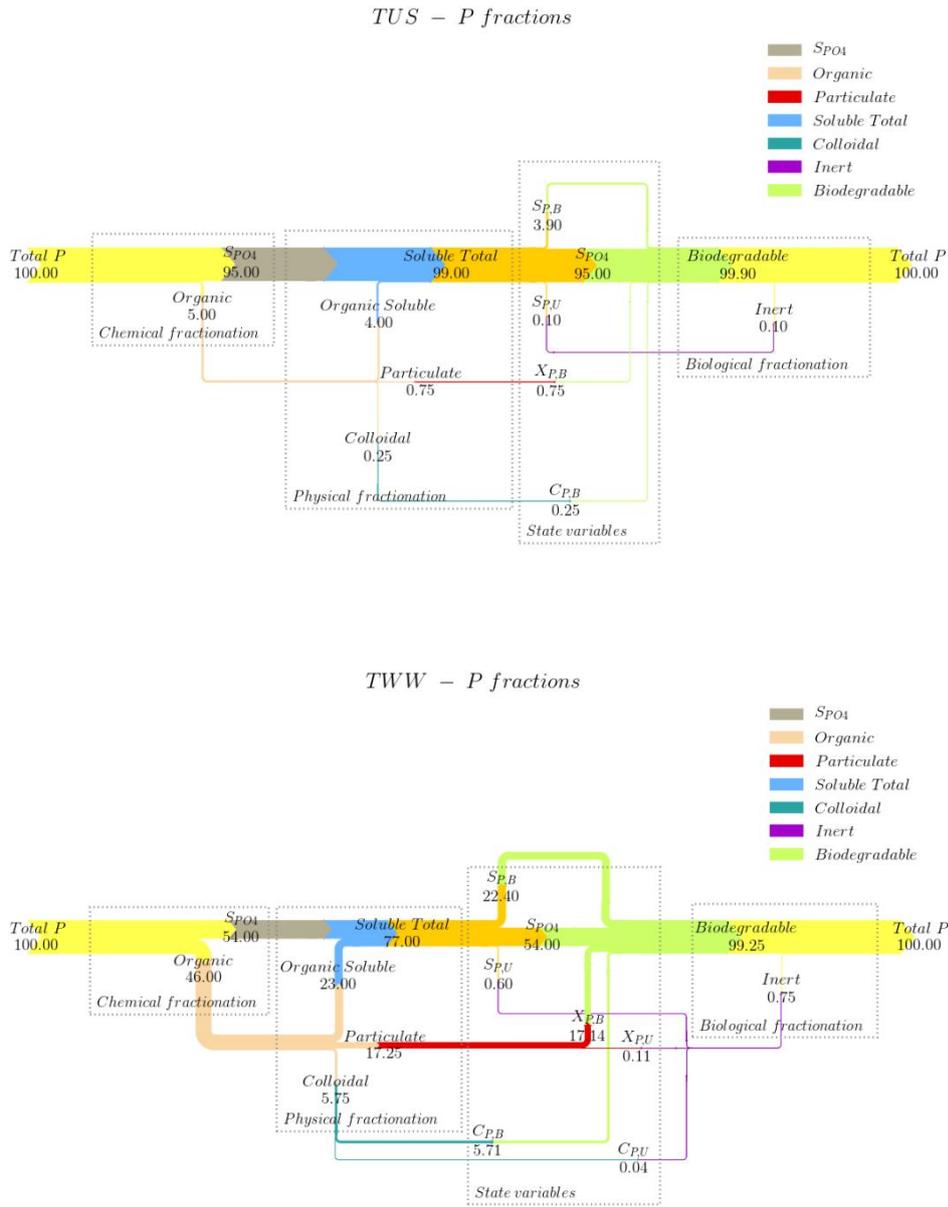


Figure III.6. Sankey diagram for phosphorus fractions in urine versus phosphorus in total wastewater

Table III.3. Ionic species molar ratio to ammonium for total wastewater and total urine stream

Variable	Ratio to $\text{SNH}_x$	
	TWW	TUS
$S_{\text{CO}_2}$	4.2	1.6
$S_{\text{Ca}}$	1.2	0.026
$S_{\text{Mg}}$	0.23	0.022
$S_{\text{Na}}$	1.7	0.39
$S_{\text{Cl}}$	3.8	0.56

### III.5. Noise addition

In order to add realistic conditions to the generated flows and avoid correlation between variables, noise was added to flowrates (domestic, industrial and rain flowrates) as well as to composite and state variables. This was done following the approach of Gernaey et al. (2011): a zero mean white noise is added using the random number block of Simulink that outputs a Gaussian distributed random signal. Attention was paid in order to select different seeds for each noise added and variance was calculated using a variation factor specified by the user that is multiplied to the average value and squared. Thus, this specified factor might be comparable to the percentage standard deviation. Also, the considered sampling time is of 15 min. Considered values for noise factors are given in table III.4 and can be easily modified in the influent generator code in order to represent other case studies.

Furthermore, following the addition of noise values, saturation blocks were maintained in order to limit the range of obtained values by fixing a lower and upper bound.

It has to be noticed that the chosen values for noise are related to the fact that flowrate, composite variables (flux) and state variables (concentration) from household are supposed to be more influenced by noise variation than urine and industry (this variation is not anymore linked to daily, weekly or yearly profile; however it represents the noisy variation of values). However, it has to be noticed that when considering the transport by truck to the plant, the user might add a storage tank and thus, daily dynamic is not any more important.

Table III.4. Noise factors considered in this study

<b>Parameter</b>	<b>Noise factor</b>
<b>Domestic WW flowrate</b>	0.15
<b>Industry flowrate</b>	0.05
<b>Urine flowrate</b>	0.05
<b>Domestic WW composite variables</b>	0.1
<b>Industry composite variables</b>	0.1
<b>Urine composite variables</b>	0.05
<b>WW state variables</b>	0.1
<b>Urine state variables</b>	0.01

### III.6. Example of simulations obtained with the generated influent

The use of the obtained dynamic influent was analysed in two different ways. The first simulation consists of using two different models, ASM1 and the wide-plant model Sumo1 from SUMO (Dynamita, 2015). The case of 50% of urine retention was considered for both models. The second simulation consists in the comparison of different urine retention percentages. For this comparison, influents were dynamically generated and following fulfilled to the simulator (using the Sumo1 wide-plant model). For both case studies, the water line was simulated in order to obtain the impact on the most important WWTP parameters that might be influenced by the urine separation.

The simulated WWTP consists of a MLE (Modified Ludzack-Ettinger) process with 2 anoxic tanks (total volume of 3000m<sup>3</sup>) and 3 aerobic ones (Total volume of 9000 m<sup>3</sup> with fixed DO of 2 g.m<sup>-3</sup>) similarly to BSM1. Also, a secondary clarifier with fixed solids removal efficiency was simulated, the internal recycle was set to approximately 300% of influent flowrate and the SRT was fixed to approximately 15 days.

The simulation was conducted dynamically during 2 weeks with an initialization on steady state for each case study with the corresponding non-dynamic influent.

It has to be noticed that as ASM1 model does not consider either inert nitrogen or phosphorus species, those were not added to the adapted ASM1 influent. In order to obtain ASM1 correspondent influents, state variables were adapted as showed in Table III.5. Additionally, in order to be comparable, kinetic and stoichiometric Sumo1 parameters were modified to be in accordance with those from ASM1 (Henze et al., 1987).

Finally, when considering different levels of urine retention, percentages of 0% (no urine separation), 20%, 50%, 80% and 100% (all urine is retained in households) were studied.

Table III.5. Adapted inputs for ASM1 simulation

ASM1 state variables	Influent generator state variables
$S_I$	$S_U$
$S_S$	$S_{VFA}+S_B+S_{MEOL}$
$X_I$	$X_U+C_U$
$X_S$	$X_B+C_B$
$X_{B,H}$	$X_{OHO}$
$X_{B,A}$	$X_{AOB}+X_{NOB}$
$X_P$	$X_E$
$S_{NO}$	$S_{NO_2}+S_{NO_3}$
$S_{NH}$	$S_{NH_x}$
$S_{ND}$	$S_{NB}$
$X_{ND}$	$X_{NB}+C_{NB}$

## III.7. Discussion

### III.7.1. Average results

Initially, as expected, the effect of recovering urine does not influence mainly the new flowrate entering the WWTP. However, the effect in state variables is markedly present. As an example, the effect of 50% of urine retention in the wastewater inputs (considering the concentration of state variables in average) is presented in Figure III.7. The most important reductions are to be considered, especially regarding soluble COD (mainly VFA - 36%), total nitrogen (29%) and total phosphorus (13%). Considering N reduced species, important abatements are obtained in ammonia (35%), as urine is the main contributor of this pollutant entering the WWTP. However, the biodegradable and the inert soluble organic forms of nitrogen are also well reduced (by 20% and 15% respectively). Following, phosphorus species reductions are mainly due to soluble phosphate (23%).

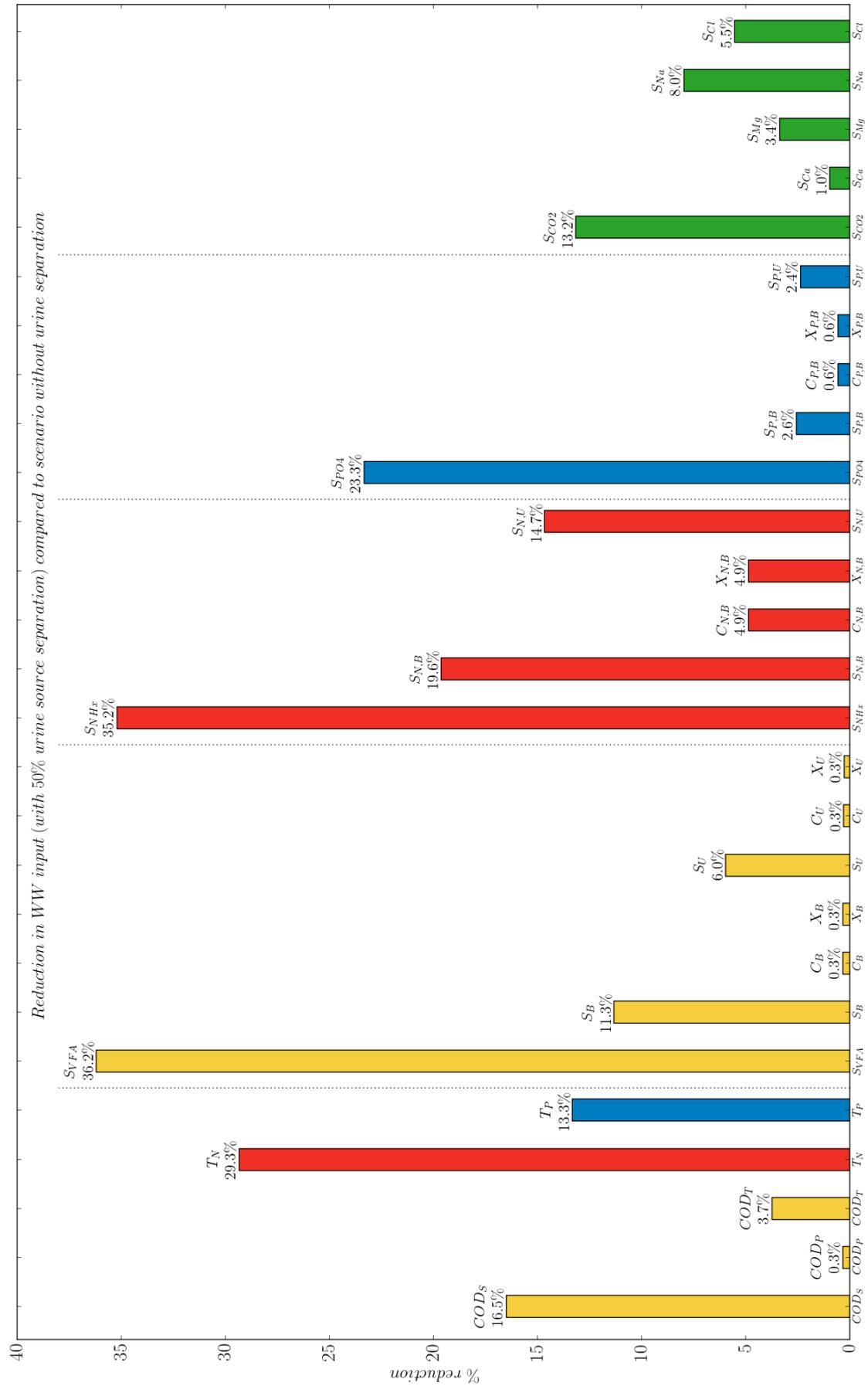


Figure III.7. Reduction of WW input variables when considering 50% urine source separation

It has to be noticed that values of major species present in urine, ammonia and phosphate, were initially expected (according to the literature) to decrease more than the previously showed values as, according to Larsen and Gujer (1996), urine contributes to 88% of TKN and 57% of TP in wastewater. This effect is due to the fact that industry represents a contribution of 20% (and thus when separating 50% of urine in households, in reality, only 40% of a urine corresponding stream is separated) and values for a non-ecological life style (important quantities of N and P in households comes from other sources rather than urine) were adopted and thus the total urine contribution is less important to the total wastewater pollutants than the described in some case theoretical case studies in literature (in this study: 73% of TKN, 88% of ammonia, 34% of TP and 58% of phosphate comes from urine – cf. table III.1).

### *III.7.2. Daily and weekly profiles*

The obtained dynamic profiles for both wastewater input (WW) and urine stream (US) for the simulated case of 50% of urine retention are showed in figure III.8 (Weekly profile of flowrate as well as daily variation of  $S_{VFA}$  and  $S_{NHx}$ ). Also, the average value of each variable is showed in coloured boxes together with its coefficient of variation (percentage).

When comparing any of the presented profiles for US and WW it can be seen that the variance of WW flowrate is smoothed in relation to urine stream. This is due to the addition of the sewer effect in the WW stream that is not applied to urine stream. Also, as discussed previously, a small delay is present in WW flowrate in relation to USS flowrate profile and to the pollutants profiles in order to account correctly for the generation of a mass of pollutants against a latter volume of diluted wastewater.

Also, when analysing pollutants, the dynamic profile (with the morning and afternoon peak for daily dynamics and the weekend effect for the last two days of the week) is markedly present for all pollutants in WW stream. However, this effect is less evident in urine concentration. This is in accordance to the assumption described previously that urine pollutants concentration are not assumed to vary importantly during the day (this assumption can also be checked by the coefficient of variation that is more than two times less important for the urine stream).

Finally, the addition of noise achieved the effect of decreasing the correlation between variables and thus the generated influent represents better real life influent streams.

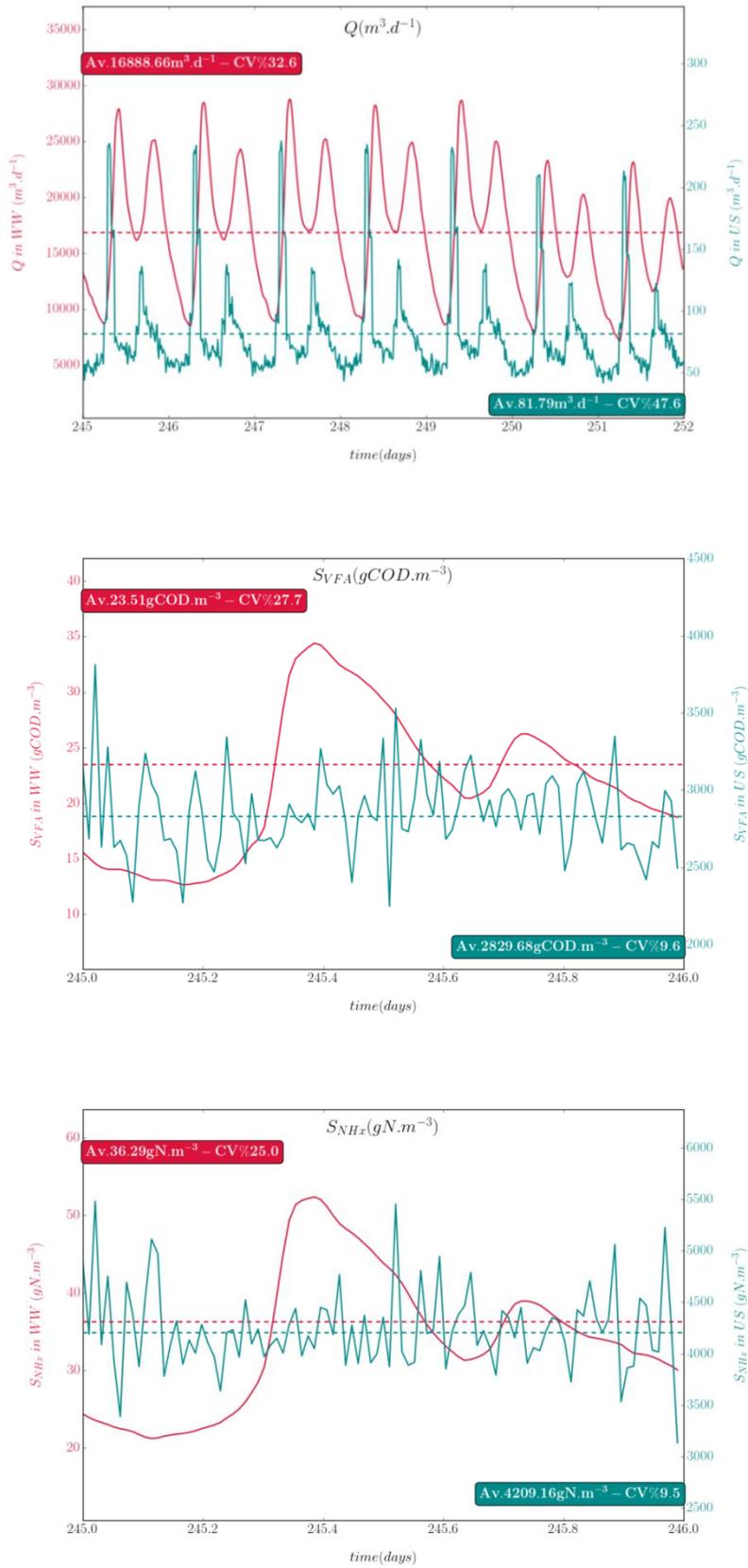


Figure III.8. Weekly profile of flowrate; Daily variation of  $S_{VFA}$  and  $S_{NHx}$

### **III.8. Use of the generated influent for process simulation**

In order to verify the applicability of the generated influent to a simulation platform, two different case studies comparison were done. The first consists of evaluating the feasibility of using the generated influent with 50% of urine retention to fulfil two different types of model (wide-plant models versus ASM family models). The second comparison case study is based on different urine retention percentages that are evaluated according to different performance parameters and operational requirements.

#### *III.8.1. Comparison between different models*

According to the flexibility idea of the influent generator, general results for the simulation using the wide-plant model Sumo1 are proposed in figure III.9 together with the ones generated by using ASM1.

Results for the considered operational parameter, airflow input, showed to be very similar for both models. Even when calibrated, effluent outputs present a small difference that is explained by the different model approach itself. As it can be noticed in figure III.9, peaks are smoothed in Sumo1; however, the average result is similar. Furthermore, results showed that the generated influent might be used for both platforms. In the case of ASM1 model, a sum of the originally proposed state variables in the influent generator is required in order to obtain the correct input variables.

Finally, none of the discussed simulations were sensitive to either phosphorus treatment or ionic species. Indeed ASM1 does not consider those species and the processes which could be sensitive to those species were not considered in simulations with sumo1 model as well. Basically the addition of phosphorus removal modelling would be more sensitive to ionic species and this could be the case of future extended simulations.

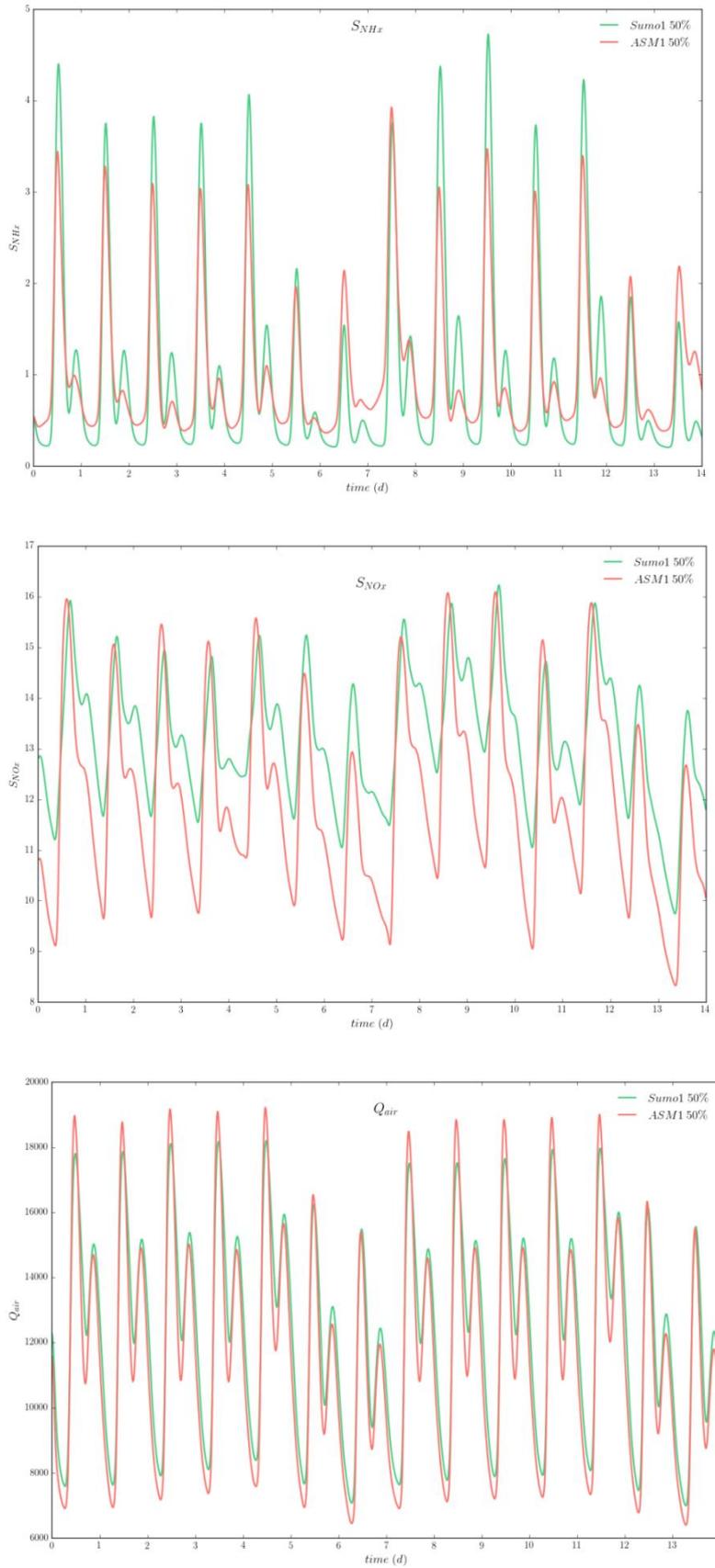


Figure III.9. Performance (Effluent ammonia and effluent nitrate and nitrite) and operational (Air flowrate) results for Sumo1 and ASM1 models

### *III.8.2. Effect of urine retention levels*

Comparison results between different urine retention percentages are showed in figure III.10. Scenarios consisting of no urine retention, 20%, 50%, 80% and the total urine retention in households were compared.

Results showed that even the retention of only 20% of urine is already capable of shaving the ammonia peaks importantly. When increasing the urine retention and achieving 80%-100% of separation the distribution of ammonia output in the WWTP is almost smoothed without any more peaks. An important reduction in air flowrate due to reduction of oxygen needs for nitrification was also noticed as a consequence of reducing the ammonia input peaks. Finally, NO<sub>x</sub> (nitrate and nitrite) output is also markedly reduced and the difference between the minimum and the peak value is also importantly reduced. This leads to two major consequences: more stable outputs in the plant could be achieved and potentially, the size of the WWTP can be reduced.

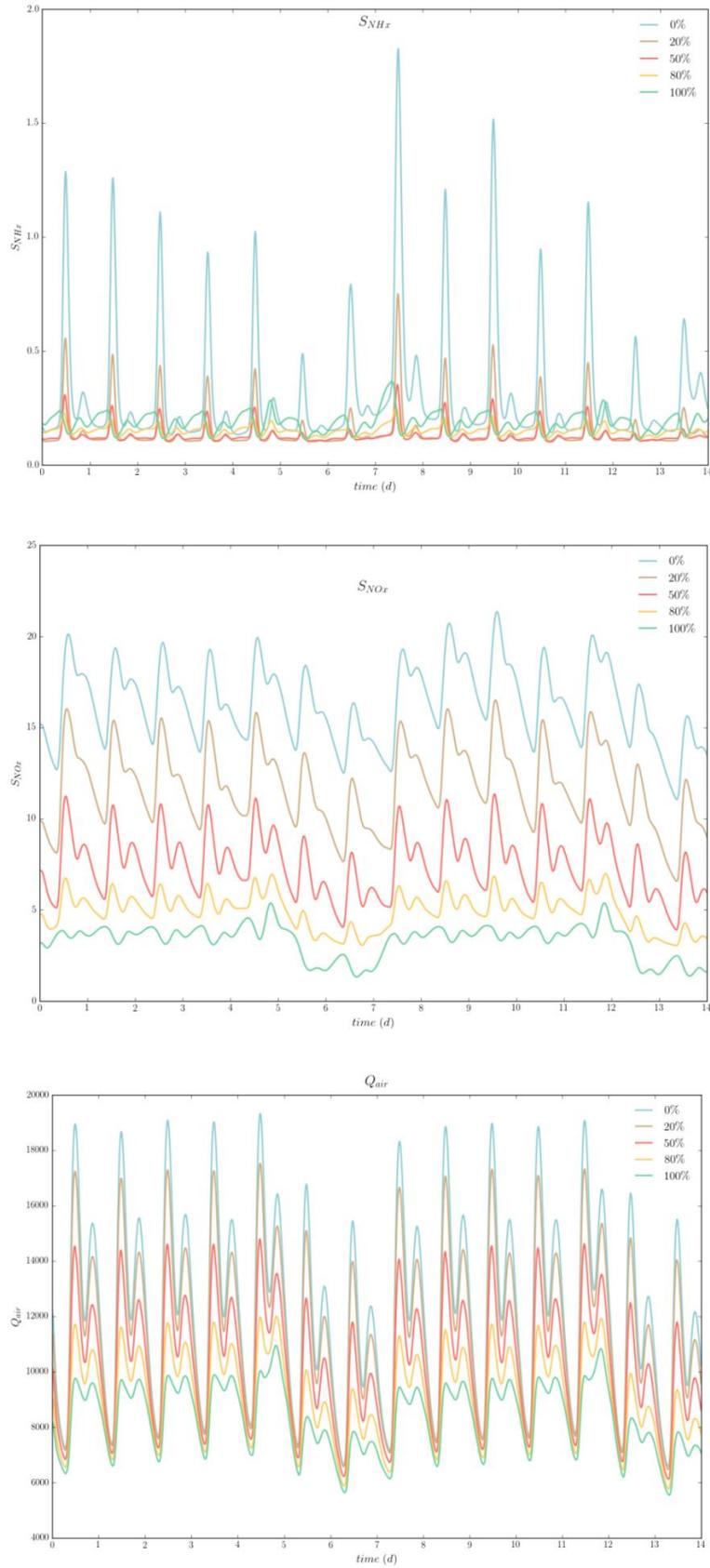


Figure III.10. Comparison of different urine retention levels considering performance (Effluent ammonia; Effluent nitrate and nitrite) and operational (Air flowrate) results

### III.9. Conclusions

Influent generators are a non-expensive and a low time consuming way to obtain input data for modelling and simulation instead of traditional sampling campaigns. This is especially true when non-conventional modifications are aimed to be evaluated and thus there is a no real world installation where measurements can be done neither it is a laborious task. However, considering dynamics and predictive data is a bottleneck of this kind of approach.

The proposed modified phenomenological influent generator for the case of urine source separation allows the evaluation of this alternative scenario of wastewater management and treatment at different urine retention levels in a reliable way and considering a wide view as both urine and wastewater streams are considered.

Moreover, due to its flexibility, if other alternatives in wastewater management are envisaged such as different retention levels or even other separation scenarios (e.g.: ammonia releasing in the sewer during the night, black water separation, unconventional greywater treatment) the tool is flexible enough and it is easy to modify the hypothesis to generate other streams. Following on the flexibility of the influent generator, the use of an extensive set of state variables allows simulating with different models such as the compared ASM1 model against the Sumo1 wide-plant model.

The important benefit of urine separation is demonstrated by dynamic simulation of a typical WWTP, reducing the daily nutrients peak load, improving the quality of rejected water, and reducing the energy needs for aeration. Finally, results showed that the tool is able to generate dynamic, long-term and predictive data for both urine and wastewater streams. The tool is now available for future simulations including innovative wastewater and urine management scenarios and optimization of plant design and operation depending on source separation level.



# **Chapter IV. Feasibility of Multi-Objective Optimization**



*“The formulation of the problem is often more essential than its solution, which may be merely a matter of mathematical or experimental skill.” (Albert Einstein)*

When considering the high environmental restrictions on the discharge of polluted waters and the strengthening of regulation laws, the process optimization becomes a potential solution, both to compromise between different treatment technologies (conventional and innovated) and to readjust the operating conditions of plants up to their optimal functioning level.

When an automated tool is available for the quantification of performance, costs and environmental impacts such as the previously described platform, one might want to analyse a wide range of available scenarios and operational alternatives. However, given the rigorous and time-consuming aspect of dynamic simulators, the problem might easily become expensive and complex to solve, with considerable requirement in terms of computational budget and calculation time. As function simplifications were avoided in order to provide realistic and predictive WWTP model, the optimization approach has now to deal with an expensive simulation-based problems. Therefore, efficient algorithmic techniques must be used to obtain the optimal results with markedly reduced number of simulation runs (or what we call the computational budget in the present thesis).

In the context of optimization, the quality of optimal results is expected to depend directly on the relevance of problem formulation. A wide review on optimization of activated sludge systems in WWTPs was provided by Hreiz et al. (2015) through which the problem formulation has been recognized as one of the major element to ensure the quality of optimal solutions. The same authors (Hreiz et al., 2015) stressed the main challenges when conducting a WWTP optimization. According to the authors, besides tackling the mismatches between the modelling and the real world results and the unpredictable variations in wastewater inputs, it is important to consider the slow dynamics of the plant and the correct formulation (flowsheet, decision variables, objective functions, constraints and flowsheet) of the problem to achieve reliable results.

The study of feasibility was conducted considering 3 objective functions: operational cost (represented by OCI), effluent quality (represented as the quantity of rejected pollutants by EQI) and environmental impacts (LCIA). EQI were based on standardized correlations proposed by the Benchmark Simulation Model N°2 Group and represent an effort of considering also ecological aspects as, for instance, rejected TKN and ammonium ions have different weights in order to move towards non ammonium species. OCI was based on plant expertise from industrials and literature in order to reflect the real world conditions. Finally, LCIA results consider, as previously described in chapter 2, the whole life cycle of the system (foreground and background emissions as well as avoided ones). Moreover, the impact of adding constraints is analysed on the basis of European reject limits. Moreover, the

feasibility study was conducted using an alternative scenario (with urine source separation and its treatment by struvite precipitation and nitrification/ anammox) to ensure the optimization of a more complex problem than the conventional WWTP by ASP.

Once an optimization problem is properly structured and formulated, the second critical step is the choice of resolution method. Rigorous modelling allows a better understanding of the interactions between decision variables and therefore, the results are more realistic and represents the real efforts to be made in order to improve the system and its functioning. However, the consideration of highly non-linear dynamic models that represents processes operating at considerably different rates - for instance, the biological and chemical reactions - makes the resolution of the whole system a stiff task.

Additionally, a crucial condition has to be fulfilled, that is to ensure the global optimality of obtained solutions. In this case, genetic algorithms are a good option as, besides ensuring the global optimality, they do not require derivative information to optimize a function, due to their stochastic mechanism of search. Moreover, they are adapted for black-box or simulation-based systems with noise. In simulation-based systems, noises are mainly due the use of a fixed tolerance to approve the convergence of each simulation run.

However, the use of genetic algorithms in their original form to solve expensive optimization problems is completely irrelevant, due to their considerable requirements in terms of computational budget. That's the reason why in the present work a novel hybrid evolutionary algorithm, called AMOEA-MAP and developed by Ahmadi et al. (2016), was used to deal with expensive optimization problem.

This chapter provides, in fact, a feasibility study - from computational time and reliability perspectives - of an efficient multi-objective approach to optimize alternative wastewater management and treatment plants with integrated LCA and rigorous dynamic modelling. This chapter has been recently accepted for publication in the journal of Chemical Engineering Research and Design.

## **Entitled of the paper: Feasibility of rigorous multi-objective optimization of wastewater management and treatment plants**

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### **Abstract**

The present paper describes a study on the feasibility of coupling rigorous dynamic modelling (DM) and its extended boundaries through life cycle assessment (LCA) with an efficient multi-objective optimization (EMOO) tool. The combined framework (DM-LCA-EMOO) was then applied to a real-world dynamic system: the wastewater treatment. To give a global view of all environmental, economic and technological performance, three objectives were considered: Effluent Quality Index (EQI), Operational Cost Index (OCI) and environmental impacts quantified through Life Cycle Impact Assessment (LCIA). Legally imposed constraints, including total nitrogen, total phosphorus, total chemical oxygen demand, total suspended solids and ammonium ion were also taken into account. Given the contradictory nature of objectives, the presence of constraints and the time-consuming simulation-based calculations, an efficient multi-objective optimization framework, namely Archive-based Multi-Objective Evolutionary Algorithm with Memory-based Adaptive Partitioning of search space (AMOEAMAP) was used. The practicality of such a combined DM-LCA-EMOO tool for the evaluation of wastewater management and treatment was then addressed and demonstrated through a case application.

*Keywords: LCA-integrated dynamic modelling, expensive multi-objective optimization, WWTP*

## IV.1. Introduction

Wastewater treatment plants (WWTPs) are a complex combination of biological, chemical and physical processes aiming to minimize damages caused by sewage discharge. Besides the variety of compounds to be treated (soluble, colloidal and particulate compounds that might be biodegradable or not), current directives are nowadays imposing stricter reject limits especially for nitrogen and phosphorus. Additionally, the conventional wastewater management, where several streams of wastewater are mixed, do not lead to an integrated solution as pollutants are diluted and nutrients recovery is complicated to accomplish (Balkema et al., 2002). To achieve an adequate performance together with minimum costs, there is an important need for optimal integration of these unit processes.

However, WWTPs have traditionally been optimized considering only cost and quality performance aspects. The inclusion of sustainable criteria in the choice of plant operation has some challenging points such as the inclusion of the background processes by extending the life cycle boundaries of the system, the assessment of all economic, environmental and social spheres and the choice of the appropriate indicators to quantify the achievement of objectives targeted (Azapagic et al., 2006).

Following the increasing interest for more sustainable processes, one should consider the quantification of the gains and the drawbacks of each alternative considered. Among the available methodologies to assess the sustainability of processes, Life Cycle Assessment (LCA) presents the advantage of taking into account the full process lifetime and thus the cumulative effect of emissions from foreground and background processes.

When conducting a complete LCA, it is fundamental to evaluate the inventory emissions during the whole process lifetime. While background data can be obtained from databases, foreground data inventory is usually obtained by data collection at the plant. However, given the interaction between a great number of parameters, possible scenarios and treatment objectives, data collection cannot be used for outlining general trends or for process optimization. Modelling and simulation is thus an interesting alternative that can be very useful when predictive results or eco-design proposals are sought (Mery et al., 2013).

Numerous LCA-integrated modelling have been published so far in several fields, comprising the water field. In the wastewater field, for instance, Corominas et al. (2013b) evaluated the environmental impact of strategies for nutrient removal in WWTPs by considering LCA, while Flores-Alsina et al. (2010) conducted a study of control strategies in a plant where environmental impacts through LCA were evaluated together with economic, technical and legal criteria. With a view to LCA-based

process evaluation, Foley et al. (2010) used steady state simulation results obtained from Biowin® for a systematic evaluation of several WWTP scenarios using LCA; Further, Mery et al. (2013) developed a LCA-integrated process modelling tool, named EVALEAU dedicated to the environmental evaluation of drinking water treatment processes and Loubet et al. (2016) proposed a framework for the modelling of urban water systems coupled to LCA for assessing its environmental impacts according to the services provided.

In a previous study, Bisinella de Faria et al. (2015) developed a LCA-integrated dynamic modelling applied to WWTP scenarios in order to obtain reliable and predictive LCA results. The framework allowed evaluating the environmental performances of different treatment scenarios together with its performance in an automated way, leaving the possibility to be subsequently used for other case studies. Accordingly, two main research streams - one generic to eco-design independently of the application, and the second specific to the field of wastewater management – remain to be further explored: (1) a practical integration of LCA calculation and dynamic process modelling with an efficient Multi-Objective Optimization (MOO) framework for appropriate process evaluations within a reasonable calculation time, (2) the achievement of reliable globally optimized performance in wastewater management with reduced costs.

With a view to the first stream, efforts have been made in the most diverse fields to consider environmental aspects in the multi-objective optimization of process and specifically, using LCA to quantify these impacts. Ahmadi and Tiruta-Barna (2015) presented an approach to combine process modelling, LCA and MOO applied to potable water resulting in a set of alternative solutions. Carreras et al. (2015) applied a MOO in order to optimize the building insulation thickness considering economic and environmental impacts using the evolutionary algorithms. Guillen-Gosalbez and Grossman (2010) proposed a modelling and computational framework in the MOO of sustainable chemical supply chains and the effect of uncertainty in the environmental evaluation. Zhang et al (2015) presented the optimal design of microgrids using  $\epsilon$ -constraint and weighted sum method for both environmental (using LCA) and economic concerns. Tascione et al (2016) proposed a coupled approach of LCA and linear programming to identify the optimal scenario for integrated waste management. Khoshnevisan et al (2015) studied the combined LCA and genetic algorithm applied to crop systems. Miret et al. (2016) proposed an approach that integrates, besides economic and environmental aspects, the social context in the MOO and the goal programming to solve the problem applied to bioethanol supply chain. In all works mentioned, the mathematical programming and the complexity related to its resolution as well as the calculation time can be seen as the most critical limitations.

Considering the second stream, Hreiz et al. (2015b) proposed a review of the available literature on optimal design and operation of Activated Sludge Processes (ASP). Authors highlighted that the

optimality of results depends on the problem formulation. Unfortunately, there is no standardisation either on cost functions or on constraint selection (in order to respect feasibility along with physically relevant operations and on the uncertainty of models). Process dynamics is also an important aspect to be taken into account for the achievement of a sustainable functioning and for an appropriate consideration of units with slow dynamics.

In the field of wastewater treatment, some interesting approaches in MOO can be mentioned. Hakanen et al. (2011, 2013) proposed an interactive optimization tool for the wastewater treatment plant design where decision-maker can express his preferences for the optimal solution while better understanding the problem. Iqbal and Guria (2009) presented the optimization of a WWTP from both single and multi-objective points of view (using thus SGA-II and NSGA-II) being the first authors to apply this MOO technique to this field. Three objective functions were considered in their study: maximization of influent flow rate, minimization of exit BOD and minimization of operational costs. Egea and Garcia (2012) have proposed to use advanced metaheuristics in order to tackle the optimization of a benchmark WWTP showing that this approach is capable of overcoming the multimodality and noise problems that appeared when a dynamic operation is supposed. Similar approaches on the optimization of WWTP have been widely discussed in the literature (Beraud et al., 2008; Costa et al., 2011; Hreiz et al., 2015a; Guerrero et al., 2012; Fu et al., 2008), nevertheless to the best of authors' knowledge, there has usually been lack of information on non-conventional treatment scenarios and on the multi-objective optimization of full plants with regard to the time consuming issues of such computation (long time is necessary due to units with slow dynamics). Moreover, there is also no information available on optimization by considering environmental impacts together with water quality and operational costs. As showed in a previous study, background processes and recovery strategies (for instance, avoided raw material requirement when nutrient recovery takes place) present high impact values for several impacts categories (Bisinella de Faria et al, 2015) and should thus be considered for a further improvement of functioning conditions.

When adding up different - usually conflicting - objectives in an optimization, it is recommended to handle it through a multi-objective optimization (MOO) approach rather than aggregating objectives into a single composite objective to be optimized. This is because a MOO context primarily allows the decision-maker to obtain more than only one possibility as scenario, and additionally when a single composite objective is used, the quality of optimal result is directly proportional to weighting factors used for the aggregation of objectives. A MOO approach is especially interesting in the case of WWTPs as the objectives are conflicting by nature and the optimal solution for a given context may be different in another future context. However, traditionally, WWTPs have been optimized using single objective optimization in view of minimising for example a total cost function. As discussed by Hakanen et al. (2013), this approach may lead to loss of information and interdependencies between

functions. Moreover, obtaining a non-dominated Pareto front (composed of a set of non-inferior solutions) allows the decision making process to be independent.

Even if ASP is well studied, given the stricter limitations for reject water, the complex interactions between system variables and the non-conventional alternatives available nowadays, it is a difficult task to decide between several sets of operations and design parameters. The predictive modelling of WWTPs represents, in this context an interesting tool in order to give insights in decisions for future eco-design and implementations. However, computationally speaking, these simulation-based problems are to be seen as black-box systems, usually with expensive calculation-time requirements, where several variables interact in a complex and non-linear way. However, in the knowledge that these problems are often treated as simulation-based modules, the numerical approximation of gradient would be unreliable, which highlights the importance of using gradient-free optimization techniques. Thus, the two most challenging aspects in the optimization of such systems are to provide an appropriate problem formulation and to use suited optimization methods that allow relevant convergence accuracy and speed: the achievement of globally optimal results under multiple legally-imposed constraints and within a reasonable calculation-time.

Genetic algorithms have proven to be powerful tools for multi-objective optimization of real world problems such as in wastewater field (Fu et al., 2008). The use of a genetic algorithm present some advantages, for instance they are derivative-free therefore suited for non-linear black-box problems, and they are capable of ensuring the global optimality of results. Additionally, because they are population-based, they promote a diverse set of optimal solutions, called the non-dominated Pareto front. However, genetic algorithms as well as other evolutionary methods are extremely time-taking and it is quite impractical to apply them, in their original structure, to expensive optimization problems.

When considering the optimization of computationally expensive problems - usually simulation-based where, mathematical programming of processes cannot be directly applied - the availability of suited meta-heuristics and acceleration techniques is markedly reduced. Ahmadi et al. (2016) have given an extensive literature survey on the enhancement of convergence speed in multi-objective optimization of expensive problems. For these specific problems, some promising improvements have been reported in the literature, for instance the hybrid and memetic Multi-Objective Evolutionary Algorithms (Kim and Liou, 2014; Lara et al., 2010), the interactive and surrogate problem construction (Ojalehto et al., 2015; Capitanescu et al., 2015) and the Gaussian stochastic process modelling (Knowles, 2006). Regarding the first two approaches, despite the multiple advantages in improving the convergence issues, their main limitation is either a still impractical computation budget or a lack of accuracy. In Gaussian stochastic process modelling, the computation budget can be set to a very low value; however, the complexity of the algorithm itself can become a limitation.

The present study aims to trigger and discuss the feasibility of optimizing a full alternative WWTP - simulated via rigorous LCA- integrated dynamic models - through an efficient multi-objective optimization (EMOO) algorithm. Therefore, here the attention is paid solely to the practicality of such an optimization for expensive rigorous WWTP problems, and to the analysis of the 3D Pareto optimal front yielded by comprising outlet water quality, costs and environmental impacts as three main process objectives, helpful for the understanding of objectives' dependencies and for the identification of main treatment drivers.

The remaining of this paper is organized as follows: First, the structure of dynamic modelling with integrated LCA for the alternative WWTP is presented. Then, the efficient multi-objective approach is described. This work uses the Archive-based Multi-Objective Evolutionary Algorithm with Memory-based Adaptive Partitioning of search space (AMOEAMAP) framework, to deal with the optimization of expensive systems (Ahmadi et al., 2016). At the end, important issues, related to the formulation of optimization problem (interactions between objectives in the optimal region, and constraints), the general guidelines for future design of innovative WWTPs, and the question of practicality and computational feasibility are addressed and discussed.

## IV.2. Materials and methods

### IV.2.1. Dynamic Modelling (DM) approach

The plant under study is based on Benchmark Simulation Model N°2 (BSM2) with several modifications: Enhanced Primary Clarification (EPC) was added to enforce biogas production, post-anoxic denitrification dedicated to achieve effluent quality limitations and a cogeneration module for the sake of energy sustainability (heat and electricity). Following the idea of an integrated wastewater management, an alternative collection of 50% of urine was applied. The urine is treated by struvite precipitation for the sake of nutrients recovery and nitrification coupled to anaerobic deammonification in order to treat the N-rich effluent from the precipitation.

Configuration details are showed in figure IV.1. The considered WWTP comprises in the mainstream a pre-treatment (PT) unit for grit removal followed by a primary treatment unit (PRIM:  $\eta_{\text{removal}} = 80\%$ ), 2 anoxic tanks (ANOX1 and ANOX2) and 3 aerobic ones (AER1, AER2 and AER3 with oxygen controlled at 1.5, 2.0 and 0.5 gO<sub>2</sub>.m<sup>-3</sup> respectively for the reference case). A post denitrification zone was also added to achieve acceptable effluent limits. Nitrate was recycled ( $Q_{\text{INT}}$ : ~35500 m<sup>3</sup>.d<sup>-1</sup> for the reference case) from the aerobic to the anoxic zone and the sludge was separated in a secondary

clarifier (SEC), which was also partly a wastage flow ( $Q_W$ :  $\sim 300 \text{ m}^3 \cdot \text{d}^{-1}$  for the reference case) redirected to a thickener (THK), and partly recycled in the anoxic zone. The primary clarifier and thickener underflows were redirected to an anaerobic digester (AD). Finally, biogas from anaerobic digestion was used in a cogeneration unit for electricity and heat production (COGEN:  $\eta_{\text{electrical}} = 35\%$ ;  $\eta_{\text{heating}} = 48.5\%$ ). The inlet flows of external carbon ( $Q_{\text{CARBON}}$ : methanol to improve denitrification;  $0.75 \text{ m}^3 \cdot \text{d}^{-1}$  in the reference case) and coagulant ( $Q_{\text{METAL1}}$  and  $Q_{\text{METAL2}}$ : iron chloride for chemical precipitation of phosphorus;  $2 \text{ m}^3 \cdot \text{d}^{-1}$  and  $1 \text{ m}^3 \cdot \text{d}^{-1}$  respectively in the reference case) were also dynamic and followed a constant daily profile. Sidestream comprises a storage tank (ST), struvite precipitation tank (PPTSTRUUV), a nitrification tank (NITRITATION: dissolved oxygen controlled at  $2.0 \text{ gO}_2 \cdot \text{m}^{-3}$  for the reference case) and an anaerobic deammonification tank (ANAMMOX) with external alkalinity input.

Plant was dynamically simulated using SUMO (Dynamita, 2015). The used model is an adapted version of original Sumo2 and includes more than 70 equations including biological growth and decay of 8 microbial populations, hydrolysis and flocculation reactions, chemical precipitation of phosphorus with several species of hydrous ferric oxides (HFO), struvite and vivianite precipitation, gas transfer reactions and pH modelling resulting in more than 60 state variables.

The dynamic influent comes from the simulation of an adapted version of influent generator from Gernaey et al. (2011) including dry and rainy periods. This influent generator was modified by authors in order to consider urine source separation. Flows are generated by households (with separation of urine and flush water) and a minor contribution of the industry. Infiltration due to rain and groundwater is also considered. Pollutant values are based on European average per person equivalent (PE) with also a minor contribution of industry. First flush effects and sewer transport was also considered for the influent (without urine separated part, which is collected and transported by lorry). Finally, simulation is conducted for 100000 PE. Average values for the WWTP influent are given in table IV.1.



Table IV.1. Average influent characteristics

<b>Composite variable</b>	<b>Unit</b>	<b>Mainstream input</b>	<b>Sidestream input (Urine)</b>
<b>Q</b>	$\text{m}^3.\text{d}^{-1}$	17692	82
<b>TCOD</b>	$\text{gCOD}.\text{m}^{-3}$	607.4	5232.3
<b>TKN</b>	$\text{gN}.\text{m}^{-3}$	50.0	4597.4
<b>NHx</b>	$\text{gN}.\text{m}^{-3}$	33.4	4135.3
<b>TP</b>	$\text{gP}.\text{m}^{-3}$	10.4	347.0
<b>PO<sub>4</sub></b>	$\text{gP}.\text{m}^{-3}$	4.8	328.4

Previously to all dynamic simulations a standard steady-state (using reference values in order to start from the same initialization) was applied and simulations were run during 21 days (7 days of process stabilization followed by 14 days of dynamic simulation which were integrated to be used in optimization).

Reject limits were imposed to 10 mgN.L-1 for total nitrogen, 1 mgP.L-1 for total phosphorus, 100 mgCOD.L-1 for total chemical oxygen demand, 35 mgTSS.L-1 for total suspended solids and 4 mgN.L-1 for ammonium ion. Therefore, the process performance will be evaluated through technological, environmental and economic criteria, formulated as described later in section 2.3.2, and under the legally imposed restrictions in terms of reject limits mentioned above.

#### *IV.2.2. Life Cycle Assessment (LCA) approach*

LCA was conducted considering  $1\text{m}^3$  of treated wastewater as functional unit. When defining boundaries, which were considered to be as broad as possible, background processes were separated from foreground ones. More, the source of data for each type of process was different, being specific simulation results for foreground processes and from Ecoinvent v2.2 for background processes.

As discussed previously, considering the whole WWTP system means taking account not only of the benefits and drawbacks of coupled water and sludge lines but also of all background processes such as disposal of by-products, consumption of energy and chemicals, and transport and the avoided impacts when valuable by-products can be obtained. In this sense, boundaries expansion was considered to include the secondary function of fertilizers (sludge and struvite were all used in agriculture and therefore substitute triple super phosphate and ammonium nitrate) and the production of an excess of electricity when appropriate (which is reinjected in the network).

The inventory took into account all flow types proposed by the reference study included in the Ecoinvent 2.2. database (Doka, 2009) and also some others judged sensible in our case, such as a cogeneration system with electricity and heat production, external carbon source addition and production, fertilizer production from urine and its utilization.

As emphasized by several authors, WWTPs are important producers of greenhouse gases (GHG) and thus gas transfer of carbon dioxide (CO<sub>2</sub>), which is 100% biogenic, was considered as well as methane (CH<sub>4</sub>) and dinitrogen monoxide (N<sub>2</sub>O) with a ratio of 0.5% of ammonia nitrified flows in dynamic conditions.

The amounts of chemicals consumed (FeCl<sub>3</sub> for P precipitation (coagulant), methanol, MgO, NaOH) that would consequently need to be produced in background processes were calculated according to simulation demands and the electricity consumption was calculated by taking the sum of all electricity requirements (aeration, mechanical mixing, pumping, scrapping and dewatering). Transports were also considered for grits collected, sludge to be disposed, chemicals used, conventional fertilizers in extended boundaries, urine from houses to the WWTP and struvite to the spreading site.

It should be noted that this study does not consider the modification of the basic infrastructure as only operation parameters are studied in an existing WWTP.

The environmental impacts were calculated in Umberto® v5.6 software using the LCA Ecoinvent database v2.2 and ReCiPe 2008 (Goedkoop et al., 2009) with endpoint (H,A) as in the LCIA method.

Further details of LCA approach can be found in Bisinella de Faria et al., 2015.

### *IV.2.3. Efficient Multi-Objective Optimization (EMOO)*

#### *IV.2.3.1. Problem formulation: objective functions, constraints and range of decision variables*

As previously discussed, 3 objective functions were taken into account: (1) Operational Cost Index (OCI) to minimize (Eq. 1); (2) Effluent Quality Index (EQI) to minimize (as this index represents the amount of pollutants being reject to nature after treatment – Eq. 2) and (3) Life Cycle Impact Assessment (LCIA) to minimize (Eq. 3).

Equation 1 was taken from the original OCI formulation in BSM2 (Alex et al., 2008) and adapted to this case study. The constants are given in table IV.2. To provide a realistic approximation of the net

operational cost of the plant, nutrients recovery and electricity production from biogas cogeneration were also taken into account together with costs related to the consumption of raw materials and energy (In equation 1, C stands for consumed and P for produced and all values are obtained from energy and mass balances that follow process simulation).

$$OCI = \alpha_1 C_{electricity} + \alpha_2 C_{methanol} + \alpha_3 C_{FeCl_3} + \alpha_4 C_{MgO} + \alpha_5 C_{NaOH} + \alpha_6 C_{heat} - \alpha_7 P_{electricity} - \alpha_8 P_{struvite}$$

Equation 1

Where,  $C_{electricity}$  represents the amount of consumed electricity,  $C_{methanol}$  represents the amount of methanol added for post-denitrification,  $C_{FeCl_3}$  represents the total amount of iron chloride added for phosphorus precipitation,  $C_{MgO}$  represents the amount of magnesium oxide added for struvite precipitation,  $C_{NaOH}$  represents the amount added for alkalinity required for nitrification process,  $C_{heat}$  represents the amount of additional heat required for the plant,  $P_{electricity}$  represents the amount of electricity produced by anaerobic digestion in the plant and  $P_{struvite}$  represents the amount of produced struvite.

Table IV.2. Proposed  $\alpha$  values for OCI function

	Unit	Value
$\alpha_1$ Consumed electricity	€/KWh	0.07
$\alpha_2$ Methanol	€/kg	0.412
$\alpha_3$ FeCl <sub>3</sub>	€/kg	0.4
$\alpha_4$ MgO	€/kg	0.188
$\alpha_5$ NaOH	€/kg	0.35
$\alpha_6$ Consumed heat	€/MJ	0.008
$\alpha_7$ Produced electricity	€/kWh	0.175
$\alpha_8$ Produced struvite	€/kg	0

Equation 2 (EQI) also was initially taken from the original BSM2 (Alex et al., 2008). The reference set of equations to describe the physico-chemical interactions as well as the complete set of chemical reactions taken into consideration were previously provided in Bisinella de Faria et al. (2015), in

accordance with the original BSM2 following several relevant improvements. However, it was completed by including a new pollutant index (TP) designating the total phosphorus released in effluent, as this reject must respect specific regulation law. Coefficients used in Equation 2 are given in table IV.3.

$$EQI = \beta_1 NO_x + \beta_2 BOD + \beta_3 COD + \beta_4 TKN + \beta_5 TSS + \beta_6 TP$$

Equation 2

Where,  $NO_x$  stands for the sum of rejected nitrate and nitrite amount, BOD stands for the rejected Biochemical Organic Demand amount, COD stands for the rejected Chemical Oxygen Demand amount, TKN stands for the sum of rejected Kjeldahl forms of nitrogen amount, TSS stands for the rejected total suspended solids amount and TP stands for the rejected total phosphorus amount.

Table IV.3. Proposed  $\beta$  values for EQI function

		<b>Value</b>
$\beta_1$	<b>Nitrate + Nitrite</b>	10
$\beta_2$	<b>BOD</b>	2
$\beta_3$	<b>COD</b>	1
$\beta_4$	<b>TKN</b>	30
$\beta_5$	<b>TSS</b>	2
$\beta_6$	<b>TP</b>	100

In the present work, current cost coefficients ( $\alpha_i$ ) and pollutant indexes for effluent quality ( $\beta_i$ ) have been precisely suited for the current global scenario in Europe. However, considering the structure of the developed framework, these values can be easily modified for other case studies in order to fit, for example, geographical market prices (e.g.: when consumed and produced electricity prices have a higher or lower ratio) or specific reject areas (e.g.: where the reject of important quantities of phosphorus may lead to significant problems).

Equation 3 (LCIA) represents the calculation of the environmental impacts using ReCiPe Endpoint 2008 where  $m_i$  is the magnitude of intervention  $i$ ,  $Q_{ei}$  is the characterisation factor that connects the

intervention  $i$  with the respective endpoint impact category  $e$  and  $I_e$  is the indicator result for endpoint impact category  $e$  (Goedkoop et al., 2009).

$$I_e = \sum_i Q_{ei} m_i$$

Equation 3

As described in section 2.1, legally imposed reject limits should be respected. To impose the respect of the average legislative compliance, constraints on the integrated value during the last 14 days were explicitly added and formulated in problem. However, as system is simulated dynamically, it is also important to count the number of violation days in order to ensure that, for example, there are no extremely high pollutant peaks. It should be noted that above the reject constraints defined explicitly, all balance equations and chemical equilibriums are to be seen as implicit hard constraints, from a mathematical point of view. Accordingly, the main problem is in fact highly constrained both explicitly and implicitly: (1) explicitly, due to the few soft reject constraints and (2) implicitly, due to the large number of hard balance and chemical equilibrium equations.

As discussed by Hreiz et al. (2015b), problem formulation is one of the major influencing elements in generating optimized solutions. The 9 decision variables chosen in this study, listed in table IV.4, are the most influencing parameters following expert decision. Aeration is well known to represent about 70% of electricity consumption in WWTPs and has high influence on nitrogen performance. Carbon flow can have an interesting impact when COD available is not enough for denitrification. Coagulant addition influences on both enhanced clarification and phosphorus precipitation in order to achieve low P concentration in effluent. Finally, recycling ratios may influence WWTP performance as internal recycle ratio allows nitrate to be recycled to denitrification zone and external ratio allows more or less biogas production as well as modifying the sludge retention time that influences plant performance.

Table IV.4. Decision variables considered in this study

<b>Parameter</b>	<b>Description</b>	<b>Unit</b>	<b>Reference value</b>	<b>Lower level</b>	<b>Higher level</b>
<b>AER1 DO</b>	Dissolved oxygen concentration in the first aerated reactor	$\text{g O}_2.\text{m}^{-3}$	1.50	0.25	4.00
<b>AER2 DO</b>	Dissolved oxygen concentration in the second aerated reactor	$\text{g O}_2.\text{m}^{-3}$	2.00	0.25	4.00
<b>AER3 DO</b>	Dissolved oxygen concentration in the third aerated reactor	$\text{g O}_2.\text{m}^{-3}$	0.50	0.25	4.00
<b>NITRITATION DO</b>	Dissolved oxygen concentration in the nitrification reactor	$\text{g O}_2.\text{m}^{-3}$	2.00	1.00	4.00
<b>CARBON Q</b>	Methanol addition in the post denitrification zone	$\text{m}^3.\text{d}^{-1}$	0.75	0.00	6.00
<b>METAL Q1</b>	Iron chloride addition in headworks (EPC)	$\text{m}^3.\text{d}^{-1}$	2.00	0.50	6.00
<b>METAL Q2</b>	Iron chloride addition for polishing (post denitrification zone)	$\text{m}^3.\text{d}^{-1}$	1.00	0.00	4.00
<b>TP1 pumped flow ratio</b>	Internal recycle ratio to denitrification (recycled output/input)	Ratio (0-1)	0.50	0.05	0.76
<b>TP2 pumped flow ratio</b>	External output ratio to thickener (output/input)	Ratio (0-1)	0.0165	0.0042	0.0370

In this sense, decision variables reference values and boundaries were chosen in order to respect the desired plant functioning. Aeration (by means of dissolved oxygen set point) was fixed in the reference to achieve a correct ammonium decrease; for the first three reactors, dissolved oxygen was initially based on BSM1 open-loop dry weather scenario and then tuned to achieve the desired performance; also, the minimum value was set to achieve non anoxic conditions; however, in the case of nitrification reactor it was fixed to a higher level as high nitrogen concentrations are expected and thus, low oxygen concentration might lead to high N<sub>2</sub>O emissions. Carbon and the two metal addition were set to 0.75, 2.0 and 1.0 respectively in order to achieve the legal reject limits specified by the constraints for, respectively, nitrogen after the post-denitrification and phosphorus in effluent. Also, considering phosphorus, it might be noticed that for the first addition, the lower boundary was not fixed to zero as at least some iron chloride is required in order to achieve enhanced primary

clarification. Finally, internal recycle ratio was fixed to be less than 3 times of the influent (pumping limitation) and the reference value was set to 0.5 to be sufficient for the denitrification of available nitrate; external ratio recycle reference value and boundaries were fixed to maintain correct and feasible sludge retention time (SRT).

#### *IV.2.3.2. Expensive optimization algorithm and general settings*

The dynamic rigorous modelling of the alternative plant together with the LCA calculation on its extended boundaries is time consuming and therefore the global problem has to be treated as an expensive black-box system. In this sense, Archive-based Multi-Objective Evolutionary Algorithm with Memory-based Adaptive Partitioning of search space (AMOEAMAP) was used here (Ahmadi et al., 2016).

Figure IV.2 illustrates the structure of the algorithm. The left side in Figure IV.2, represents the Archive-based MOEA (AMOEAMAP), while the Memory-based Adaptive Partitioning of search space (MAP) corresponds the bloc highlighted in grey on the right side.

As described in detail in Ahmadi et al. (2016) and Ahmadi (2016), this algorithm is hybrid (evolutionary and metaheuristics) and presents two main modifications from the original structure of the state-of-the-art fast and elitist non-sorting genetic algorithm (NSGAII) of Deb et al. (2002):

- i. the use of two populations that are evolved simultaneously: a large archive population to store the best optimal solutions previously achieved, and a small operational population to intervene genetic operations with lower computation budget,
- ii. the use of an adaptive partitioning algorithm for a dynamic reticulation of the search space in order to markedly decrease the number of required evaluations. As a result, the optimal Pareto front can be yielded within a fixed computation budget of 300 function evaluations only, for a tri-objective optimization problem.

Further, following the idea of the adaptive partitioning of the search space, a new mutation operator, dubbed Importance-based Mutation Operator (IAMO), was included in order to balance exploration and exploitation tendency of the search algorithm while the small population is submitted to the genetic operations.

As illustrated in figure IV.2, through AMOEAMAP, the best optimal solutions previously evaluated are stored in an archive matrix and therefore only the operational population will intervene in the genetic operations with fewer function evaluations. On the other side, MAP offers a dynamic and realistic

partitioning of the search space, with the discretization being dynamically refined in an adaptive and probabilistic fashion, from coarse to finer partitioning when the need to attain better accuracy arises (Ahmadi et al., 2016; Ahmadi, 2016).

For constraint handling, the concept of constraint domination was used at the level of genetic selection. Three criteria are therefore used to discriminate between solutions of a population: dominancy, diversity and constraint violation.

General settings for AMOEAMAP algorithm were set as follows. The population size was set at 36, four times the number of decision variables; to be large enough compared to the total number of variables and the size of the small operational population was set equal to the number of decision variables. As AMOEAMAP is dedicated to expensive problems, the stopping criteria is the computation budget, which is here set to 300 function evaluations for the tri-objective optimization problems, described in Section 2.3.1. According to the crossover operation, the simulated binary crossover (SBX) was chosen with the original parameter settings as in NSGAI, ( $\eta_c=15$  and  $p_c=1$ ), set by Deb and Agrawal (1995). The mutation operator – the Importance Adaptive Mutation Operator (IAMO) - is self-tuned internally in accordance with the information coming from the MAP algorithm.

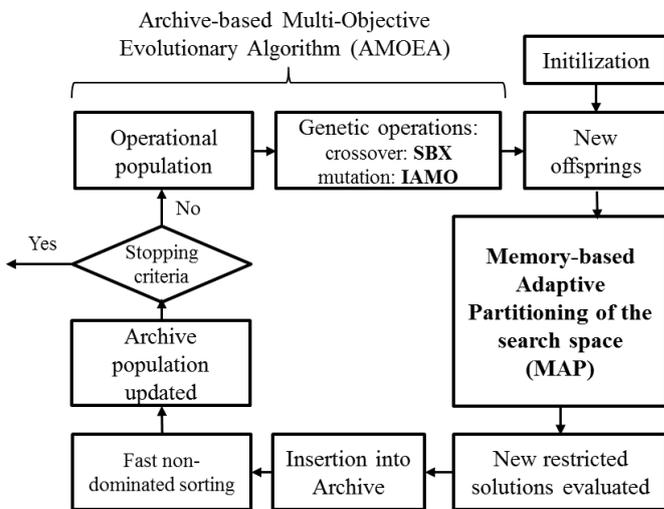


Figure IV.2. Structure of AMOEAMAP framework used in this WWTP problem optimization

#### IV.2.4. Integrated framework: DM-LCA-EMOO

The combined/integrated framework comprises the three tools presented previously as well as the connections between those tools, performed via Python interfacing. Figure IV.3 details the combined

framework. Initially, model parameters were fixed and dynamic influent data was provided to the simulator (Fig. 2, data flows 1, 2, 3). Following the dynamic simulation, process inventories were generated with their own inputs and outputs (data flow 4). After the dynamic simulations, data are passed through a Python interface (data flow 5) and the results are integrated over the simulation time. Python scripts also perform complementary calculations (e.g. calculation of cogeneration and energy requirements) and adjust assignments between the output flows resulting from the SUMO simulation and Umberto® input flows (data flows 6-9). The results are then converted to an Umberto®-compatible input file for foreground and background processes (data flow 10).

LCA calculations are then performed within Umberto® using the Ecoinvent database (data flows 11 and 13). This last step completes the LCI (data flow 12) by adding the contribution of background processes to WWTP ones. Following, the environmental impacts (data flow 14) are calculated using the chosen Life Cycle Impact Assessment valuation system. Further, the modules mentioned above, are connected to the Efficient Multi-Objective Optimization tool. EMOO is carried out through the AMOEA-MAP algorithm, where the results are received from the simulation and LCA blocks (data flows 15-20) and decision variables are steered via data flows 19-20 to the corresponding blocks. Regarding DM, Python interface and LCA modules, four main types of results are generated as output: effluent concentrations and quality violations (data flow A), operational cost along with energy parameters and nutrient recovery (data flow B), environmental impact results (data flow C). Finally, the non-dominated Pareto front serves as the final result, suited for decision making (data flow 21).

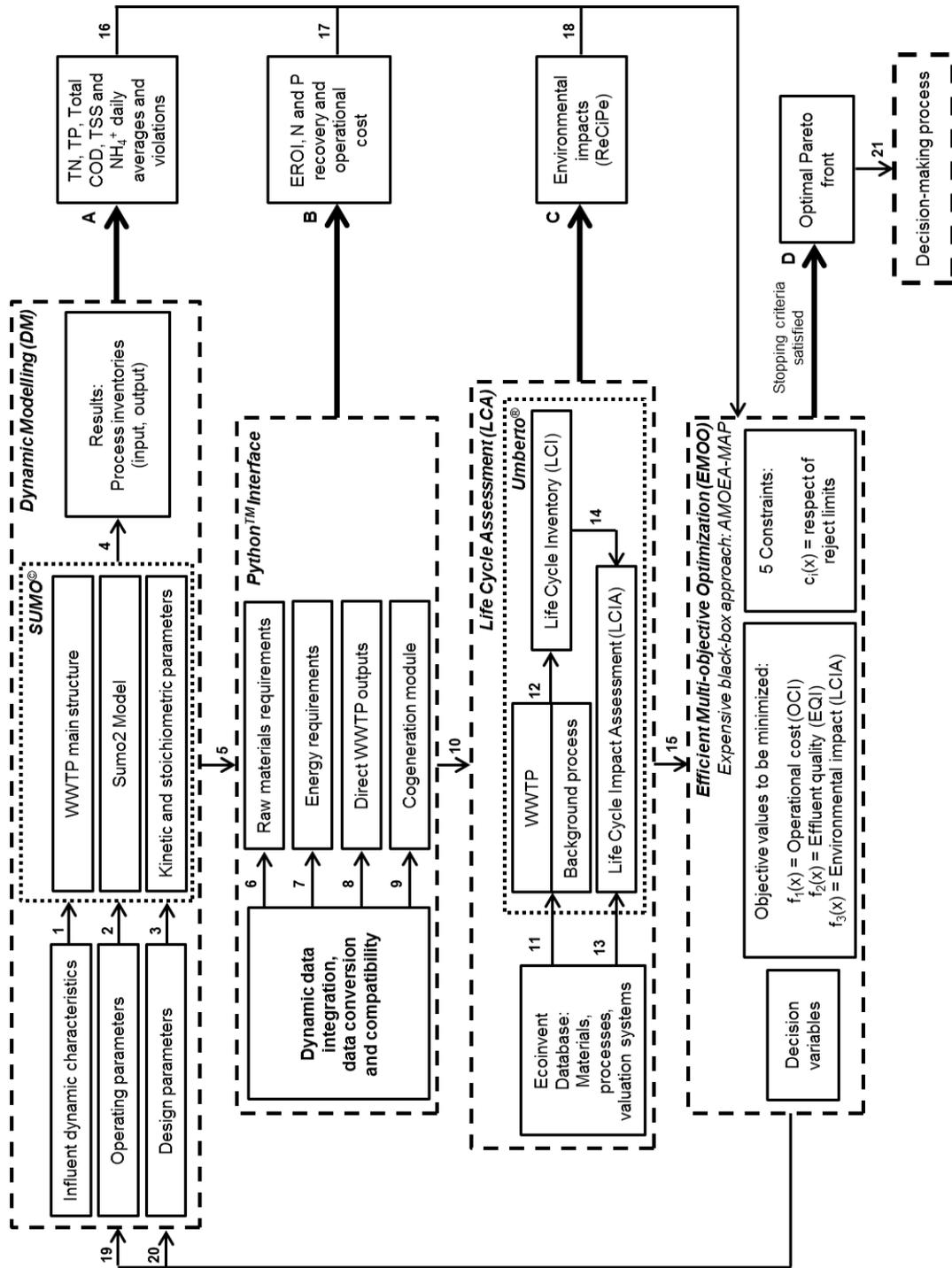


Figure IV.3. Structure of the integrated framework (Dynamic Modelling - Life Cycle Assessment - Efficient Multi-Objective Optimization)

### IV.3. Results and discussion

#### IV.3.1. WWTP optimization and objectives' dependencies

In this section, results of the optimization of alternative wastewater management and treatment (DM-LCA-EMOO) are illustrated, where both the feasibility and practicability of the optimization approach and the importance of problem formulation on the quality of results are emphasized and discussed. Graphical representations were all carried out within the Matplotlib (Hunter, 2007) under Python.

Figure IV.4 presents the 3D Pareto optimal curve (black dotted line) obtained with a low computation budget of 300 function evaluations. These results have been achieved by minimizing the three objective functions (Eq. 1-3), previously discussed, without additional reject limit constraints in order to give an overall view of the shape of Pareto front and to better illustrate the correlation between different objective functions all over the objective space. In this figure, axes present operational cost represented by OCI, quality index (pollutants being rejected) represented by EQI and environmental impacts represented by LCIA. Additionally, a 3D surfacing fitting was conducted to better illustrate the shape of Pareto optimal curve on the tri-dimensional objective space (Figure IV.4).

The correlation between objective functions can be directly drawn from figure IV.4. Over the whole Pareto curve, OCI and LCIA showed to be positively correlated meaning that when one increases the other increases also. In contrast, EQI and LCIA showed to be negatively correlated, which is to say that when EQI is reduced (outlet water quality increases), environmental impacts increase. Following the previous discussion, OCI and EQI are also negatively correlated (an increase in operational costs is required in order to deliver a better quality of the outlet water).

If reject limit constraints are also included explicitly (constrained optimization), a reduced Pareto curve will be achieved (red dotted line showed in figure IV.4). Therefore, in figure IV.4 three zones can be distinguished over the overall Pareto optimal curve (represented by grey arrows): zone I, II and III. Zone I corresponds to a region where quality is not acceptable as constraints are violated ( $EQI > 0.22$ ). However, in this zone it is relatively easy to obtain a substantial gain in water quality (EQI decreases) without significant increase in costs (OCI) and in environmental impacts (LCIA) as the system is not really forced to deliver the best treatment performance. On the other side, in Zone II and III, operating conditions are forced to respect the legally imposed reject constraints. Nevertheless, Zone II and III are distinguished by the amount of operational efforts required to attain better quality of outlet water. In Zone II, a moderated increase (relative to Zone III) in OCI and LCIA results in a satisfactory improvement in EQI (water quality). At this level, operator reaches the optimum quality of

treated water for the alternative wastewater treatment plant studied in the present study ( $EQI = [0.19-0.22]$ ). Beyond this quality ( $EQI < 0.19$ ), a small improvement in the quality of treated water induces an important increase in costs (OCI) and environmental impacts (LCIA). Hence, based on the configuration of wastewater treatment process proposed in the present study, it is industrially impractical to operate at the conditions belonging to Zone III.

With the aim of detailing each zone, a zoom is provided for Zone I (figure IV.5a) and Zones II and III (figure IV.5b). With regards to Zone II, the practical optimal zone from the decision making point of view, the most sensitive parameters/variables to provide a reasonable improvement in the quality of treated water can be identified. For this purpose, a zoom on Zone II and III was provided in figure IV.5b where all reject constraints and the legally imposed quality of treated water are respected.

It should be noted that running a minimization on EQI (maximizing the quality of treated water) instead of considering water quality as constraint is helpful when evaluating technological limits related to innovative wastewater treatment processes. By minimizing EQI, Zone III will also appear on the Pareto curve, where the limit of a reasonable (economic and environmental) treatment for a chosen wastewater management technology can be identified. This is to say that independently of the legally imposed quality for treated water, it is impractical to yield EQI below 0.19. As can be seen in figure IV.5b, in Zone III, EQI remains practically constant where both costs and environmental impacts are markedly increased. This zone is thus not an optimal operational zone; nevertheless, it offers the possibility to explore the limits of the chosen wastewater management technology. Additionally, the previous explanation suggests that to attain higher outlet water qualities ( $EQI < 0.19$ ), new treatment technologies shall be brought out.

Moreover, according to figure IV.5a-b, EQI and LCIA are significantly different by looking into their Pearson product-moment correlation coefficients (Figure 5a-b, bottom illustrations on the correlation between objective functions), as there are negatively and significantly correlated. However, based on the present definition of OCI function, OCI and LCIA seem to be correlated positively (correlation coefficient  $> +0.97$ ). The conclusion is that for the present case-study and based on the improved OCI function used in this work, LCIA and OCI are not significantly different. It should be noted that a tri-dimensional optimization with the simultaneous integration of the three objective functions is the only way to check such a positive correlation between economic and environmental functions for a given case-study. Nevertheless, this result cannot provide any generic suggestion on the exclusive use of either OCI or LCIA function in the context of multi-objective optimization. The reason is that the correlated behaviour between OCI and LCIA functions in the present work may be purely case specific and may also depend on the relevance of OCI definition.

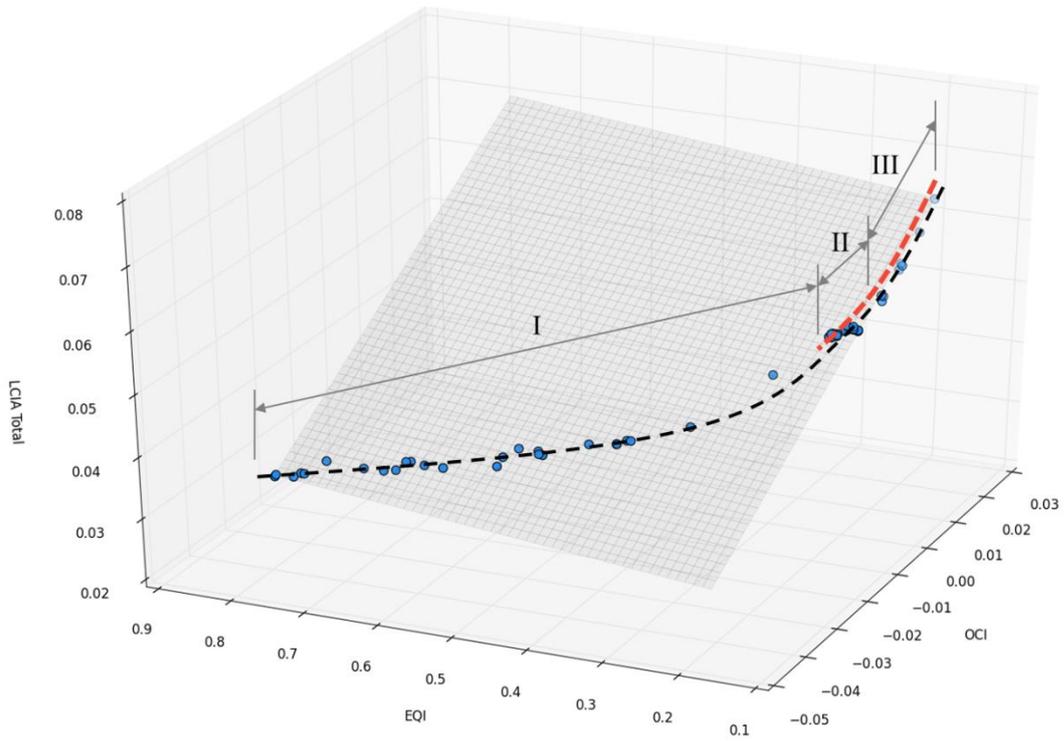


Figure IV.4. Pareto optimal curves for constrained and unconstrained optimization of WWTP

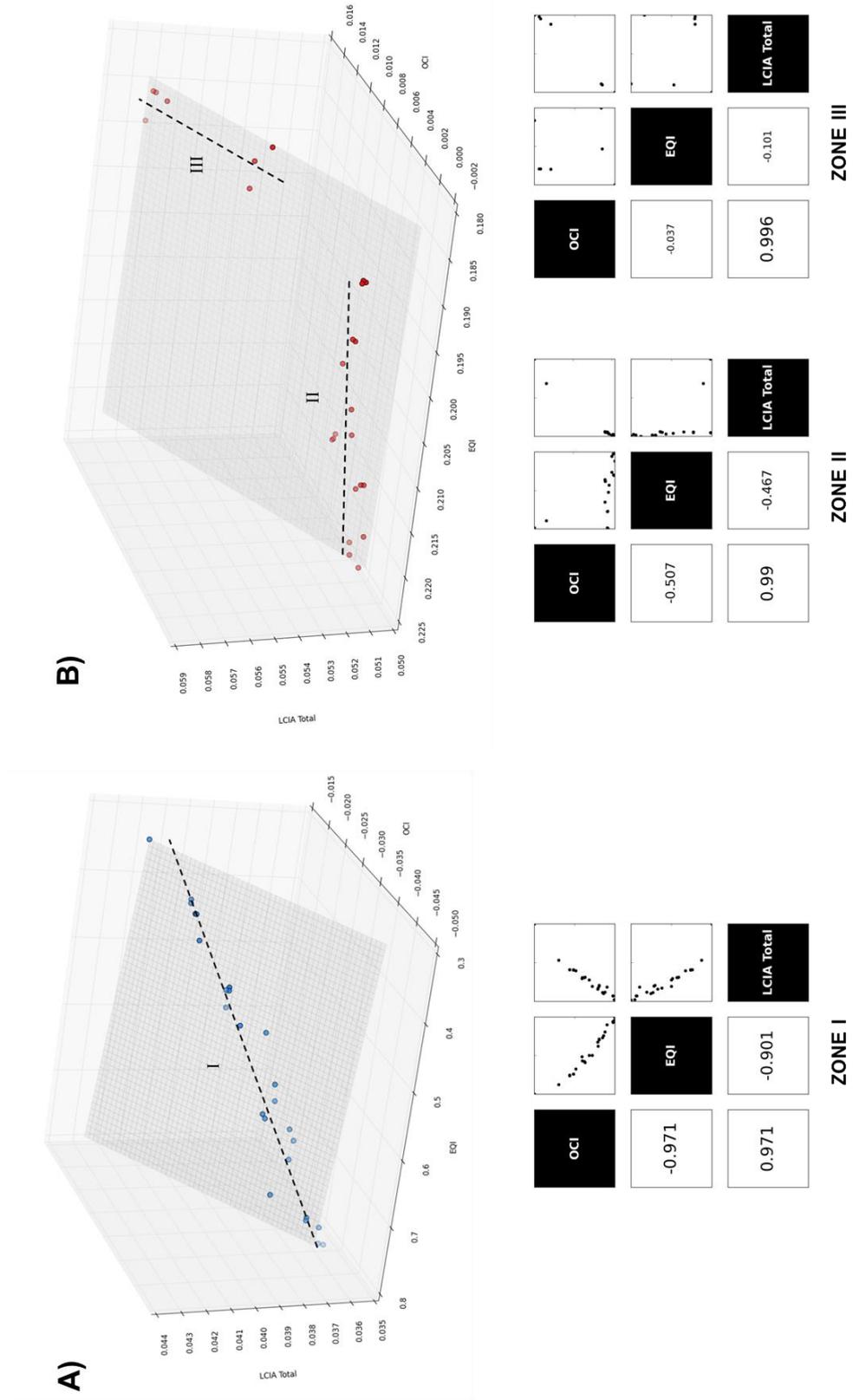


Figure IV.5. Zoom on optimal zones with water quality beyond the legally-imposed limits

(A) Zone I: feasible improvement of water quality without respecting the legal reject limits; (B) Zone II: feasible improvement of water quality without significant increase of cost and environmental impacts, Zone III: technological limitation of the proposed treatment) [bottom illustrations represent Pearson product-moment correlation coefficients]

### IV.3.2. Drivers for an optimal treatment

Given the Pareto optimal front for a WWTP where reject limits as well as the outlet water quality suit the legally imposed thresholds (constrained formulation); it is subsequently important to identify the main drivers (sensitive variables on the Pareto front) to the optimization.

For instance, driver variables in Zone III indicate where a design modification should be conducted.

Figures IV.6 and IV.7 presents the dependencies between objective functions and the main optimal process drivers: carbon addition and metal addition in the WWTP studied. Given the first optimal zone in figures IV.6 and IV.7, related to Zone II on the Pareto optimal curve (figure IV.5b), methanol added must remain the same at its optimum value while an increase in water quality up to  $EQI=0.19$  can be yielded by increasing the amount of iron chloride added. Therefore, metal addition is the main treatment driver in this zone (Zone II) due to its effect on phosphorus removal.

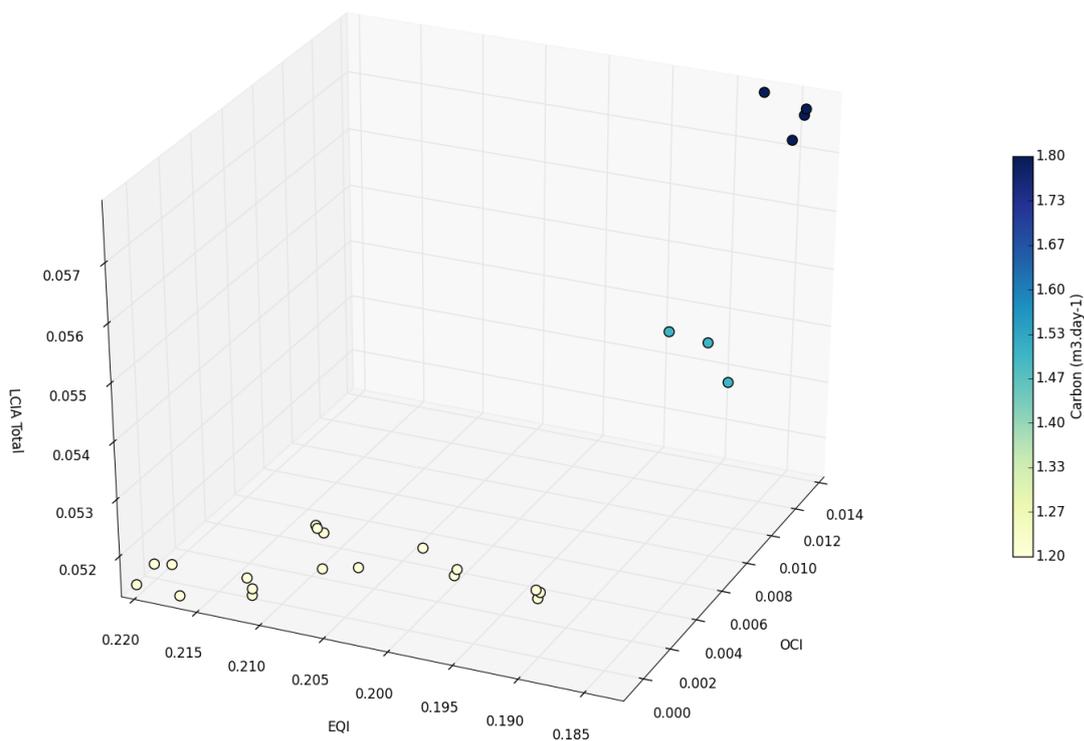


Figure IV.6. Level of methanol addition - driver for N treatment - for all solutions belonging to the Pareto optimal front

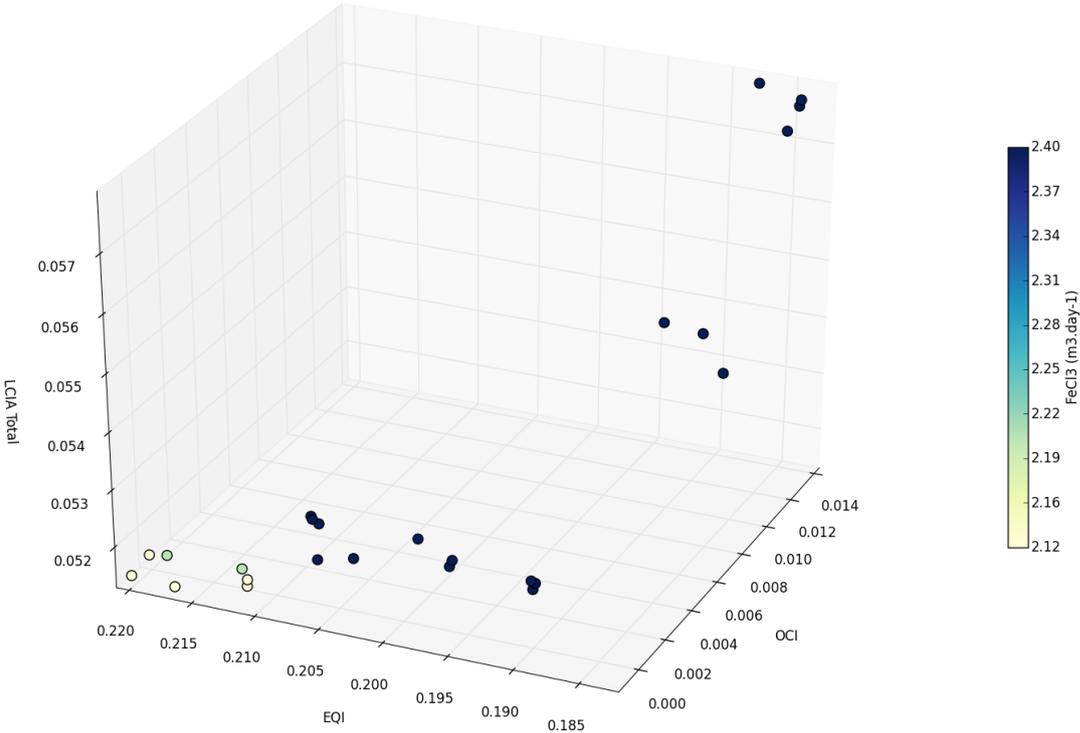


Figure IV.7. Level of iron chloride addition – driver for P removal – for all solutions in the Pareto optimal front

Table IV.5. Decision variables values for chosen optimal points

Parameter	Unit	A	B	C	D
<b>AER1 DO</b>	g O <sub>2</sub> .m <sup>-3</sup>	0.25	0.625	0.625	0.625
<b>AER2 DO</b>	g O <sub>2</sub> .m <sup>-3</sup>	0.25	0.25	1.0	1.0
<b>AER3 DO</b>	g O <sub>2</sub> .m <sup>-3</sup>	0.25	1.0	1.0	1.0
<b>NITRITATION DO</b>	g O <sub>2</sub> .m <sup>-3</sup>	1.6	1.6	1.6	1.6
<b>CARBON Q</b>	m <sup>3</sup> .d <sup>-1</sup>	0.0	1.2	1.5	1.5
<b>METAL Q1</b>	m <sup>3</sup> .d <sup>-1</sup>	0.5	2.125	2.4	2.4
<b>METAL Q2</b>	m <sup>3</sup> .d <sup>-1</sup>	0.0	0.8	0.8	0.8
<b>TP1 pumped flow ratio</b>	Ratio (0-1)	0.121	0.334	0.334	0.405
<b>TP2 pumped flow ratio</b>	Ratio (0-1)	0.017	0.021	0.024	0.031

In contrast, the increasing dose of methanol is responsible for a great increase in costs and environmental impacts in Zone III without any sensitive impact on the water quality (figure IV.6). As discussed previously, if water qualities beyond EQI ~ 0.19 (Zone III) are targeted, the technology

chosen in the management and/or treatment train has to be changed. As methanol addition plays an important role in denitrification, two design improvements could thus be carried out: i) managing differently the nitrogen input in the WWTP considering, for instance, the increase in urine source separation, and ii) treating more efficiently the nitrogen (using other process combination, for instance) in the sidestream and in the mainstream line. Both alternatives would allow thus the reduction in the addition of methanol at post denitrification level.

Additionally, aiming to better identify the weight of decision variables to differentiate the optimal solutions over the Pareto front, table IV.5 was provided which compiles the decision variables values for 4 chosen points A, B, C and D on the boundaries of Zone I, II and III (Figure IV.4): the point A and B to restrict Zone I (minimum OCI value in relative to Zone I and II, respectively), the point C to separate Zone II and III, and the point D as the highest treated water quality obtained (minimum EQI value in Zone III). As showed in table IV.5, all the variables increase with the decrease of EQI (better wastewater treatment); however, the most influencing decision variables (drivers) providing a change from one functioning zone to a new one, are the carbon and iron chloride addition. This result is also confirmed by Figure IV.8 which presents the correlation between variables and objective functions with the scatterplots in the upper triangle, Pearson product-moment correlation coefficients in the lower triangle, and the corresponding variable or function name on the main diagonal.



through normalized hypervolume difference indicator ( $I_H^-$ ) as a function of computation budget (number of function evaluations already made). The efficient multi-objective optimization method was therefore necessary to make the optimization of rigorous DM-LCA system computationally feasible with no loss of accuracy.

The optimization results, for both a constrained and an unconstrained formulation, were provided in figure IV.4. The unconstrained optimization (black disconnected line in figure IV.4) provided a wider distribution of optimal solutions, and clearly illustrated the contrast between three optimal zones (Zone I, II and III). The two Pareto optimal fronts (constrained and unconstrained) are superposed with the sole difference that the results based on a constrained problem formulation provide EQI below 0.22. This proves that in case the reject limits are explicitly defined as constraints, optimal results can be attained more quickly (less computation effort), with the same level of accuracy and with no additional constraint-related complexities. EROI (energy return on investment) for all solutions belonging to the Pareto optimal front, remain practically constant at 1.2, which shows that the suggested cost formulation in terms of OCI, allowed additionally a proper optimization of energy recovery throughout the treatment process.

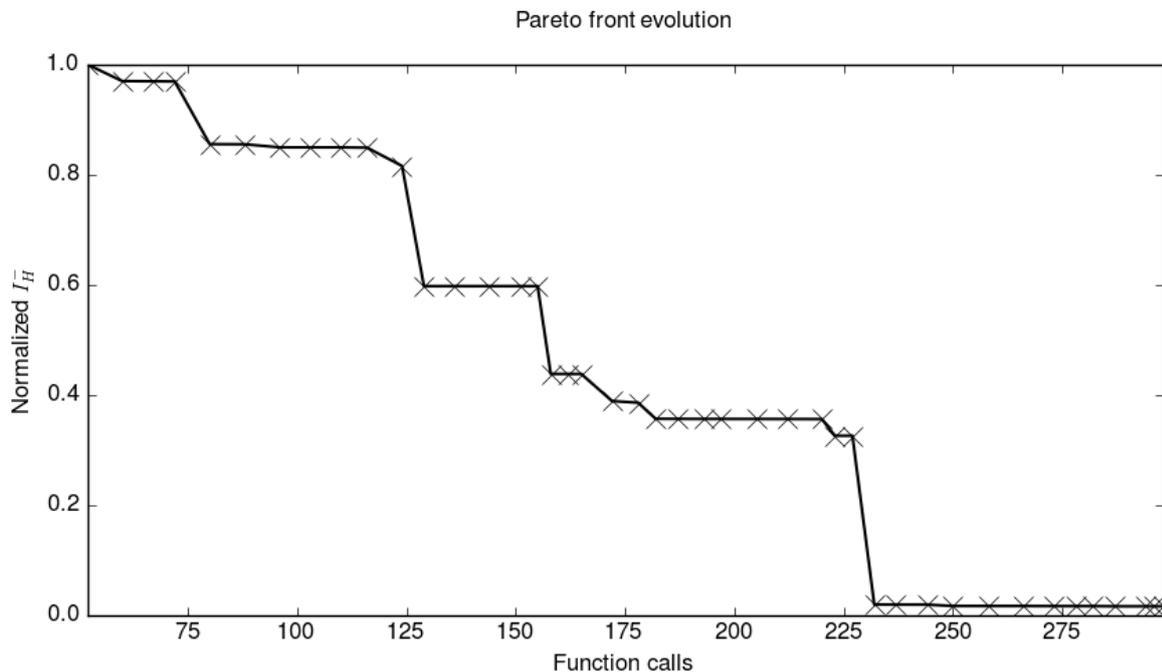


Figure IV.9. Optimization improvement based on hypervolume distance indicator ( $I_H^-$ ) calculations (computation budget of 300 function evaluations for constrained problem)

#### IV.4. Conclusion

The present study fulfils the current concerns for more eco-friendly and sustainable processes and the wide range of available combination of alternatives in the wastewater management field. Given the interconnected objectives and parameters as well as the great quantity of data that can be yielded using a predictive modelling, it becomes a difficult task for decision makers to visualize all options and choose among multiple optimal scenarios. Thus, the integrated DM-LCA-EMOO framework helps to compromise between technological aspects (process performance), operational costs and environmental impacts. However, when optimizing time-consuming simulation-based systems, efforts have to be made in order to reduce the number of function evaluations required, for the optimization to be practical and computationally feasible. The practicability of such an integrated framework (DM-LCA-EMOO) was demonstrated when a relevant optimization approach, suited for expensive problems (AMOEAMAP), is used. Conducting optimization with and without legally imposed constraints on reject limits, allowed a deeper analysis on the technological limits of a given treatment process. When applied to a real world case study in the wastewater treatment field, OCI showed globally to be positively correlated with LCIA as both costs and environmental impacts are mainly generated by background processes (supply chain). In contrast, OCI (and also LCIA) showed to be negatively correlated with EQI, as improvements in quality require increasing operational costs and environmental impacts. Throughout the Pareto optimal curve with acceptable water quality (Zone II and III), two situations were discussed: i) a water quality (EQI) belonging to [0.19-0.22], where an improvement in treatment can be achieved by increasing the amount of metal added, which is to say that the water quality can be improved with less requirement in costs and less environmental damages; and ii) a EQI below 0.19 (extremely good water quality), where the treatment has already arrived to its limitation, which is to say that a slight improvement in water quality by increasing the amount of methanol added with result in an excessive increase in costs and environmental damages. The latter shows that to attain higher water qualities ( $EQI < 0.19$ ), the technology itself has to be improved or changed.

# **Chapter V. Case Studies on Multi-Objective Optimization**



*“Climate change, demographics, water, food, energy, global health, women's empowerment – these issues are all intertwined. We cannot look at one strand in isolation. Instead, we must examine how these strands are woven together.” (Ban Ki-moon)*

As previously described in chapter IV, when rigorous modelling of WWTPs and WRRFs together with its extended life cycle boundaries is considered for the optimization of economic, environmental and performance aspects, the problem becomes easily complex from the optimization point of view, and therefore requires an efficient optimization tool. However, such a multi-criteria approach is unavoidable, as WWTP problems involve usually conflicting objectives with somehow unpredictable interconnections between them.

When a rigorous and integrated tool is available and the feasibility of the approach has been previously validated, the appropriate analysis of different real-world case studies can be carried out, in order to understand, for instance, how process objectives, constraints or dynamics are influenced by a functioning point of the plant. Moreover, comparative optimization-based studies on different alternative scenarios against the conventional ones are thereafter practical and reliable to bring about. Indeed, in this case, the optimization becomes a powerful tool to help learning about system interactions and objectives interdependencies.

The role of a wastewater treatment plant (WWTP) is to avoid the contamination caused by wastewater discharge. Whereas, WWTPs are constantly facing perturbations in influent flow rate and nutrient loads; therefore, they shall be systematically subject to the regulations. The nutrient limitations of the receiving water body, that are getting tighter due to the ever increasing environmental concerns, involves especially nitrogen and phosphorus. However, achieving low levels of pollutants demands high energy (notably regarding the aeration for nitrification) and chemicals consumption (e.g. in phosphorus removal). It is thus important to find a way to compromise between ensuing advantages and drawbacks arising out of a new alternative scenario. Moreover, whatever the scenario (conventional or alternative), the decision-making is a difficult task, as parameters are often interconnected and the problem is highly non-linear. As a consequence of this interaction, results might be influenced at different levels and at all objective functions.

The system optimization for the sake of performance and sustainability is receiving more and more attention, nowadays. Nevertheless, restricted comparisons against conventional facilities, when the new optimal operating conditions were not necessarily provided, are often inaccurate. The reason is that alternative systems might sometimes generate irrelevant environmental impacts due often to an underestimation of benefits arising from the recovery of certain valuable by-products. Therefore, when assessing these alternative scenarios based on comparative studies, it is fundamental to adopt rigorous

predictive models together with the quantification of involved benefits and drawbacks through the whole process life cycle.

A review on single and multi-objective optimization of WWTPs was conducted by Hreiz et al. (2015). Authors showed that MOO approaches are still scarce and problem formulation remains as one of the most important issues to be addressed. Moreover, not many optimization studies based on wide-plant modelling were found in the literature, with an appropriate multi-objective approach to preserve the true interactions between the conflicting objectives involved. Also, to the best of the author knowledge, for the moment, there are no alternative scenarios optimization studies available on literature.

Accordingly, one aim in this chapter is to study different problem formulations together with their consequences on optimal results, when applied to the reference or alternative scenarios. Then, based on a reference conventional scenario, comparative studies on dynamic versus steady-state simulation are provided. Moreover, the impact of constraint formulation on the quality of optimal solutions is discussed. The difference between the ReCiPe Endpoint method and the ReCiPe Midpoint for environmental analysis is also brought about as an independent comparative study. Finally, a through comparison between the reference and an alternative scenario (urine source separation followed by nitrogen treatment by nitrification/ anaerobic deammonification, dubbed ANA) is provided.

This chapter is thought to be submitted for publication in the journal Water Research.

## **Entitled of the paper: LCA based multi-objective optimization of conventional and innovative wastewater management and treatment scenarios**

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### **Abstract**

A comparison has been made between a conventional wastewater treatment plant (WWTP) and an alternative water resource recovery facility (WRRF) by using a plant-wide efficient multi-objective optimization tool, with the objectives being the effluent quality (expressed as a sum of rejected pollutants, EQI), the operational cost (OCI) and the environmental impacts (LCIA) through Life Cycle Assessment (LCA). The alternative scenario included the Enhanced Primary Clarification (EPC) and the Urine Source Separation (USS). In the latter, urine is treated afterwards by struvite precipitation (P recovery) and by partial nitrification coupled with anaerobic deammonification (to treat residual nitrogen). For the multi-objective optimization, an efficient Archive-based Multi-Objective Evolutionary Algorithm with Memory-based Adaptive Partitioning of search space (AMOEAMAP), tailored to deal with expensive simulation-based problems was used. The analysis proved the efficiency of the innovative scenario studied and demonstrated that the results of such an analysis would be reliable when, (i) the optimal results are achieved with no pre-defined aggregation of objectives in problem formulation, (ii) the life cycle inventories are appropriately integrated through LCA, and (iii) the plant dynamics together with the main operating parameters are taken into consideration via predictive models. The optimization-based approach allowed, additionally, the achievement of fruitful conclusions on several critical issues: the importance of problem formulation and constraint definition in WWTP optimization, the actual interdependencies between objective functions through Pearson product-moment correlations on optimal results, the choice of suited environmental impact categories, and the identification of the main process drivers with regards solely to optimal operating conditions.

*Keywords: Expensive multi-objective optimization; alternative wastewater treatments; LCA-integrated dynamic modelling; water resource recovery facility*

## V.1. Introduction

Wastewater treatment plants (WWTPs) are, by definition, facilities aiming to treat wastewater before their discharge into the environment. However, the treatment process itself as well as ancillary materials and energy requirements would become responsible for additional environmental footprints, as new pollutants would appear if a proper environmental analysis based on the whole process life cycle is established. Especially for the assessment of innovative alternative scenarios in wastewater treatment and management, it is fundamental to account for these newly generated impacts

Activated sludge process (ASP) is the most widely used technique for sewage treatment. However, this conventional wastewater treatment is being more and more criticized nowadays, because of its high consumption of energy and chemicals and the substantial amounts of sludge that it produces (that is considered sometimes as a waste). Therefore, scientific and industrial communities are moving towards a more sustainable way of wastewater treatment where more attention is paid to the recovery of valuable products. This might be conceived by applying some alternative processes to the existing WWTPs that uses a conventional ASP with extra process units, resulting in water resource recovery facilities (WRRFs).

The importance of a rigorous modelling as a powerful tool can be understood, when dealing with complex interactions generated due to the related modifications brought in the plant's configuration. However, the unit processes involved are highly influenced by dynamic inputs as the flows and nutrient fluxes in influent can vary depending on daily, weekly, seasonally and even yearly fluctuations. Moreover, interactions between the mechanical, biological, chemical and physical aspects of the processes involved leads to a highly non-linear modelling system. The resulting system is indeed computationally expensive, requiring specific calculation strategies for its resolution.

Since the publication of Azapagic and Clift (1999), the literature reviews have been depicting the importance of considering environmental aspects when assessing and evaluating processes. However, technical and economic aspects might not be forgotten or underestimated. In this sense, when making an effort to find the optimal operating conditions for a given system, it is fundamental to compromise between all genuine criteria, including the process performance, cost and environmental footprints. Specifically in the field of wastewater, Flores-Alsina et al. (2011; 2014) presented a complementary approach to the traditional cost and performance analysis, where greenhouse gases are also taken into account. By applying the proposed approach, authors arrived to the conclusion that, in order to have an overall assessment of the plant and to achieve the optimal conditions of operation in a more sustainable way, it is necessary to compromise harmoniously between the three criteria mentioned above.

Given the presence of several conflicting objectives in WWTPs and WRRFs optimization, multi-objective optimization (MOO) is an interesting tool to address the optimization of the problem with no pre-defined aggregation or weighting. Hreiz et al. (2015a) proposed a review on the use of single and multi-objective optimization in the context of WWTPs. According to authors, there are important challenges to be addressed when conducting an optimization, among which the problem formulation was recognized to be the most determining. Somehow, the problem formulation accounts for the unpredictable interactions between the objective functions, decision variables – whose sensitivity may change from one problem to another - and legally or environmentally imposed constraints. The problem formulation shapes indeed the quality of optimal solutions. Additionally, authors highlighted that, as the real optimality depends on the problem formulation, there is an important challenge, for instance, in the standardisation of cost functions and constraint selection (in order to respect feasibility along with physically relevant operating conditions). The process dynamics was also mentioned by authors as an important aspect to be integrated, to achieve sustainability based on reliable predictions of process behaviour as both slow and rapid dynamics are present in some treatment units. The importance of using multi-objective optimization when real-world wastewater problems are thought was thoroughly highlighted by Hreiz et al. (2015a), as the use of single objective optimization might be misleading or restricted by the weighting strategies imposed to aggregate different process objectives. The aggregation might hide the contradictory interactions between the objectives and avoid the achievement of common-sense conclusions on the real efficiency of a given treatment strategy and on its efficiency change over the adjacent operating conditions.

Another interesting aspect regarding the MOO is that instead of one single optimal solution, a set of optimal points, namely the non-dominated Pareto front, can be achieved. The Pareto front allows for further discussions on outcomes generated (both benefits and drawbacks) and decision-making. Therefore, other sensitive aspects that are sometimes not quantifiable (thus usually not included in the optimization) or that are known for their influence on the robustness of plant such as the use of a short sludge retention time (SRT), the presence of filamentous bacteria and the dysfunctioning in the secondary clarifier, could be taken into account for further analysis. Moreover, as described earlier, the decision-making can be carried out afterwards based on the generated optimal solutions and the expert of the field suggestions (Hreiz et al, 2015a; Azapagic, 1999; Hakanen et al., 2008).

To the authors' knowledge, only a few studies on the literature, that are discussed hereafter, have tackled properly the problem from a multi-objective point of view. Sweetapple et al. (2014) studied the optimization of a modified version of the Benchmark Simulation Model N°2 (BSM2) - without sludge line - and obtained Pareto sets by targeting the minimisation of greenhouse gas (GHG) emissions, operational costs and effluent pollutant concentrations. A modified version of BSM2 was chosen in order to make the problem feasible, as otherwise the complexity could not allow the

achievement of optimal solutions within a reasonable calculation time. Authors have indicated the importance of taking into account GHG emissions as only decreasing costs and pollutants in output water may lead to inadvertent increases in GHGs emissions. Hreiz et al. (2015b) proposed a multi-objective optimization of a small-size WWTP, by considering water line and sludge incineration. The study used rigorous modelling and was based on cost and nitrogen discharge as the objective functions to minimize. Authors indicated that incineration of sludge might present important benefits, especially when the discharge amount of nitrogen is high; however, the plant did not achieve energy autarky. Another study on the field was proposed by Beraud (2009) where multi-objective optimization was conducted over the Benchmark Simulation Model N°1 (BSM1) scenario considering effluent quality and energy consumption. Authors highlighted the important gains that might be achieved at the optimal operating conditions compared to the conventional control strategies applied to BSM1. Also, according to authors, in order for the optimization to be feasible, it has to be performed within a limited time horizon.

Moreover, there is no available information in the literature on optimization when considering environmental impacts together with water quality and operational cost. However, it has already been shown that background processes present important levels for several environmental impact categories (Bisinella de Faria et al, 2015; Foley et al., 2010; Yoshida et al., 2014).

Several studies in the literature brought about the question of problem formulation, even though in these studies, only cost and performance are commonly considered as objective functions. Iqbal and Guria (2009) presented a first work where the elitist non-dominated sorting genetic algorithm (NSGAI) was used in the field of wastewater. Different problem formulations were proposed by authors (single, two and three objectives) with the consideration of performance and economic criteria. According to authors, the optimal Pareto front could be achieved after 2500 generations. Such an approach is quite impractical when rigorous dynamic modelling is involved, as the average calculation time for a dynamic simulation run exceeds several minutes.

Guerrero et al. (2012) proposed a multi-criteria function optimization to take into account microbiology-related failures in the plant functioning. In a more global approach, Fu et al. (2008) proposed a study on a MOO platform applied for the control of an integrated urban wastewater system. Authors showed through a case study that including the discharging water body as a decision variable provides more information for the decision maker to compromise between objectives. Important improvements compared to the non-optimal case were found in both performance and cost objectives. Authors showed that NSGAI is a powerful and effective algorithm to be used in this type of problem. However, modelling was conducted through BSM1 scenario and using ASM1 modelling approach.

As opposed to the above-mentioned works, Kim et al. (2015) considered not only the water line but also sludge train. When modelling the plant, authors used a modified version of ASMN model that includes the GHG emissions and the Anaerobic Digestion Model (ADM) to simulate the anaerobic digestion. However, when solving the optimization problem, targeting the minimization of GHG emissions, cost and discharged pollution, an integrated performance index was calculated by normalizing the objectives and applying a weighted aggregated sum. Results were thus obtained between 300 and 2000 simulation runs and it was claimed that even in already tuned facilities, new optimal points can be achieved (with the optimal system reducing 31% of GHG emissions, 11% of cost and 2% of discharged pollutants). Nevertheless, the results were achieved based on a single objective reformulation of the problem, and therefore no solid conclusion can be drawn on the real sensitivity of original objective functions towards the decision variables.

Finally, an interesting approach from Hakanen et al. (2011; 2013) proposed the use of an interactive tool to consider decision makers' preferences during the optimization of WWTPs. The tool was meant to be used for the design of new plants or for the optimization of existing ones. According to authors, there is no need in converting evaluation criteria into specific functions that might lead to loss of information. Also, it was claimed that, as the decision maker can express her/his own preferences, it is possible to learn reciprocally about the interdependencies in the problem. However, authors indicated that further research is still necessary when the consideration of process dynamics and rigorous modelling is targeted.

Having in mind the available approaches in the literature and, to the best of authors' knowledge, there is still a lack of comprehensive information on the interest in an appropriate multi-objective approach for the optimization and the understanding of WWTPs when dynamics and rigorous predictive modelling are involved. The rigorous modelling and simulation being time consuming, more efficient algorithms have to be developed and used. Moreover, nowadays, multi-objective optimization is almost applied to reference treatment systems, only. However, there exists an increasing interest in sustainable systems in order to reduce the environmental damages resulting from a WWTP plant, while ensuring the optimal conditions of the plant (minimal cost and maximal performance).

Currently, several alternatives to conventional ASP have been proposed in order to achieve flexibility and stability during the treatment and to maximize the resource recovery. Among the proposed options, urine source separation has been highlighted as one of the promising alternatives to promote sustainability in the wastewater management (Maurer et al., 2006). A great interest in this type of collection is that when the urine is collected separately, it allows also the recovery of certain nutrients, notably nitrogen (N) and phosphorus (P), thanks to its high composition (Larsen and Gujer, 1996). Subsequently, urine can be treated with magnesium in order to form struvite ( $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$ ), a slow-release fertilizer (Maurer et al., 2006). In addition to the recovery possibilities, the urine source

separation leads to the avoidance of ammonia peaks in the plant which will logically result in a more stable plant and therefore a redesign would be feasible when new infrastructures are envisaged (Rauch et al., 2003). Urine separation can also decrease the consumption of chemicals used for P-elimination and reduce the consumption of energy and external carbon sources in WWTPs through a reduction in advanced N-removal requirements. There is also treatment options proposed nowadays for nitrogen rich streams such as nitrification/ deammonification by *Anammoxidans* bacteria.

Another feature with a view to enhanced sustainability in WWTP plants is to achieve energy autarky. The energy autarky is gaining interest from both economic and environmental points of view. When the anaerobic digestion is implemented, one way to improve biogas production is to accentuate the enhanced primary clarification where, with the addition of chemicals, a more efficient flocculation takes place and thus more organic matter can be dedicated to anaerobic digestion. This strategy helps to turn the energy balance of WWTPs into a net positive energy. Accordingly, Flores-Alsina et al. (2014) proposed the enhancement of total suspended solids (TSS) removal in the primary clarifier, which led to a higher chemical oxygen demand (COD) for the digestion and consequently more biogas production was produced. Additionally, if coupled with a less rich nitrogen influent (when considering, for instance, a fraction of urine that is separated at the source), enhanced primary clarification represents an important benefit, as less organic matter is required for N-removal.

Accordingly, beyond the predictable advantages that can easily be raised, the imposed changes in the wastewater management and treatment may require important efforts and thus, it is fundamental to provide complete life cycle assessment for any further evaluation or validation of a given alternative treatment strategy. Among the alternative scenarios for WWTPs, proposed in the literature, Remy et al. (2008) showed that the new scenarios might sometimes generate higher environmental impacts when compared to a conventional treatment scenario. In this case, it should be noticed that conventional scenarios are provided with already optimized operating conditions. Therefore, with regards to alternative scenarios, a parallel optimization of design and operating conditions must be carried out to provide a fair comparison with the conventional plants.

In order to shed light on new options of wastewater management and treatment, the goal in the present study is to apply a previously validated optimization platform – an efficient multi-objective optimization tool coupled with a rigorous dynamic modelling and life cycle assessment (Bisinella de Faria et al., 2016a) - to the reference and alternative scenarios in the field of wastewater. The practicality of such an expensive optimization and the reliability of results have been previously demonstrated for a WWTP. In the present study, the conventional WWTP and an alternative WRRFs are compared when optimized, by accounting also the operating conditions as complementary decision variables to provide a fair comparison. The proposed alternative scenario allows thus giving insights on new options of wastewater management and treatment.

## V.2. Materials and methods

### *V.2.1. Dynamic Modelling – Life Cycle Assessment – Efficient Multi-Objective Optimization (DM-LCA-EMOO) coupling approach*

The multi-objective optimization approach used in this study, which is extensively described in Bisinella de Faria et al. (2016a) together with its feasibility study, might be globally divided into 3 calculation blocks interconnected via Python™. The first part represents the Dynamic Modelling (DM) where a rigorous dynamic simulator for WWTPs - in this study, SUMO v.15 beta 69.1 from Dynamita (2016) using an adapted version of Sumo2 model - is integrated (Dynamic modelling block in figure V.1). The simulation results are then converted into a Life Cycle Assessment (LCA) compatible process inventory by integrating dynamic output results over the time. The complementary calculations, mainly related to energetic and background aspects, are also conducted in this intermediate block and managed through Python™ scripts (Python™ interface block in figure V.1). As illustrated in LCA block (figure V.1), Life Cycle Impact Assessment (LCIA) is performed within Umberto® software v.5.6 by using the Ecoinvent database v.2.2, and is fed by the Life Cycle Inventories (LCI) previously provided. Finally, the above-mentioned tools and results are connected to an Efficient Multi-Objective Optimization tool (EMOO block in figure V.1). Details on each calculation step have been provided previously in Bisinella de Faria et al. (2016a), where the whole combined platform was subject to a feasibility study based on a full WWTP configuration. In the present work, however, brief instructions will be provided through the following subsections to clarify the specificity of each modelling or calculation block.

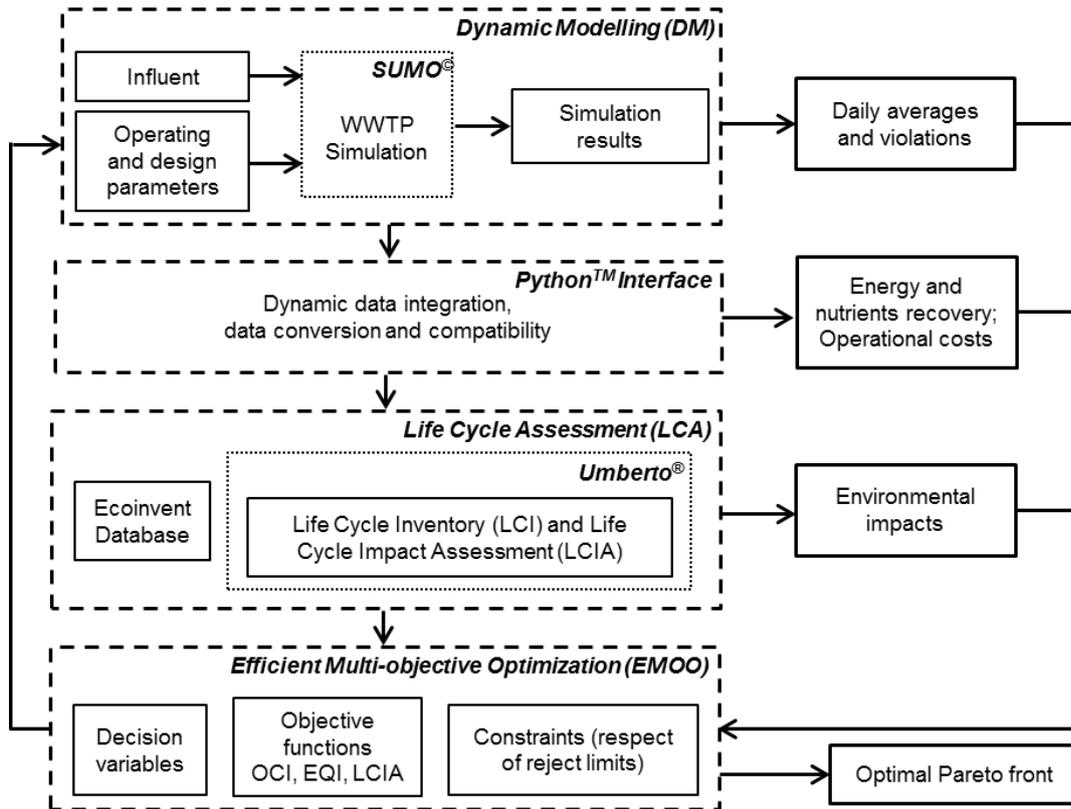


Figure V.1. Simplified structure of the integrated framework (Dynamic Modelling - Life Cycle Assessment - Efficient Multi-Objective Optimization)

### V.2.1.1. Dynamic modelling (DM)

Dynamic modelling and simulation was conducted within SUMO software (Dynamita, 2015). The chosen model is an adapted version of original Sumo2 and holds for more than 70 equations including biological growth and decay of 8 microbial populations, hydrolysis and flocculation reactions, chemical precipitation of phosphorus with several species of hydrous ferric oxides (HFO), struvite and vivianite precipitation, gas transfer reactions and pH modelling. It should be noted that the resulting system deals with more than 60 state variables.

Previously to all dynamic simulations, the initialization was conducted by the consideration of a reference steady-state condition that contains reference parameter values. The simulation was thereafter carried out, in dynamic regime for 3 weeks, whereas only the simulation results of the last 2 weeks were employed for further calculations (the first week is considered as a stabilization period between the steady-state and the dynamic period).

Details on each scenario flowsheet will be provided in section 2.2.

### V.2.1.2. *Life Cycle Assessment (LCA)*

Aiming to estimate the environmental impact calculation over the whole wastewater management and treatment system, an LCA was conducted based on the WWTP present in Ecoinvent 2.2. database (Doka, 2009) with relevant adaptations for the considered case studies. The considered functional unit was  $1\text{m}^3$  of treated wastewater. The system's boundaries were defined to be as broad as possible in order to consider detailed foreground and background emissions.

In this sense, boundaries included as the foreground process the coupled water and sludge lines with their direct emissions (e.g.: pollutants rejected to the river after the treatment; GHG emissions during treatment such as  $\text{CO}_2$  – considered as biogenic if coming from the input wastewater -,  $\text{CH}_4$  and  $\text{N}_2\text{O}$  – estimated as 0.5% of ammonia nitrified flows); Similarly, background processes included plant infrastructure, the disposal of by-products (grits from pre-treatment and sludge), the supply chain of raw materials (iron chloride for P precipitation (coagulant), methanol for post-denitrification,  $\text{MgO}$  for struvite precipitation and  $\text{NaOH}$  for alkalinity addition), energy consumption (from aeration, mechanical mixing, pumping, scrapping and dewatering) and the transport (collected grits for disposal, sludge to be disposed, chemicals coming from production, conventional fertilizers in extended boundaries, urine from houses to the WWTP and struvite to the spreading site in the alternative scenario). Moreover, modification of the WWTP infrastructure was not considered, neither for the conventional nor for the alternative scenario, as only operation parameters were included in this study.

In an effort to take into account all foreground and background processes, benefits and drawbacks were considered, beyond the calculation of direct and indirect impacts, by the addition of avoided impacts in case of by-product recovery (such as fertilizer recovery from sludge and struvite when urine is source separated that can substitute triple super phosphate and ammonium nitrate) and by the excess of produced electricity (reinjecting in the network).

Moreover, considering the obtained Life Cycle Inventory, background processes were separated from the foreground. This was done as source of data for each type of process was different: specific simulation results were used for foreground processes, while Ecoinvent v2.2 modules were used for background processes calculation (modules were fulfilled with required quantities from process simulation).

Finally, the environmental impacts were calculated via Umberto® v5.6 software using the LCA Ecoinvent database v2.2 and ReCiPe 2008 (Goedkoop et al., 2009) with endpoint (H,A) and midpoint (H) as in the LCIA method. Further details on LCA approach can be found in Bisinella de Faria et al. (2015).

### V.2.1.3. *Efficient Multi-Objective Optimization (EMOO)*

Broadly, multi-objective optimization is the process of optimizing simultaneously two or several objectives with or without constraints. Among the several proposed optimization methodologies in the literature, evolutionary algorithms are particularly sought to highlight because of their capability of ensuring the global optimality of results and their derivative-free search strategy due to the use of stochastic operators (e.g. probabilistic selection, genetic crossover, mutation and migration) (Deb, 2011).

However, in the field of eco-design and intensive process optimization, the choice of a search algorithm shall also follow the computational complexity of problem. As the dynamic modelling coupled with the LCA calculations is time consuming (20 minutes per simulation run, in average), the present WWTP optimization problem has to be treated as an expensive simulation-based system. Here, the expensive aspect refers to the computational time required for the achievement of optimal results, which is directly proportional to the computational budget (number of simulation runs needed) for a satisfactory optimization of WWTP.

An efficient multi-objective approach is thus required in order to deal with expensive simulation-based problems. To this end, Archive-based Multi-Objective Evolutionary Algorithm with Memory-based Adaptive Partitioning of search space (AMOEAMAP) was used in this work. As described in Ahmadi et al. (2016) and Ahmadi (2016), AMOEAMAP is a hybrid algorithm, result of the combination of multi-objective evolutionary algorithms with new metaheuristics to reduce the number of simulation runs required and to provide a rapid and accurate convergence to optimal Pareto front. The algorithm presents two main modifications from the original structure of the state-of-the-art NSGAII (Deb et al., 2002): (i) the use of a bi-population search strategy involving simultaneously a large archive population to store the best optimal solutions previously achieved, and a small operational population to intervene genetic operations with lower computation budget; (ii) the use of a memory-based adaptive partitioning algorithm for a dynamic self-adaptive reticulation of the search space in order to efficiently identify the zones susceptible of providing optimal solution with fewer number of function evaluations.

For constraint handling, the concept of constraint domination was used (Deb et al., 2002). Three criteria are therefore used to discriminate between solutions in a population: dominancy, diversity and constraint violation. The latter operates by integrating the constraint satisfaction as the third selection criteria within the evolutionary selection procedure, and therefore prevents a parallel handling of optimization and constraint satisfaction as two independent search strategies.

As general settings for AMOEA-MAP, the population size was set to four times the number of decision variables to be large enough compared to the total number of variables and the size of the small operational population was set equal to the number of decision variables. The stopping criteria was set to the computation budget, which is here set to 300 function evaluations. According to the crossover operation, the simulated binary crossover (SBX) was chosen with the original parameter settings as in NSGAI, ( $\eta_c=15$  and  $p_c=1$ ), set by Deb and Agrawal (1995). The mutation operator – the Importance Adaptive Mutation Operator (IAMO) - is self-tuned internally in accordance with the information coming from the MAP algorithm.

### V.2.2. WWTP scenarios (conventional vs. innovative)

The plant under study is based on Benchmark Simulation Model N°2 (BSM2). Two scenarios are accordingly proposed in this study:

- i) the reference scenario (REF);
- ii) the urine source separation scenario coupled with the sidestream recovery of phosphorus by struvite precipitation and nitrogen treatment in urine by nitrification coupled with anaerobic deammonification (ANA);

A set of brief and comprehensive flowsheets for the two above-mentioned scenarios is given in figure V.2. Further, the main detailed configuration is illustrated in figure V.3.

Starting from BSM2 configuration, some adaptations were proposed. For the ANA scenario, where less nitrogen is to be treated in the water line, Enhanced Primary Clarification (EPC) was introduced for the enforcement of biogas production (figure V.2). Also, in both scenarios, a post-anoxic denitrification zone was included which is dedicated to achieve effluent quality limitations (figure V.3). Additionally, a cogeneration module was integrated for the sake of energy sustainability (heat and electricity).

As shown in figure V.2, REF scenario does not involve the sidestream line, depicted in figure V.2 as a yellow box, and EPC (green box) is also included only in ANA scenario. Moreover, for the alternative scenario, urine source separation was considered in a proportion of 50%.

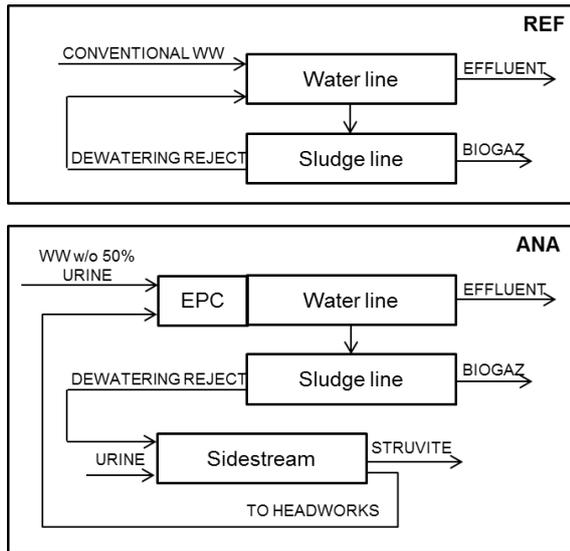


Figure V.2. Simplified flowsheet for the two WWTP scenarios studied in the present work

Basically, the considered WWTP comprises in the mainstream, a pre-treatment (PT) unit for grit removal (not showed in figure V.3) followed by a primary treatment unit (PRIM:  $\eta_{\text{solids removal}} = 50\%$  for REF and  $\eta_{\text{solids removal}} = 80\%$  for ANA), 2 anoxic tanks (ANOX1 and ANOX2) and 3 aerobic ones (AER1, AER2 and AER3 with oxygen set to  $\text{DO}_1 = 1.5$ ,  $\text{DO}_2 = 2.0$  and  $\text{DO}_3 = 0.5 \text{ gO}_2\cdot\text{m}^{-3}$ , respectively) followed by a post denitrification zone (figure V.3). Nitrate was recycled from the aerobic to the anoxic zone ( $Q_i$ ) and the sludge was separated in a secondary clarifier (SEC), which was also partly a wastage flow ( $Q_w$ ) redirected to a thickener (THK), and partly recycled in the anoxic zone. The primary clarifier and thickener underflows were redirected to an anaerobic digester – AD (figure V.3). Finally, biogas from anaerobic digestion was sent to a cogeneration unit for electricity and heat production (Cogeneration module:  $\eta_{\text{electrical}} = 35\%$ ;  $\eta_{\text{heating}} = 48.5\%$ ). Also, at this level, an input flow of external carbon ( $Q_{\text{CARBON}}$ : methanol to improve denitrification) and coagulant ( $Q_{\text{METAL1}}$  and  $Q_{\text{METAL2}}$ : iron chloride for chemical precipitation of phosphorus) were considered. Sidestream comprises a storage tank (ST), struvite precipitation tank (PPTSTRUV), a nitrification tank (NITRITATION: dissolved oxygen controlled at  $\text{DO}_{\text{NITRITATION}} = 2.0 \text{ gO}_2\cdot\text{m}^{-3}$ ) and an anaerobic deammonification tank (ANAMMOX) with external alkalinity input (figure V.3).

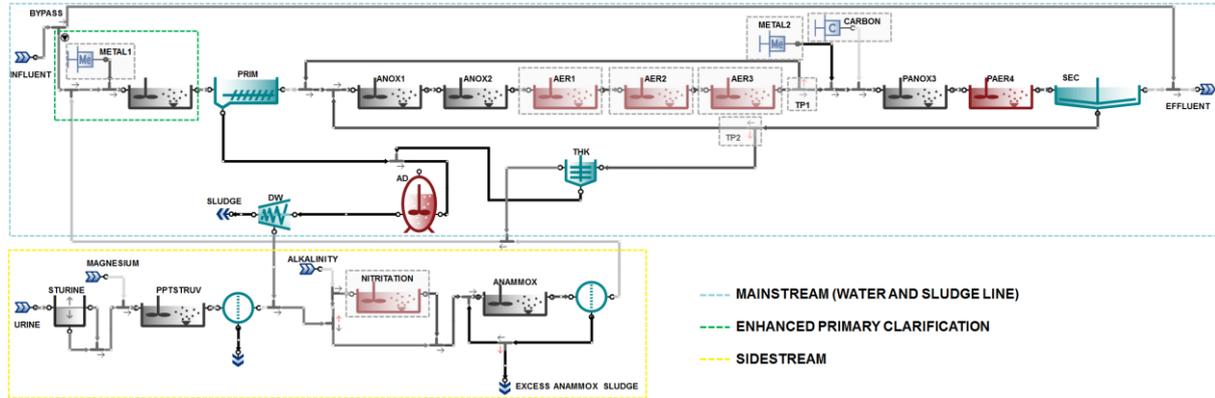


Figure V.3. Detailed configuration of the proposed WWTP scenarios in SUMO

Given the importance of dynamics on the operation of the plant, dynamic influents were considered in the simulation. Dynamic influents were generated by using an adapted dynamic and phenomenological influent generator proposed by Bisinella de Faria et al. (2016b) that considers wastewater and urine streams (in the case of urine source separation). Main characteristics of influent streams are given in table V.1.

Table V.1. Influent characteristics

Variable	Unit	REF		ANA	
		CONVENTIONAL WW	WW w/o 50% URINE	URINE	
Q	$\text{m}^3 \cdot \text{d}^{-1}$	18019.6	16991.7	82.1	
Soluble COD	$\text{gCOD} \cdot \text{m}^{-3}$	130.0	114.4	4869.8	
Particulate COD	$\text{gCOD} \cdot \text{m}^{-3}$	478.1	505.3	365.3	
Ammonium	$\text{gN} \cdot \text{m}^{-3}$	51.5	34.8	4121.0	
Organic N	$\text{gN} \cdot \text{m}^{-3}$	17.2	15.9	458.3	
Phosphate	$\text{gP} \cdot \text{m}^{-3}$	6.2	5.0	328.2	
Organic P	$\text{gP} \cdot \text{m}^{-3}$	5.4	5.5	18.8	

### V.2.3. Optimization problem formulation

#### V.2.3.1. Objective function

In order to account for all technical, economic and environmental aspects involved in the improvement of WWTP, 3 objective functions were subject to minimization: (1) Operational Cost Index (OCI) (Eq.

1); (2) Effluent Quality Index (EQI) (as this index represents the amount of pollutants being rejected to the environment after the treatment – Eq. 2) and (3) Life Cycle Impact Assessment (LCIA) (Eq. 3).

Equation 1 was taken from the original OCI formulation in BSM2 (Alex et al., 2008) and was adapted to this case study in order to account for the real market prices provided by the field experts. The corresponding constants are given in table V.2. Additionally, in order to provide a realistic approximation of the net operational cost of the plant, nutrient recovery and electricity production from biogas cogeneration were also taken into account, together with the costs related to the consumption of raw materials and energy. It should be noted that, in equation 1, C stands for consumed and P for produced.

$$OCI = \alpha_1 C_{electricity} + \alpha_2 C_{methanol} + \alpha_3 C_{FeCl_3} + \alpha_4 C_{MgO} + \alpha_5 C_{NaOH} + \alpha_6 C_{heat} - \alpha_7 P_{electricity} - \alpha_8 P_{struvite}$$

Equation 1

Table V.2. Proposed  $\alpha$  values for OCI function

	Unit	Value
$\alpha_1$ Consumed electricity	€/KWh	0.07
$\alpha_2$ Methanol	€/kg	0.412
$\alpha_3$ FeCl <sub>3</sub>	€/kg	0.4
$\alpha_4$ MgO	€/kg	0.188
$\alpha_5$ NaOH	€/kg	0.35
$\alpha_6$ Consumed heat	€/MJ	0.008
$\alpha_7$ Produced electricity	€/kWh	0.175
$\alpha_8$ Produced struvite	€/kg	0

Equation 2 (EQI) was initially taken from the original BSM2 (Alex et al., 2008). However, it was completed by including a new pollutant index (TP) designating the total phosphorus released in effluent, as this reject must respect specific regulation laws. The coefficients used in Equation 2 are provided in table V.3.

$$EQI = \beta_1 NO_x + \beta_2 BOD + \beta_3 COD + \beta_4 TKN + \beta_5 TSS + \beta_6 TP$$

Equation 2

Table V.3. Proposed  $\beta$  values for EQI function

		<b>Value</b>
$\beta_1$	<b>Nitrate + Nitrite</b>	10
$\beta_2$	<b>BOD</b>	2
$\beta_3$	<b>COD</b>	1
$\beta_4$	<b>TKN</b>	30
$\beta_5$	<b>TSS</b>	2
$\beta_6$	<b>TP</b>	100

In the present work, current cost coefficients ( $\alpha_i$ ) and pollutant indexes for effluent quality ( $\beta_i$ ) have been precisely suited for the global scenario in present Europe. However, when considering the structure of the developed framework, these values can be easily readjusted for other benchmarks in order to fit, for instance, geographical market prices and problematic reject areas where, for instance, important quantities of phosphorus are to be avoided. Moreover, it should be noticed that, a zero market price is attributed to struvite, even in case it is valorised in agriculture. This reason is to be capable of accounting for the eventual situation through which the recovery and use of this fertilizer is not well accepted. Similarly, nitrogen and phosphorus in sludge were not financially valorised. Additionally, other operational costs such as the cost of labour were not included.

Equation 3 (LCIA) represents the calculation of the environmental impacts using ReCiPe Endpoint 2008 (H, A) considering the aggregated sum that considers human health (HH), ecosystem diversity (ED) and resources availability (RA).

$$I_e = \sum_i Q_{ei} m_i$$

Equation 3

Where  $m_i$  is the magnitude of intervention  $i$ ,  $Q_{ei}$  is the characterisation factor that connects the intervention  $i$  to the respective endpoint impact category  $e$ , and  $I_e$  is the indicator result for the endpoint impact category  $e$  (Goedkoop et al., 2009). The ReCiPe Endpoint indicator resulted from the aggregation of normalized and weighted endpoint impacts and was used in this study as an environmental objective to be minimized.

Moreover, in an effort to respond to different decision makers' requirements, on a complementary problem formulation, environmental impact was also optimized based on the ReCiPe Midpoint 2008 (H) Global Warming Potential (GWP) indicator.

### V.2.3.2. Decision variables and constraints handling

The set of chosen decision variables in the present work depends on the choice of scenario studied. The decision variables in REF and ANA scenario are listed in table V.4. The choice of decision variables was made based on their sensitivity through expert analysis and was previously justified in Bisinella de Faria et al. (2016a).

Table V.4. Decision variables chosen for REF and ANA scenarios

Parameter	Description	Unit	REF reference value	ANA reference value	Lower level	Higher level
DO <sub>1</sub>	Dissolved oxygen concentration in the first aerated reactor	g O <sub>2</sub> .m <sup>-3</sup>	1.50	1.50	0.25	4.00
DO <sub>2</sub>	Dissolved oxygen concentration in the second aerated reactor	g O <sub>2</sub> .m <sup>-3</sup>	2.00	2.00	0.25	4.00
DO <sub>3</sub>	Dissolved oxygen concentration in the third aerated reactor	g O <sub>2</sub> .m <sup>-3</sup>	0.50	0.50	0.25	4.00
DO <sub>NITRITATION</sub>	Dissolved oxygen concentration in the nitrification reactor	g O <sub>2</sub> .m <sup>-3</sup>	-	2.00	1.00	4.00
Q <sub>CARBON</sub>	Methanol addition in the post denitrification zone	m <sup>3</sup> .d <sup>-1</sup>	0.80	0.80	0.00	6.00
Q <sub>METAL1</sub>	Iron chloride addition in headworks (EPC)	m <sup>3</sup> .d <sup>-1</sup>	-	2.00	0.50	6.00
Q <sub>METAL2</sub>	Iron chloride addition for polishing (post denitrification zone)	m <sup>3</sup> .d <sup>-1</sup>	4.00	0.80	0.00	4.00
Q <sub>I</sub>	Internal recycle flowrate to denitrification	m <sup>3</sup> .d <sup>-1</sup>	50,000	40,000	1,000	55,000
Q <sub>W</sub>	Sludge wastage	m <sup>3</sup> .d <sup>-1</sup>	400	300	50	500

DO<sub>NITRITATION</sub> is not included as variable in case of REF scenario as sidestream does not exist; Q<sub>METAL1</sub> variable is also excluded for REF scenario as no EPC is envisaged in this scenario.

Finally, in the context of WWTP optimization, the legally imposed limits on rejects shall be, in average, respected. For the problem formulation under constraints, the reject limits were set to 10

$\text{gN.m}^{-3}$  for total nitrogen,  $1 \text{ gP.m}^{-3}$  for total phosphorus,  $100 \text{ gCOD.m}^{-3}$  for total COD,  $35 \text{ gTSS.m}^{-3}$  for total suspended solids and  $4 \text{ gN.L}^{-3}$  for ammonium ion.

To satisfy these conditions, constraints were explicitly included in the problem formulation to check their violations during the last 14 days of simulation. However, as system is simulated dynamically, it is also important to check the number of daily violations in order to ensure, for instance, the absence of high pollutant peaks in daily rejects.

### V.2.3.3. *Recall on optimization problem formulation*

Several combinations of scenarios and problem formulations are hereafter proposed (table V.5). The first aim in this regard is formerly to observe the relevance of different problem formulations and assumptions in case of WWTP optimization (case studies A to D in table V.5). At this level, the following comparisons have been carried out: constrained *versus* unconstrained problem formulations, dynamics *versus* steady-state (with averaged influent) simulations and total Endpoint *versus* the Midpoint GWP as the choice of environmental impacts assessment method. Given the first set of comparative studies, the second goal is to evaluate the consistency of an innovative WRRF scenario (case study E in table V.5) while a suited problem formulation is used, under the most realistic conditions of simulation.

Table V.5. List of comparative studies on different problem formulations and innovative scenarios in the field of WWTP optimization

Case study	Scenario	Dynamics	Constraints	LCIA
A	<b>REF</b>	Yes	No	Endpoint
B	REF	Yes	<b>Yes</b>	Endpoint
C	REF	<b>No</b>	No	Endpoint
D	REF	Yes	No	<b>Midpoint GWP</b>
E	<b>ANA</b>	Yes	Both	Endpoint

### **V.3. Results and discussion**

In this section, results of the conducted optimization will be presented together with the corresponding interdependencies between objective functions. The optimal decision variables together with the main drivers of the proposed configurations as well as the consequences of different problem formulations will be pointed out. Here, the graphical representations were all carried out through the Matplotlib (Hunter, 2007) under Python.

#### *V.3.1. Reference scenario*

##### *V.3.1.1. General results*

Before the analysis of the alternative optimization scenario, results over the reference scenario were presented. Figure V.4 presents the 3D Pareto optimal curve achieved for the reference scenario. As previously highlighted, this curve was obtained with a low computation budget of 300 function evaluations (simulation runs). The complexity of objective functions as well as their interdependencies resulted in a tri-dimensional curve instead of a tri-dimensional surface. A tri-dimensional curve is usually attained where the adjacent solutions are dominated, from a multi-objective optimization point of view, and therefore, the condition of global optimality is hard to achieve. This is another proof on the importance of choosing evolutionary algorithms for optimization instead of conventional local search methods.

In figure V.4, axes present the operational cost represented by OCI, the quality index (pollutants rejected) represented by EQI and the total environmental impacts calculated by the total aggregated ReCiPe Endpoint approach via LCIA. Two sets of points, obtained from two different problem formulations were presented in figure V.4. The first problem formulation, namely the case study A (table V.5) was illustrated by yellow and green points in figure V.4 (Zone Ia and Ib). This formulation represents an unconstrained problem for the reference scenario. The second problem formulation, namely the case study B in table V.5 was shown in figure V.4 through blue and rose points (Zone II and III). The latter corresponds to a constrained problem formulation where better output water quality is expected to be obtained.

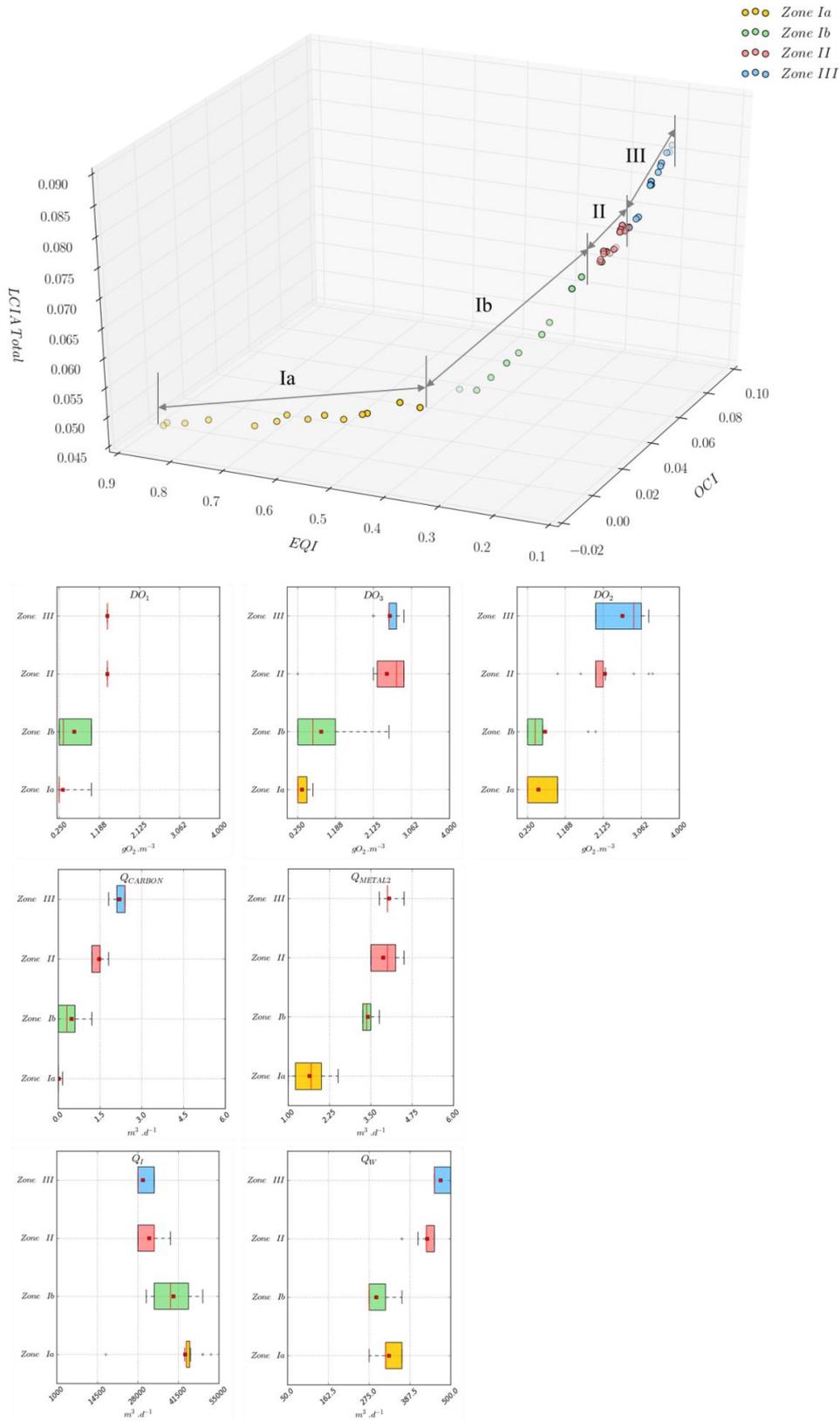


Figure V.4. Pareto-optimal curves for constrained and unconstrained optimization of the reference WWTP

[bottom illustrations are the box-and-whisker plots on decision variables]

Box-and-whisker plots were given on each decision variables and for each zone, through complementary illustrations (bottom graphics in figure V.4). In each box, the small red square represents the average value and the red line represents the median. The 25<sup>th</sup> and the 75<sup>th</sup> quartile were represented by the edges of the box and the whiskers were extended to the most extreme data that are not considered as outliers (represented by '+' sign beyond the whiskers). Also, in order to represent the distribution of decision variables over the lower and higher boundaries, ranges through the x-axis of the plot were set to the same boundary values fixed for the optimization.

From figure V.4, a direct correlation between objective functions can be seen. In general, OCI and LCIA showed to be positively correlated, as both have the same direction of increase. However, EQI and LCIA showed to be negatively correlated. Moreover, when EQI is reduced (less pollutants rejected) the global environmental impact increases. This behaviour might be justified by the important impact of background processes, already described in the literature, which influence both costs and environmental impacts. Consequently, OCI and EQI were negatively correlated, where an increase in quality – reduction of EQI – lead to more energy and chemicals consumption and consequently to higher operational costs.

As a result of individual efforts made by each objective function to achieve its own condition of optimality despite the contradictory effects between the objectives, four main zones, namely Zone Ia, Ib, II and III, appeared on the overall Pareto optimal front. The constrained zone (Zone II and III) represents the legal compliance imposed to more than 100,000 person equivalent WWTPs ( $TN < 10\text{gN.m}^{-3}$  and  $TP < 1\text{gP.m}^{-3}$ ). However, in order to give insights on plants functioning with less strict constraints, discussion will be also provided for Zones Ia and Ib concerning pollutants concentration. Nevertheless, it has to be noted here that no comparison over objective function results between different zones might be done as reject limits are different and thus the function of the system is not anymore the same (functional unit defined in this study:  $1\text{m}^3$  of treated water respecting  $10\text{gN.m}^{-3}$  for total nitrogen,  $1\text{gP.m}^{-3}$  for total phosphorus,  $100\text{gCOD.m}^{-3}$  for total COD,  $35\text{gTSS.m}^{-3}$  for total suspended solids and  $4\text{gN.m}^{-3}$  for ammonium ion).

Initially, it should be noticed that Zone I (points that do not respect the strict reject limits) was divided into Ia and Ib depending on the level of cost required to achieve a better quality (the shape of cost increase in each zone was represented by the average slope of the curve). Globally, Zone Ia and Ib correspond to a region where quality is not acceptable and the strict constraints are not respected. However, in these zones, important gains can easily be achieved without important increase in costs and environmental impacts. Actually, in zone Ia, TN objective for less strict constraints in WWTPs was reached ( $TN < 15\text{gN.m}^{-3}$ ); however, phosphorus elimination was not satisfactory ( $TP > 3.5\text{gP.m}^{-3}$ ). When considering Zone Ib, the constraints were all respected for the less strict regulation limits

( $TN < 15\text{gN.m}^{-3}$ ,  $TP < 2\text{gP.m}^{-3}$ ); in contrast, they were not respected for this study constraints. Details on each effluent concentration were given in figure V.5.

Zone II represents the real-world optimal operating zone for the considered plant in this study, as in this region, operating conditions are pushed to respect the legally imposed European reject limits (especially  $TN < 10\text{gN.m}^{-3}$ ,  $TP < 1\text{gP.m}^{-3}$ , figure V.5) with reasonable efforts regarding the environmental impacts and cost. Finally, Zone III was represented by extremely low quantities of pollutants rejected and thus by a great effluent quality ( $TN < 5\text{gN.m}^{-3}$  and  $TP < 1\text{gP.m}^{-3}$ ). Nevertheless, despite achieving the highest quality in this zone, a slight increase in quality resulted in considerable increase in environmental impacts and operational costs, which is not necessarily desired.

These results are in accordance with the previous ones proposed by authors (Bisinella de Faria et al., 2016a) throughout a feasibility study of the WWTP optimization platform. One of the major conclusions that might be drawn here is that, even in the case of a well established technology, such as a conventional wastewater activated sludge treatment process, there is a limit point up to which the treatment is still reasonable and practical. Beyond this limit point, if one wishes to still improve the quality (decreasing EQI above the Zone II), a new technology should be conceived.

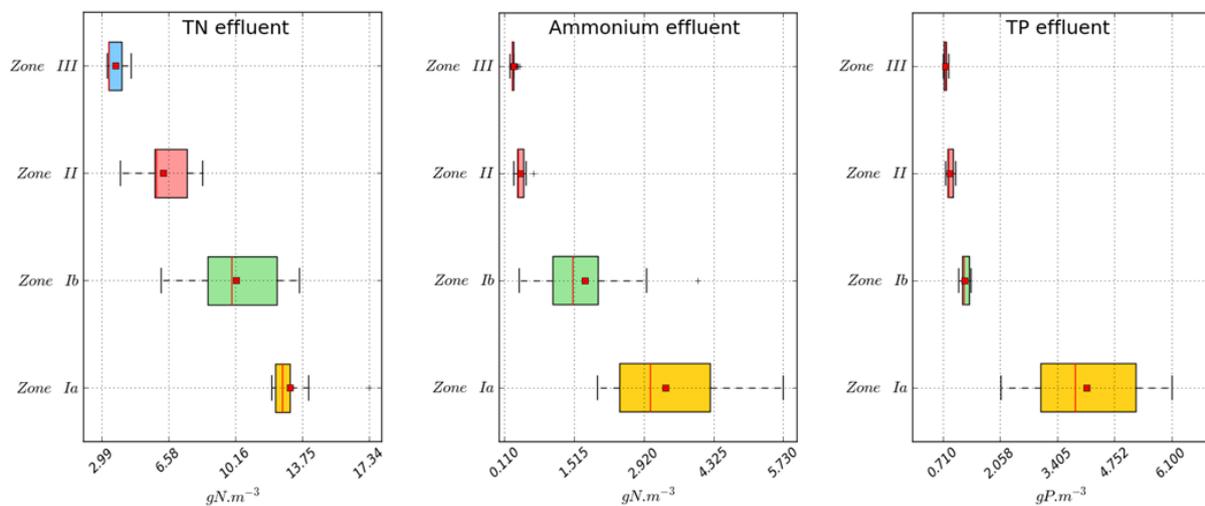


Figure V.5. Box-and-whisker plots for total nitrogen, ammonium ion and total phosphorus concentrations in effluent for the optimized reference scenario (REF)

Moreover, in order to better understand the limitation of the technology, disaggregation of the total Effluent Quality Index was presented in figure V.5 for total nitrogen, total phosphorus and ammonium in effluent. Also, even if Total Suspended Solids (TSS) and Chemical Oxygen Demand (COD) are

included in the quality index and as constraints, they were not given in figure V.5 as they respect reject limits all along the Pareto front.

It has been previously indicated that, strict constraints were respected only in Zone II and III. However, the total nitrogen started already having a reasonable level in Zone Ib, while for phosphorus the acceptable level was only achieved in Zone II and III. This might represent the great difficulty of achieving low phosphorus concentration in effluent without adaptations in plant (as only chemical precipitation is applied in this WWTP). Instead, the nitrogen treatment had more important operation flexibility, as more variables are involved with their own interactions (DOs, carbon addition, internal recirculation). Accordingly, there was no increase in quality from Zone II to III, due to the decrease in phosphorus reject concentration (figure V.5).

Also, when considering the nitrogen conversion from ammonium ion to nitrite/nitrate and finally to  $N_2$ , it might be concluded that the shift from Zone II to Zone III (where low EQI is achieved with more important cost) represent an advanced post-denitrification, where ammonium cannot be further reduced and thus nitrite/nitrate are tackled (figure V.5). This behaviour might also be explained from two points of view. Firstly, the weights were attributed differently in the EQI function, for instance, TKN presented a greater weight (30) than  $NO_x$  species (10), and therefore, in order to minimize EQI, it is preferable to minimize TKN before the  $NO_x$  minimization. Similarly, when minimizing OCI, electricity contribution seemed to increase slightly from Zone II to III while carbon addition contribution increased markedly (figure V.6)

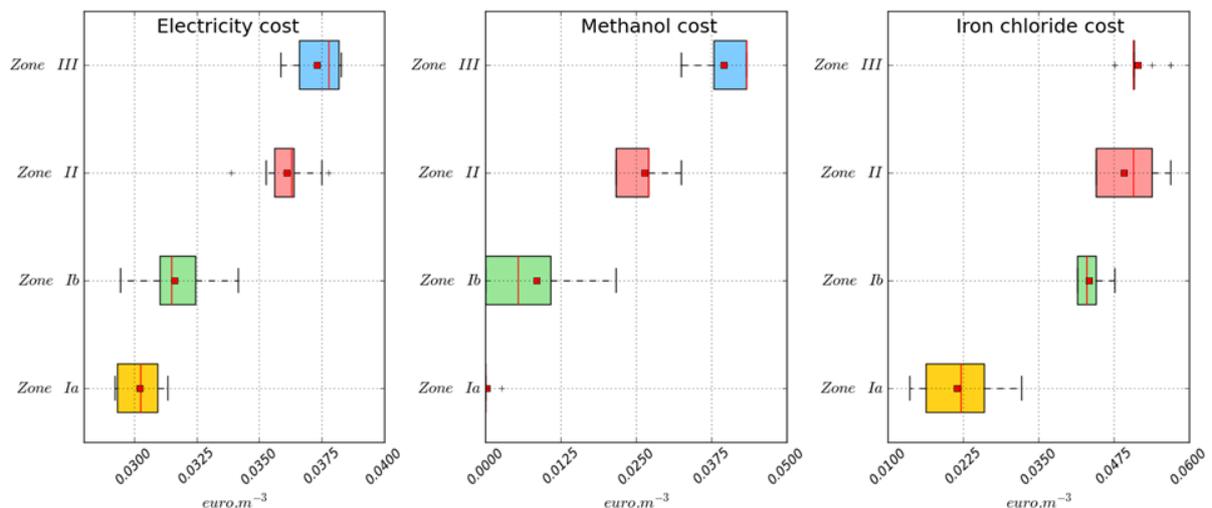


Figure V.6. Box-and-whisker plots for the main cost contributors in Operational Cost Index (OCI) function for the optimized reference scenario (REF)

The constraint violation for ammonium happened only in Zone I and when low DO was fixed. This is the case, when all three DOs were set to  $0.25\text{gO}_2\cdot\text{m}^{-3}$ .

Further, when comparing the constrained *versus* the unconstrained Pareto fronts, it should be noted that given the fixed population size for the optimization, the same number of points will be used to describe the diversity in Pareto fronts. Consequently, for an unconstrained problem formulation (case studies A, C and D), the Pareto fronts were mainly concentrated around the Zone I, and were not necessarily intended to provide more details (optimal solutions) over the zones where the strict reject limits were satisfied. The identification of Zone I is important due to the minimum operational cost associated to this zone. However, an unconstrained optimization formulation, where no reject constraint is explicitly imposed to problem, might result in a set of optimal solutions, as in Zone I. Such a formulation is quite impractical to use, due to the unacceptable level of effluent quality in results.

#### V.3.1.2. *Analysis on decision variables*

In order to analyse the influence of decision variables over the 4 zones in the Pareto front, as previously illustrated in figure V.4, box-and-whisker plots were provided. These plots (bottom plots in figure V.4) allowed studying the variability of decision variables per Pareto optimal zone. Globally, when considering average values of dissolved oxygen set points, a correlation with EQI can be observed, as the increase in DO values leads to a shift from one zone to another. Moreover, a markedly increase, passing from zone Ib to II, was observed for all the three DO set points (figure V.4). This DO increase was responsible for the great conversion of ammonium nitrogen through other forms of nitrogen, nitrite and nitrate, which have a lower weight than the ammonium ion in the EQI function. Deeply on  $\text{DO}_1$ , in Zone Ia, II and III, variations in the interquartile range was almost inexistent and thus variable values were almost punctual. Consequently, there was no flexibility over its set point leading to one fixed operational set point. When considering the dissolved oxygen set point for the secondary basin ( $\text{DO}_2$ ), all zones in figure V.4 presented an important variability in the interquartile range, and some outliers showed possible alternative functioning points. Finally,  $\text{DO}_3$  presented a similar behaviour as  $\text{DO}_2$ . Overall, there was not a large range for dissolved oxygen operation and, in general, DO values could be suitably set for each zone.

When considering carbon addition, an almost linear increase was noticed among the represented zones. A relatively small addition of carbon lead to a shift from one zone to another and, globally, the choice of the variable set point do not present much flexibility. Also, as previously discussed, the shift from Zone II (good quality with acceptable cost) to Zone III (good quality with exaggerated cost)

seemed to be governed by the carbon addition (leading to an advanced post denitrification). Therefore, it is possible, from a technological point of view, to obtain a very high water quality in terms of nitrogen rejects. However, the latter would lead to inadvertent increases in cost and environmental impacts and therefore, new ways of managing nitrogen in the plant (or avoiding its entrance in the plant) are required.

The amount of metal addition had also an important influence on the shift between different zones over the Pareto optimal front (figure V.4). This was especially the case when going from Zone Ia to Zone Ib, as when a great amount of phosphate is available, in the beginning of the treatment, it is quite easy to eliminate it. Therefore, in this case, the plant required an increase in the amount of iron chloride added in order to markedly decrease phosphorus concentration in effluent. However, from Zone II to Zone III, there was almost no increase in metal addition. This might be justified, as previously discussed, by the limitation of P-elimination technology in the reference case - P is mainly eliminated by chemical precipitation of phosphate, whereas residual P is also organic. Thus, in Zone II, constraints were already respected and almost no more phosphorus was eliminated in Zone III. It is also important to notice the variation of metal addition along its fixed boundaries (the molar ratio of  $Fe/P_{Total}$  varies from 0.5 to 2.3). Globally, lower and higher averages were quite far from the extreme boundaries, which validate the choice of wide ranges for variables during the optimization of the WWTP.

The only variable presenting an opposite trend compared to all others was the internal recycle,  $Q_I$ . This is mainly explained by the increase in carbon addition that was required to achieve good treatment.  $Q_I$  must indeed decrease as denitrification will take place afterwards in the post-anoxic zone. However, there is still a flexibility in the operation of the internal recycle, represented by boxes boundaries, except for Zone Ia, where treatment is really poor (together with the low DOs and the low carbon addition) and thus high recirculation is required to achieve the best, however not sufficient, treatment.

Finally, the wastage, represented by  $Q_w$ , presented a dispersed behaviour with lower values for Zone Ia and Ib and, with higher values for Zone II and III. Globally, higher sludge wastage was allowed in Zone II and III, as more organic matter was available and thus more biomass was expected in the reactors allowing more sludge wastage in order to increase biogas production and to compensate the increase in electricity consumption.

Complementary to figure V.4, the correlation between decision variables and objective functions is provided in figure V.7. Results, which are represented through scatterplots in the upper triangle, Pearson product-moment correlation coefficients in the lower triangle, and the corresponding variable or function name on the main diagonal, are in accordance with the previously discussed correlations among objective functions and decision variables. Furthermore the Pearson product-moment

correlation coefficients over the whole Pareto (lower triangle in figure V.7, without distinction on zones), showed that OCI and EQI were mostly driven by carbon and metal addition, followed by DOs set points. This behaviour was also confirmed by the chosen gradient of  $Q_{\text{CARBON}}$  and  $Q_{\text{METAL2}}$ , presented through the bottom illustrations in figure V.7.

### V.3.1.3. *Steady state versus dynamic modelling approach*

Aiming to reinforce the reliability of results, a comparative study was conducted by considering dynamics of the plant, as opposed to a steady state condition of run. This problem formulation is justified by the importance of understanding the trends of objectives and decision variables when steady state conditions are considered.

In figure V.8, a comparison of the optimal Pareto front resulting from problem formulation A and C (table V.5) is presented. Accordingly, it can be observed that for high EQI values (poor treatment), the optimal results for the steady state conditions seemed to be close to the Pareto front obtained by the consideration of plant's dynamics and followed similar trends. However, an important gap can be noticed when EQI starts decreasing (where treatment started to effectively take place). The gap was followed in the region where constraints become stricter. From the authors' point of view, this trend is mainly related to the fact that, when constraints are stricter and thus, treatment is intensified to further improve the quality, steady state regime underestimates significantly costs and environmental impacts, as the influent flow and concentration peaks are not taken into account. Therefore, fictive water qualities would be obtained for the same operational cost. Moreover, when considering the distribution of decision variables over the optimal Pareto front, they seemed similarly to be underestimated. It was especially observed for the dissolved oxygen in the third basin  $DO_3$ , the metal addition and the internal recycle. Additionally, it should be noted that simulation runs based on steady state conditions do not allow the identification of daily violations of constraints.

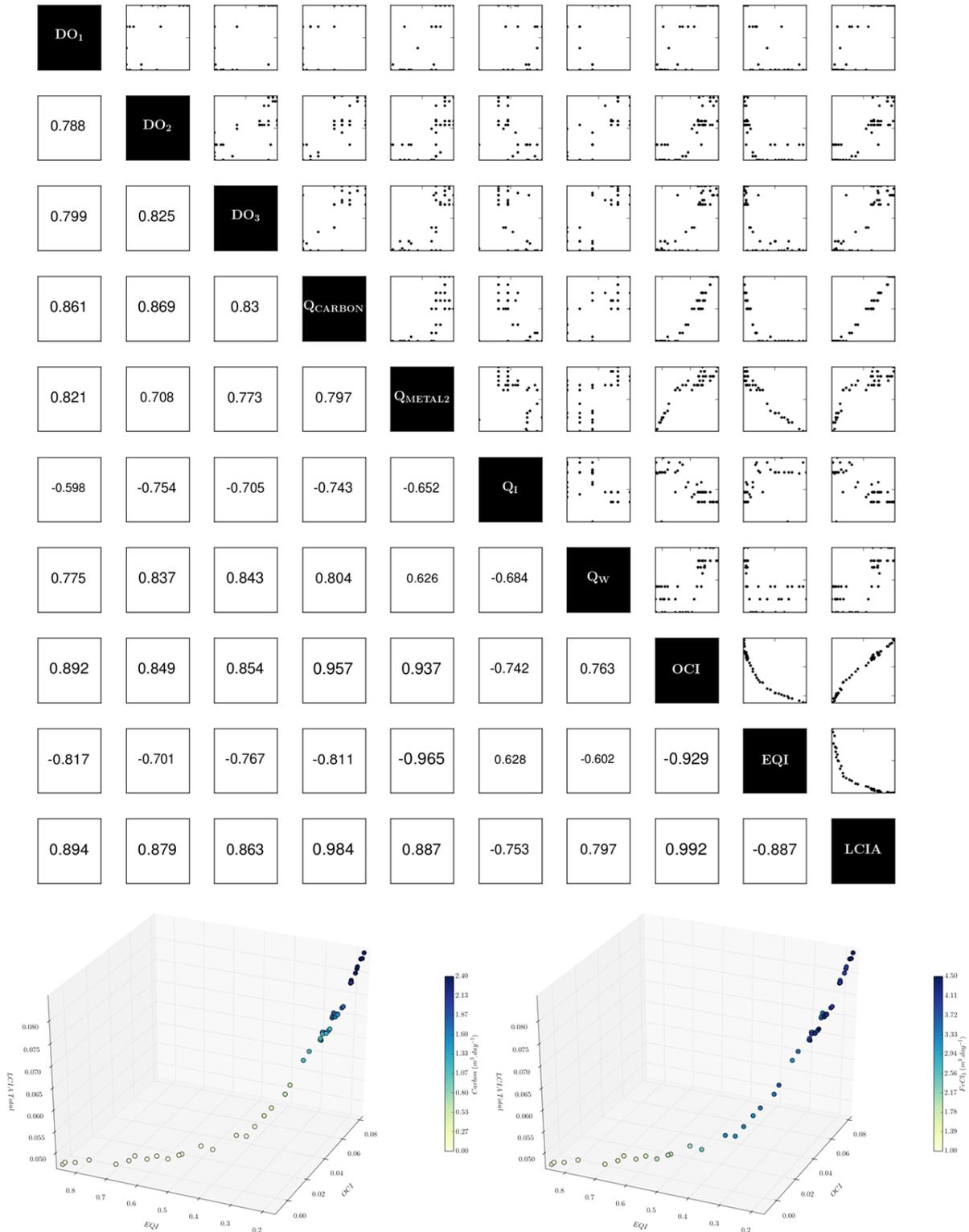


Figure V.7. Correlation scatterplots on decision variables and objective functions (optimized REF scenario)

[bottom illustrations represent the gradient of carbon and metal addition over the whole Pareto optimal front]

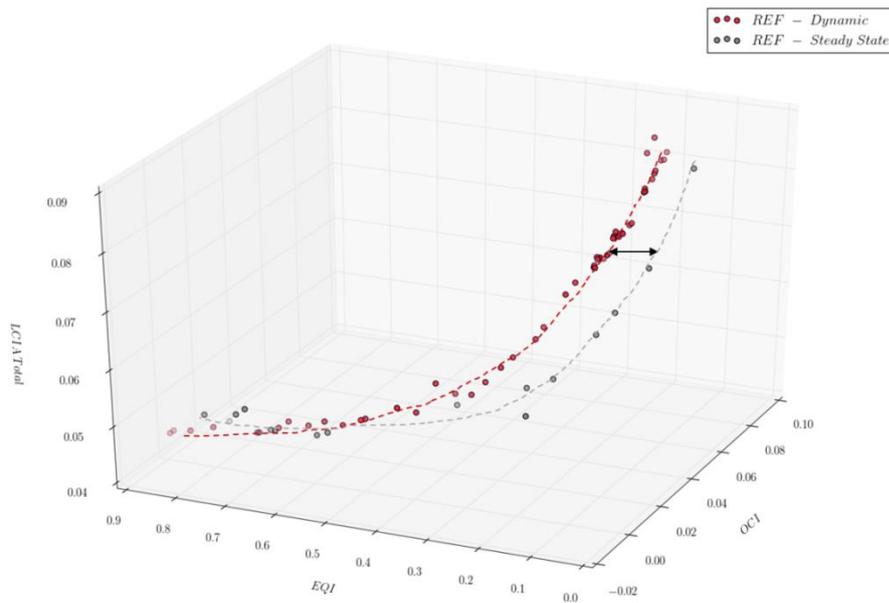


Figure V.8: Pareto-optimal fronts resulting from steady state *versus* dynamic simulations (REF scenario)

#### V.3.1.4. Total Endpoint versus Midpoint Global Warming Potential

As previously discussed, decision-making might become a difficult task in complex problems such as in WWTPs where not only several operational parameters (represented by decision variables) are involved, but also several conflicting objectives have to be optimized simultaneously. To provide comprehensive and visually descriptive results for decision-making, it is recommended to limit the number of objectives to 3 objective functions maximum. Nowadays, in the field of WWTPs, GHG emissions are one of the major issues to be minimized together with cost and performance. In order to show the contrast between an aggregated ReCiPe total Endpoint impact and the original endpoint categories of impact, a correlation against the most influencing impact categories in human health (HH), ecosystem diversity (ED) and resources availability (RA) was provided in Figure V.9. In this figure, the upper triangle represents the scatterplots, while the Pearson product-moment correlation coefficients were given in the lower triangle. The name of corresponding impact categories can be found on the main diagonal.

Pearson product-moment correlation coefficients in figure V.9 demonstrate that several endpoint impact categories are well represented by the aggregated ReCiPe total Endpoint impact. Actually, only one category, freshwater eutrophication (FEP ED), is negatively correlated to the aggregated index. However, as this impact is by nature linked to the discharge emissions, it was expected that their values would be correlated to the Effluent Quality Index, instead of the total environmental impact. As a result, it can be concluded that all main endpoint impacts presented a positive correlation to LCIA

(and consequently OCI), and a negative correlation to EQI. The latter indicates that the chosen aggregated ReCiPe total Endpoint impact category represents correctly the majority of the impacts categories. Finally, the strongest correlation was found between the aggregated ReCiPe total Endpoint impact and the Global Warming Potential (GWP) indicator for both human health (HH) and ecosystem diversity (ED). This might be explained by the important influence of GHG emissions in a WWTP's Life Cycle Analysis, as already shown by several authors in the literature.



Figure V.9. Pearson product-moment correlations between different impact categories in LCIA

[HH - Human Health; ED - Ecosystem diversity; RA - Resources availability; GWP - Global Warming Potential; HTP - Human Toxicity Potential; PMFP - Particulate Matter Formation Potential; FEP - Freshwater Eutrophication Potential; ALOP - Agricultural Land Occupation Potential; FDP - Fossil Depletion Potential]

By following the same idea of providing decision makers with complete and comprehensive information on each case study, it is important to verify for the present case study if the optimal solutions depend on the choice of impact categories or not. For this aim, a comparative study was carried out based on the use of the aggregated total ReCiPe Endpoint impact and the ReCiPe Midpoint GWP (scenarios A versus D in table V.5). Results, which consider also the two other common

objectives - OCI and EQI - showed Pareto fronts well fitted, which is to say that both impact categories resulted in almost the same optimal solutions. When comparing the 3D Pareto fronts, in general, similar trends on the curve were found and thus, the total endpoint represents a good approximation of the total GHG minimization (including direct and indirect emissions). This observation, however, is case specific, and might not be generalized. According to the scenarios studied in the present work, it should be noted that in order for the midpoint GWP impacts to fit the same trends as in total ReCiPe endpoint impact, all relevant emissions through the life cycle in foreground and background processes must be accurately taken into account.

### V.3.2. *Alternative scenario (ANA)*

The final part of this study is dedicated to the comparison of the conventional wastewater management and treatment (REF scenario) against an alternative WRRF (ANA scenario). The comparative results on these scenarios were provided in figure V.10. Regarding the ANA scenario, two optimization runs were carried out, one unconstrained (Zone Ia and Ib) and one with strict constraints (Zone II and III). The same distinction of 4 zones over the optimal Pareto front was done for this alternative scenario. The bottom graphics in figure V.10 represent the box-whisker plots over the decision variables.

Globally, the alternative scenario showed to offer an interesting gain in the functioning of the wastewater treatment in terms of performance, operational cost and environmental impacts. For instance, for a fixed water output quality, fewer costs were achieved together with less environmental impacts through ANA scenario.

Also, from figure V.10, it is important to indicate that in both technologies, a high water quality can be attained (lowest EQI equal to 0.18 in Zone III), and if the decision maker wishes still to decrease EQI below 0.18, compromises have to be made, as cost and environmental impacts would exaggeratedly increase through both technologies.

Similarly to the reference scenario, OCI showed to be positively correlated to LCIA while EQI is negatively correlated to the previous. By following the trends in decision variables, the metal and carbon addition presented a similar behaviour, with a limited flexibility in the variable operation. Also, similarly to the trend observed in REF scenario, there was no increase in metal addition between Zone II and III; however, the carbon addition increased aiming to eliminate the residual nitrite and nitrate. Regarding the metal addition, the presence of a quite fixed optimal point for the distribution of metal in headworks (for the enhanced primary clarification) and by the end of the mainstream (for polishing of phosphorus treatment) was observed.

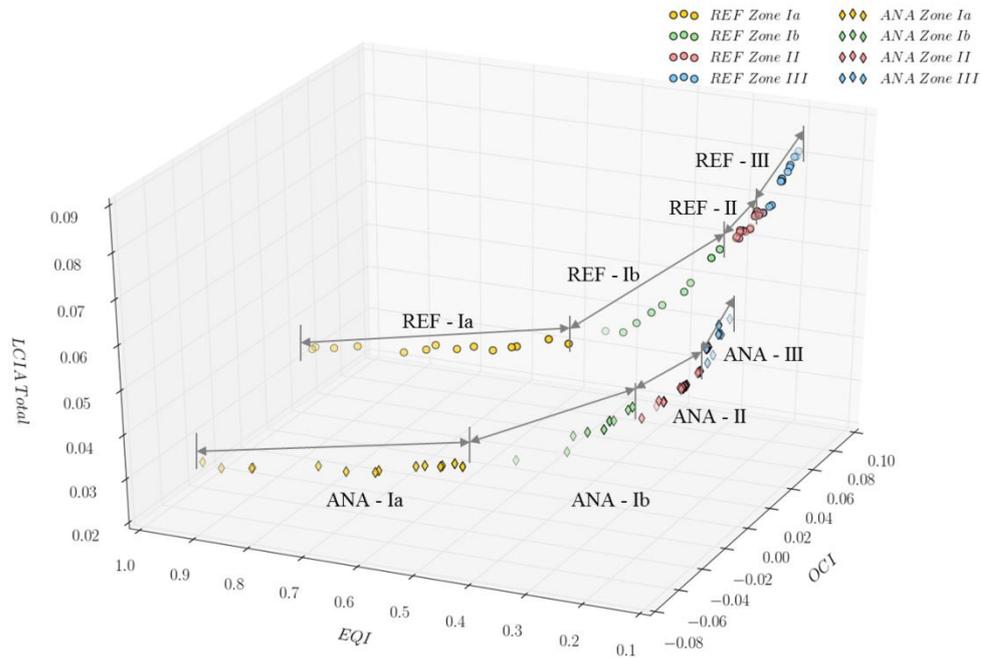


Figure V.10: Comparative optimal Pareto fronts on the reference scenario (REF) *versus* the urine treatment by nitritation/ anaerobic deammonification (ANA)

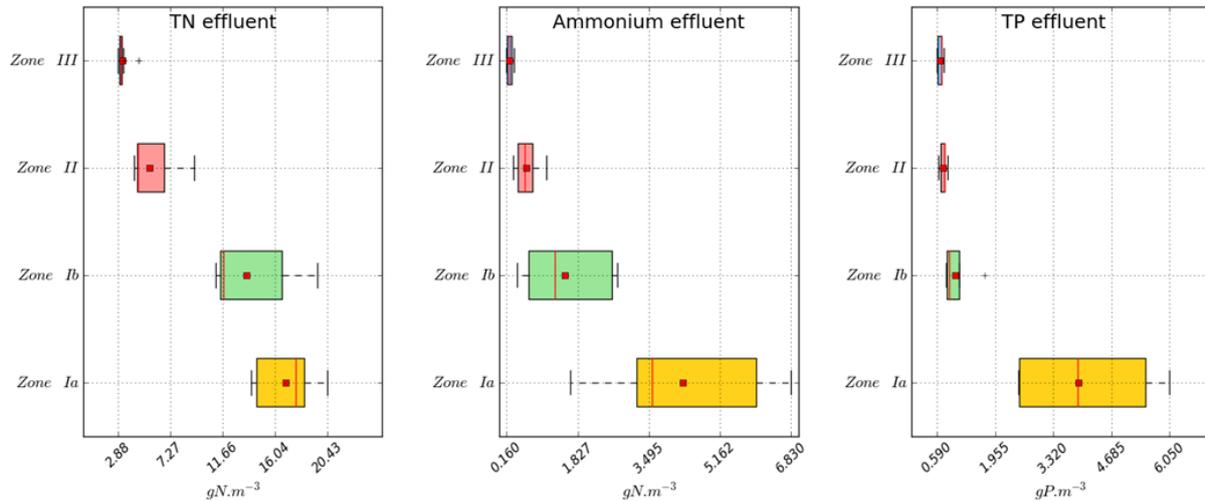


Figure V.11. Box-and-whisker plots on total nitrogen, ammonium ion and total phosphorus concentrations in effluent of the optimized ANA scenario

Considering the dissolved oxygen values for the first three basins, results followed the expected trends, with fewer requirements in aeration as less nitrogen was present. However, DO values seemed to be extremely low for some optimal points bringing in the question of plant redesign when urine source separation is envisaged at a proportion of 50% coupled to enhanced primary clarification.

When considering  $DO_{\text{NITRITATION}}$ , values seemed to be stable around  $2\text{gO}_2.\text{m}^{-3}$  for all zones (figure V.10); however, even if an unexpected large range in Zone Ia and Ib was noticed, it did not seem to considerably influence the performance and energy consumption in the plant. Finally, the optimal solutions were not recognized as being sensitive to internal recycle ( $Q_I$ ) and wastage ( $Q_W$ ).

Regarding the effluent concentrations over the optimal zones in figure V.11, it should be noticed that in Zone Ia, neither nitrogen nor phosphorus reject limits were respected. However, in the following zone (Zone Ib), less strict reject limits ( $\text{TN} < 15\text{gN}.\text{m}^{-3}$  and  $\text{TP} < 2\text{gP}.\text{m}^{-3}$ ) were fully satisfied. In addition, Zone II and III respected the strict constraint limits imposed in this study ( $\text{TN} < 10\text{gN}.\text{m}^{-3}$  and  $\text{TP} < 1\text{gP}.\text{m}^{-3}$ ) with an extremely low amount of nitrogen reject in Zone III (TN around  $3\text{gN}.\text{m}^{-3}$ ).

### V.3.3. Consequences on energy autarky

With a view to energy autarky in wastewater treatment plants, one might propose the addition to the optimization problem of a supplementary objective function or constraint based, for instance, on the ratio between the recovered amount of energy and the consumed one. This parameter is hereafter

called as Energy Return On Investment (EROI). However, given the results provided earlier, it was found that EROI is fully driven and optimized via the previously chosen objectives. Figure V.12 presents the improvement in EROI (by colour gradient) along with the Pareto-optimal front in the reference case. Box-and-whisker plots were presented for electricity consumption and production in both REF and ANA scenarios through the bottom illustrations in figure V.12. As it might be noted, even without considering EROI explicitly among the objective functions for the REF scenario, it was optimized implicitly as followed the changes in three other functions. There is thus no need for a systematic integration of EROI in the problem formulation, unless the cost and LCIA were not genuinely approximated.

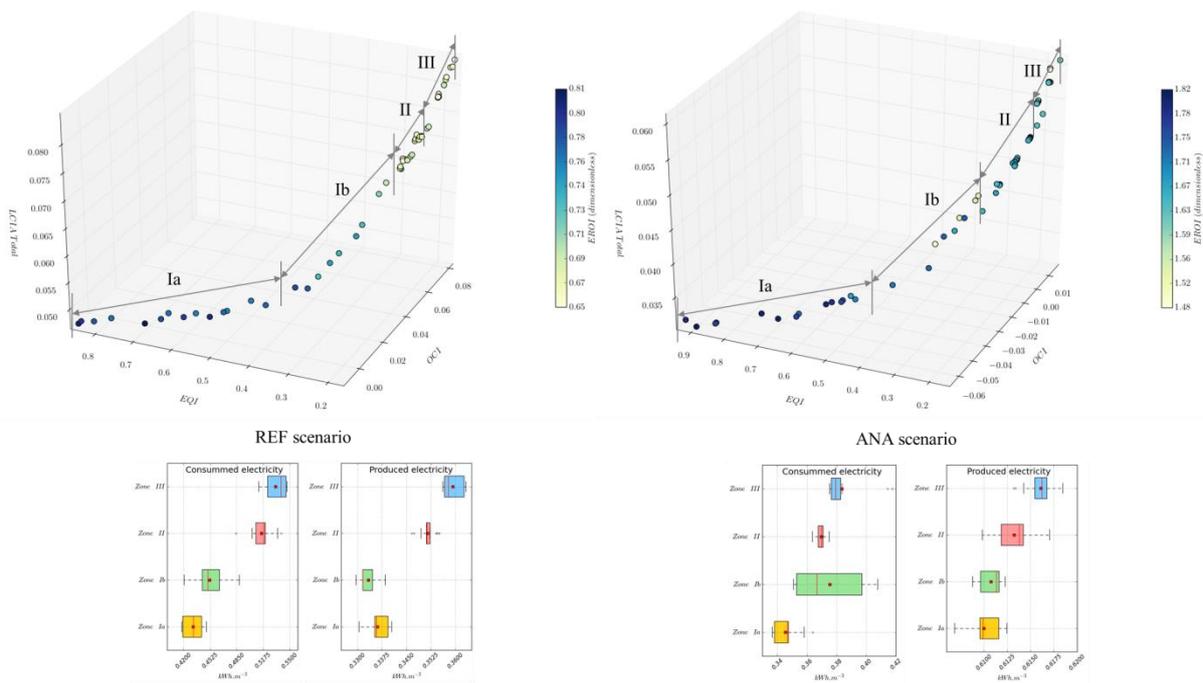


Figure V.12: EROI (Energy return on investment) calculations for all solutions belonging to the optimal Pareto front (REF and ANA scenarios)

[bottom graphics are box-whisker plots on consumed and produced electricity for REF and ANA scenarios]

Moreover, it is important to state that, for the reference scenario, the optimal values did not allow the energy autarky to be achieved (EROI ranging from 0.65 to 0.81) and more specifically, EROI faced a decrease in Zone II and III, as a consequence of consuming more energy to provide better qualities. In reality, regarding the reference scenario, to achieve a relevant treatment, EROI cannot attain high values as the electricity consumption increases rapidly whereas its production encounters a slight increase only. From Zone Ia to Zone III, the electricity consumption rose from 0.43 to 0.53 kWh.m<sup>-3</sup>

while the produced electricity faced a slight increase from 0.34 to 0.36 kWh.m<sup>-3</sup>, which is to say an increase of 19% and 6%, respectively.

As opposed to REF scenario, the alternative ANA scenario did not present a strong correlation of EROI with quality over the optimal Pareto front (figure V.12), as DOs were not highly correlated with objective functions. The problem drivers were indeed identified to be mainly the methanol and iron chloride addition.

However, with a view to box-whisker plots (bottom figure V.12), it might be noted that, similarly to REF scenario, the shift from one zone to another (in the sense of decreasing EQI), increased the energy consumption; however, the produced electricity did not face any significant change during the shift. Moreover, ANA scenario allowed, for all zones, the energy autarky with EROIs evolving from 1.48 to 1.82 due to an important increase in energy production compared to REF scenario.

#### *V.3.4. Benefits achieved from REF and ANA scenarios*

Table V.6 summarizes the main differences found when comparing REF and ANA scenarios with the objective functions being the effluent quality index, the operational cost and the environmental impacts, and by accounting for the amount of produced and consumed electricity, the addition of chemicals (iron chloride and methanol), the main reject concentrations (Total Nitrogen and Total Phosphorus) and GHG emissions by the endpoint category climate change for human health and ecosystem diversity. Also, general gains, which were presented in table V.6 (% gain is represented by (ANA-REF)/REF) passing from REF scenario to ANA scenario were shown throughout Zone II and III (figure V.10).

As previously discussed, comparison might not be established for Zones Ia and Ib as the functional unit of the system is not the same considering the respected constraints. Throughout this study, it has been demonstrated that for Zone II and III, which represent the most relevant operating zones, all process parameters and objective functions were improved. Among the main gains, it is important to highlight the improvement in OCI by approximately 100% (due to the “negative cost” of electricity production), in quality by 10% and in environmental impacts (using the total aggregated ReCiPe Endpoint indicator) by 30%.

Both consumed and produced electricity presented important gains. Considering the consumption, it was decrease by 28% and an increased of more than 70% was observed for produced electricity. Moreover, chemical addition decreased by more than 20% for methanol and 21% for iron chloride due, respectively, to less nitrogen and less phosphorus entering the plant to be conventionally treated.

When considering reject limits, even if in both scenarios constraints were respected for Zones II and III, ANA scenario allowed a decrease of 12% in rejected total nitrogen and of approximately 15% in total phosphorus.

Finally, for the GHG emitted over the total life cycle (foreground and background together with avoided impacts), an important decrease of approximately 30% in climate change impact was noted for both human health and ecosystem diversity category.

Table V.6. Benefits derived from ANA scenario when compared with REF scenario

Average value for each zone	REF		ANA			
	II	III	II		III	
<b>OCI</b> ( $\text{€} \cdot \text{m}^{-3}$ )	0.056	0.071	-0.009	<b>-116%</b>	0.006	<b>-91%</b>
<b>EQI</b> ( $\text{kg poll-Eq} \cdot \text{m}^{-3}$ )	0.207	0.179	0.189	<b>-9%</b>	0.165	<b>-8%</b>
<b>LCIA</b> (points)	0.073	0.081	0.051	<b>-31%</b>	0.058	<b>-28%</b>
<b>Consummed electricity</b> ( $\text{kWh} \cdot \text{m}^{-3}$ )	0.52	0.53	0.37	<b>-28%</b>	0.38	<b>-28%</b>
<b>Produced electricity</b> ( $\text{kWh} \cdot \text{m}^{-3}$ )	0.35	0.36	0.61	<b>+74%</b>	0.62	<b>+72%</b>
<b>Methanol addition</b> ( $\text{m}^3 \cdot \text{d}^{-1}$ )	1.46	2.19	1.07	<b>-27%</b>	1.73	<b>-21%</b>
<b>Iron chloride addition</b> ( $\text{m}^3 \cdot \text{d}^{-1}$ )	3.87	4.06	3.04	<b>-21%</b>	3.19	<b>-21%</b>
<b>TN effluent</b> ( $\text{gN} \cdot \text{m}^{-3}$ )	6.29	3.72	5.52	<b>-12%</b>	3.29	<b>-12%</b>
<b>TP effluent</b> ( $\text{gP} \cdot \text{m}^{-3}$ )	0.88	0.76	0.74	<b>-16%</b>	0.66	<b>-13%</b>
<b>Climate change – Human health</b> (points)	0.022	0.024	0.015	<b>-32%</b>	0.017	<b>-29%</b>
<b>Climate change – Ecosystem diversity</b> (points)	0.015	0.016	0.010	<b>-33%</b>	0.011	<b>-31%</b>

## V.4. Conclusions

When evaluating WWTP scenarios, the decision-making is at the same time a crucial and difficult task. Commonly, there are several interconnected parameters and variables as well as multiple conflicting objectives. In this sense, the multi-objective optimization allows for a harmonious optimization of each objective despite their intrinsic contradictions, and therefore, provides a diverse set of optimal solutions. Throughout this study, it has been demonstrated that a coupled Dynamic Modelling - Life Cycle Assessment - Efficient Multi-Objective Optimization (DM-LCA-EMOO) platform is truly needed to provide a proper evaluation and comparison between different conventional and innovative WWTP scenarios, to allow further discussions on functions interdependencies, and to construct a reliable basis for decision-making.

With regards to optimal wastewater treatment and management scenarios, the main process drivers were identified to be carbon and metal addition followed by dissolved oxygen set points. Throughout the optimal solutions, four main zones were particularly highlighted over the Pareto-optimal front where treatment performance depended on the achievement of more or less strict constraints. Energy aspects were also discussed by means of the consumed and produced electricity and the energy return on investment (EROI). It was proved that the alternative scenario ANA is capable of achieving energy autarky by decreasing electricity consumption and increasing its production.

Moreover, the consequences resulting from the problem formulation, the simulation conditions (steady state *versus* dynamic) and the choice of environmental impact category throughout LCIA (ReCiPe Midpoint GWP *versus* the aggregated total ReCiPe Endpoint) were discussed and clarified. Accordingly, the major outcomes were that steady state importantly underestimates all the three objectives and the use of the aggregated total ReCiPe Endpoint is capable of representing almost all impact categories, except eutrophication which is linked to the discharge of pollutants.

The benefits in case of an alternative scenario, at optimal conditions, which considers the urine source separation coupled with nitrogen treatment by nitrification and anaerobic deammonification (ANA), were compared with the conventional reference scenario (REF). The comparison showed that when managing nitrogen differently, significant gains might be achieved: approximately 100% in operational cost (OCI), 10% in water quality (EQI) and 30% in environmental impacts through the LCIA. Finally, presented results provided insights on a requirement for redesigning the plant when an alternative scenario is aimed at, for instance, really low dissolved oxygen set points were found for ANA scenario.

Finally, an important aspect of this work to be emphasized is that the developed platform was conceived to be flexible to other case studies. Therefore, the consistency of other conventional or alternative wastewater treatment plants can be evaluated with few modifications in framework's flowsheet.

# **Chapter VI. Conclusions and perspectives**



*“Everything we think about regarding sustainability - from energy to agriculture to manufacturing to population - has a water footprint. Almost all of the water on Earth is salt water, and the remaining freshwater supplies are split between agricultural use and human use - as well as maintaining the existing natural environment.” (Jamais Cascio)*

Nowadays, wastewater might be considered as both a problem and an opportunity for recovery of nutrients and energy. When considered as a problem, in order to ensure the quality of water bodies and avoid other indirect environmental problems, wastewater is required to be correctly treated. This treatment requires the use of an important quantity of energy (especially for nitrogen treatment) and chemicals. When considering the environmental burden of the treatment, it is important thus to consider all the involved processes, from the entrance of the wastewater in the WWTP to the output of treated water and passing by the production of required raw materials and the disposal/ utilization of by-products.

However, when considering wastewater as a source of valuable nutrients and energy, it is a promising alternative and thus WWTPs are nowadays being considered mainly as water resource recovery facilities. The recovery might include different and more or less innovative options such as energy recovery by biogas production and urine source separation with recovery/ treatment of nutrients (mainly nitrogen and phosphorus).

Additionally, considering the whole urban water management as an anthropogenic activity that already allows the reutilisation of water in a cycle, it seems logical to think about nutrients recycling, especially when having in mind the future (or in some current cases) scenario of resources depletion and the need of achieving less intensified and more sustainable processes.

The presented work is a result of a coupling approach including rigorous dynamic modelling, life cycle assessment with extended boundaries and efficient multi-objective optimization. When tackling comparisons between scenarios aiming to clarify the benefits and drawbacks of each scenario, realistic aspects were considered and the proposed alternative scenarios, that include mainly enhancement of biogas production and management of source separated urine, globally showed to be more sustainable than conventional ones.

Globally, the main achievements through this study are described as follows. Concerning LCA, this work included the definition of a relevant approach according to the ISO methodology together with the correspondence between simulation results and LCA inputs. The coupling platform was developed and a range of conventional and alternative scenarios were analysed. With regards to influents, more reliability was obtained as this study considered the dynamic characterisation of urine and wastewater

followed by its inclusion in an adapted influent generator. Concerning the last part of this work - the multi-objective optimization - different problem formulations and case studies were proposed together with the application of the platform to conventional and alternative treatment scenarios. A detailed conclusion on each chapter's achievement is provided hereafter.

In chapter II, the importance of considering the environmental aspects when the eco-design of WWTPs is aimed was highlighted. A coupled platform integrating a wide-plant dynamic modelling and LCA was fully developed with data treatment by Python™. The approach was successfully applied to six WWTP scenarios. Scenarios with urine source-separation (USS) presented a positive effect on the effluent quality and decreased the energy consumption in WWTP while the enhanced primary clarification (EPC) led to important energy savings (with more energy recovery and less energy use). The coupling of these two approaches, led to energy autarky together with a better respect of reject limits. The most interesting scenarios showed to be the USS+EPC coupled to urine treatment by nitrification/deammonification (considering also feasibility and acceptability) and the agricultural valorisation as fertilizer. By the contribution analysis, hotspots were identified such as the infrastructures (which might be optimized if alternative scenarios are targeted), N<sub>2</sub>O direct emissions (which depend, among others, on the nitrogen concentration in WWTP input) and heavy metals in sludge.

Following, chapter III presented the adaptation of a dynamic and phenomenological influent generator to take into account the urine source separation at a user specified level and its impact on total wastewater stream. The use of the influent generator, allowed in a non expensive way to obtain reliable influents that might be used later for simulation of alternative scenarios. Given its flexibility, it is also possible to envisage other alternative scenarios, and the generated variables might be easily used for different modelling approaches such as wide-plant modelling and ASM family models. By the end, the benefits from the urine separation were demonstrated by the dynamic simulation of a typical plant, where daily nutrient peak load were avoided and the reject quality was improved. The developed tool is thus available for future simulations including innovative wastewater and urine management scenarios and for their optimization.

Chapter IV studied the feasibility of coupling the previously developed DM-LCA platform with an efficient multi-objective optimization (EMOO) approach dedicated to expensive black-box problems. The coupled DM-LCA-EMOO platform was capable of generating an optimal Pareto front that compromises between technological aspects (process performance), operational cost and environmental impacts. Also, the analysis of the differences between constrained and unconstrained optimization results allowed for a deeper view to the technological limitation of a given treatment process. Finally, relations between objectives were better understood: OCI and LCIA were positively correlated thanks to supply chain impacts and costs, while EQI showed to be negatively correlated

with them. Three main zones were also identified: (1) a zone with a unacceptable water quality easy to attain, (2) an intermediate zone where reject limits are respected with no exaggeration in costs and environmental impacts, (3) a zone of technological limitation where, further treatments may imply exaggerated costs and environmental impacts.

Finally, chapter V promoted the application of the previously developed platform to an alternative scenario considering the urine source separation and the nitrogen treatment by nitrification and anaerobic ammonium oxidation. Together with the major gains identified, reaching approximately 100% for operational costs, 10% for effluent quality and 30% for environmental impacts, the application of the platform also allowed identifying the differences between results when different problem formulations are available. Additionally, the platform provided also results concerning functions' interdependencies and correlations between decision variables for different case studies.

Furthermore, it is important to indicate that the major difference between this study and others found in the literature is the reliability of the framework when using dynamic simulations and a reliable dynamic input for WWTP and urine streams. Further, this study is the first one that comprises multi-objective optimization of alternative scenarios, coupling wide-plant modelling and dynamic aspects, together with a relevant integration of LCA. Also, the alternative scenarios related to the urine source separation such as nitrification/deammonification and agricultural spreading - not so far evaluated in the literature through LCA - were also studied.

In an effort to disseminate and encourage the inclusion of environmental aspects when assessing WRRFs as well as the multi-objective optimization approach to tackle wastewater management and treatment problems, this work resulted in 4 peer-reviewed papers that were already accepted or under preparation for submission. It was also communicated in 6 different conferences and seminars focusing each time on different aspects of the study, i.e. nutrient recovery and recycling, environmental assessment methodology and multi-objective optimization in order to ensure an enriching exchange between authors and the most involved researchers in each field.

The perspectives might be divided into the three main aspects of the platform: wide-plant modelling, LCA and multi-objective optimization. Before, it should be noted that the flexibility is one of the main characteristics in the DM-LCA-EMOO platform. This characteristic was particularly pursued throughout this work. Special efforts were made during the construction of the platform in order to ensure its applicability to other benchmarks or other case studies that might become relevant.

Considering modelling and simulation, the flexibility is especially important as WWTP flowsheets are frequently changing to achieve, for instance, lower required reject limits. One might also want to

evaluate a different and innovative process by comparing it with a reference one. Also, the modelling of specific parts of the process are evolving rapidly nowadays such as nitrous oxide emissions modelling that have not yet achieved a consensus in scientific and industrial communities. The latter, however, might completely revolve the choice of functioning parameters when sustainable scenarios are targeted.

According to inputs in WWTP, it is also important to increase efforts to provide more realistic information at different level (time dependency, geographical and catchment characteristics). However, this is also highly dependent on real-world data collection that would allow the comprehension of dynamics, mainly for urine generation that is not deeply studied, especially according to aspects related to the time dependency and the fate of some components. Another interesting perspective that might be considered is the generation of other streams from a household when considering other source separation scenarios.

Improving proposals in the field of LCA includes mainly the addition of dynamic aspects in the environmental assessment as well as the addition of more details – such as emerging substances - when the system is case specific. It should be noted that, currently, as LCA relies on steady state conditions, the dynamic results of WWTP operation are integrated and calculated in average. However, certain improvements in LCA would allow the consideration of the time dependency in background processes according to the operational functioning of the plant as well as long term changes in catchment and concentration changes in the wastewater input due to, for instance, population growth or water scarcity conditions.

Another important effort to be made when considering environmental analysis coupled to WWTP scenarios concerns the infrastructure involvement, as evaluations based on alternative scenarios might also include infrastructure modifications in order to reflect their real gains. However, nowadays, a great uncertainty is involved in environmental analysis and thus, slight modifications in infrastructure might not be quantified correctly. In this sense, efforts have to be made in order to consider the infrastructure modelling in a rigorous way or at least to validate the uncertainties linked to a plant size range to allow the redesign of new alternative scenarios. Accordingly, one might think of an exhaustive list of perspective scenarios (with infrastructure changes) to be evaluated and optimized such as the inclusion of anaerobic ammonium oxidation in the mainstream as well as a multitude of processes for the treatment and valorisation of urine source separated.

Considering the optimization aspects, methodology is evolving rapidly and recent advances on machine learning have been helpful in the field of expensive optimization. From the best of our knowledge, the utilisation of these tools, especially the Support Vector Machine (SVM) for efficient function recognition and approximation might represent an important gain in case of expensive

optimization such as in WWTPs, but also when the optimization is subject to multiple stiff constraints. Finally, as the optimization platform is mixed-integer, there is also the possibility of including a superstructure in the optimization problem by using binary variables, the pathway to follow in the treatment, for instance in the case of urine source separation and especially when more complex problems such as full household waste managements or elevated retention percentages of urine are envisaged.

As a final conclusion, the developed DM-LCA-EMOO tool is now available for both evaluation and optimization of any desired scenario in the field of WWTPs and WRRFs, under realistic assumptions and operational conditions. The tool is indeed flexible enough to be adapted to any related case studies and might be integrated to any existing modelling platform.



## Résumé long en français

Selon les Nations Unies, dans le monde, 40% des personnes souffrent d'une pénurie d'eau et ce nombre risque d'augmenter. En 2011, 41 pays ont connu un stress hydrique et, d'ici 2050, au moins une personne sur quatre serait touchée par des pénuries d'eau récurrentes. Globalement, encore 2,4 milliards de personnes utilisent des installations d'assainissement précaires et au moins 1,8 milliard de personnes utilisent une source d'eau potable qui est contaminée par des fèces. En conséquence, environ 1000 enfants meurent chaque jour en raison de maladies liées à l'eau et au manque d'assainissement.

Les Objectifs du Millénaire pour le Développement (en anglais, Millennium Development Goals, MDGs) proposés en 2000 par le Programme des Nations Unies pour le développement, qui comptent parmi les huit principaux objectifs, la durabilité environnementale est arrivée à son terme en 2015. Comme indiqué dans le rapport final (Nations Unies, 2015), des progrès ont été réalisés : 1,9 milliard de personnes ont accès à l'eau potable depuis 1990 ; 2,1 milliards de personnes ont maintenant accès à un assainissement amélioré et 98% de substances appauvrissant la couche d'ozone ont été éliminées depuis 1990.

Toutefois, de nombreux progrès restent à faire et certains points ont été laissés de côté. Comme indiqué dans le rapport final, le changement climatique et l'environnement se détériorent. Les chiffres relatifs aux impacts environnementaux directs sont alarmants: les émissions mondiales de dioxyde de carbone (CO<sub>2</sub>) ont augmenté de plus de 50% depuis 1990 et le taux de croissance des émissions entre 2000 et 2010 a été plus important que dans chacune des trois décennies précédentes; Les émissions de méthane (CH<sub>4</sub>) et de protoxyde d'azote (N<sub>2</sub>O), puissants gaz à effet de serre, pourraient augmenter de 50% et 25% entre 1990 et 2020 ainsi que la température moyenne mondiale qui a augmenté de 0,85 °C entre 1880 et 2012; En outre, le niveau moyen de la mer a augmenté de 19 cm entre 1901 et 2010 et environ 40% des océans sont actuellement fortement touchés par les activités humaines; Enfin, on estime que 90% des eaux usées dans les pays en développement sont rejetées sans traitement (Nations Unies, 2016).

Néanmoins, non seulement les chiffres sont alarmants. Les changements dans le contexte mondial deviennent de plus en plus évidents quand on considère la croissance de la population avec l'urbanisation et l'industrialisation, la demande alimentaire croissante, les changements de l'utilisation des terres et dans les niveaux de vie (UN-Water, 2015). Par conséquent, compte tenu de la pression croissante exercée sur les systèmes existants de collecte et de traitement des eaux usées, celles-ci sont évacuées sans traitement et la qualité de l'eau où elles sont déversées, diminue. Ce manque de traitement conduit à des impacts directs sur l'équilibre des écosystèmes aquatiques et finit en modifiant également les activités anthropiques, du développement urbain à la production alimentaire et à

l'industrie. En conséquence, l'environnement est menacé et soumis à des pressions ; également, la santé humaine est en voie de dégradation.

Par conséquent, il est de plus en plus clair que les eaux usées, en tant que flux de pollution produit par l'activité anthropique qui a besoin d'utiliser les ressources naturelles, doivent retourner à l'environnement de manière sûre. Ceci est essentiel pour mettre fin à la dégradation engendrée par ce cycle non écologique et qui entraîne l'épuisement des ressources, la dégradation des écosystèmes et enfin l'exposition de la santé humaine à un danger imminent. Il est donc impératif de trouver une gestion et un traitement des eaux usées plus consciencieux pour atteindre des niveaux de traitement plus élevés et une robustesse afin de faire évoluer ensemble le lien écosystème - santé humaine. Dans ce sens, au lieu d'être une source de problèmes, les eaux usées bien gérées devraient jouer un rôle positif dans l'environnement, ce qui améliore la sécurité alimentaire, la santé et l'économie. Cependant, cela ne peut être fait que si la gestion des eaux usées est considérée comme faisant partie intégrante d'un cycle intégré et d'un système de gestion écosystémique comprenant des aspects sociaux, économiques, environnementaux et géographiques (Corcoran et al., 2010).

Les eaux usées sont aujourd'hui décrites comme une ressource et un problème par plusieurs auteurs. Depuis 2013, des publications de la Water Environment Federation (WEF) ont commencé à utiliser le terme « WRRF – Water Resource Recovery Facility » plutôt que « WWTP – Wastewater Treatment Plant » pour « mieux cibler les produits et les avantages du traitement, plutôt que les déchets qui entrent dans ces installations » (WE & T, 2013). Dans le passé, l'objectif principal du traitement des eaux usées était d'atteindre les limites de rejet autorisées. De nos jours, les objectifs visent à maximiser la récupération des ressources précieuses bien que la qualité de l'eau soit maintenue et que la robustesse des processus soit atteinte.

Lorsque l'on considère les éléments nutritifs, la partie la plus importante vient de l'urine. Par exemple, comme discuté par Tidaker et al. (2007), l'urine de la population suédoise contient environ 36 kilotonnes d'azote et 3,3 kilotonnes de phosphore tandis que 170 kilotonnes d'azote et 15 kilotonnes de phosphore ont été consommées à partir d'engrais minéraux en Suède en 2001. Par conséquent, si l'azote, le phosphore et même le potassium de l'urine avaient été utilisés en remplacement des engrais synthétiques, la production industrielle de ceux-ci pourrait être diminuée et la décharge de ces nutriments serait également réduite (Johansson et al., 2000).

Aussi, l'extraction des ressources des eaux usées n'est pas nouvelle. Certaines solutions telles que la production d'eau adapté à l'usage à posteriori (fit-for-purpose), les biosolides utilisés dans les terres agricoles et la production d'énergie provenant de la digestion anaérobie sont déjà courantes dans les stations d'épuration. De nos jours, on commence à étudier de nouveaux procédés pour produire /

recupérer des composés spécifiques des eaux usées comme la struvite précipitée (à utiliser comme engrais), les polyhydroxyalcanoates à partir des boues et à utiliser le gaz issu de la digestion pour produire du méthanol ou de l'ammoniac (WERF, 2011).

En outre, l'utilisation des biosolides et des eaux usées elles-mêmes dans les terres agricoles est de plus en plus acceptée par la population. Dans les pays en développement, la réutilisation des eaux usées est due notamment à la capacité limitée de traiter les eaux usées et à l'absence d'autres sources d'eau acceptables pour l'agriculture. Dans les pays développés, la réutilisation et le recyclage de l'eau sont de plus en plus considérés comme un moyen de répondre à la pénurie sur place d'eau et à la réaffectation de l'eau dédiée à l'agriculture à d'autres usages. En outre, toutes les normes environnementales strictes conduisent à une utilisation agricole inévitable et économiquement faisable des eaux usées et des boues (Drechsel et al., 2010).

La digestion anaérobie est aujourd'hui un processus de valorisation dans plusieurs stations d'épurations. Dans ce procédé, la fermentation microbienne a lieu et convertit la matière organique en biogaz (principalement  $\text{CH}_4$  et  $\text{CO}_2$ ) qui peut ainsi être utilisé pour produire de l'énergie dans les systèmes de cogénération. Une autre conséquence de la digestion anaérobie est la minéralisation des composés organiques biodégradables qui conduit à une concentration élevée de  $\text{NH}_4^+$  et  $\text{PO}_4^{3-}$  en solution et à la stabilisation des boues (van Lier et al., 2008). Plusieurs études ont été menées afin d'améliorer la production de biogaz visant à inverser le bilan énergétique et à conduire les stations d'épuration à être en autarcie énergétique (Schaubroeck et al., 2015; Aichinger et al., 2015). Étant donné que la production de biogaz dépend des solides en suspension volatils entrant dans le digesteur qui seront dégradés, une possibilité d'augmenter la production de biogaz est de forcer l'entrée de plus de matière organique dans le digesteur. Ceci peut être fait en récupérant la matière organique entrant dans la station par une clarification primaire renforcée (avec une addition de produits chimiques pour obtenir une meilleure floculation), précédemment à sa dégradation dans la ligne d'eau par l'oxydation microbienne. Un autre avantage de la récupération de la matière organique à ce point est qu'il aura moins de croissance bactérienne pour traiter le carbone dans les bassins aérés et donc moins d'énergie sera nécessaire pour aérer la boue activée (Flores-Alsina et al., 2014). Des recherches plus récentes ont également été développées pour le procédé à forte teneur en boues activées (HRAS) - Jimenez et al., 2015 - travaillant à faible temps de rétention de la boue et également pour le processus de nitrification partielle et anammox sur la ligne principale (Laurenzi et al., 2016). Si le couplage des deux approches précitées réussissait, cette approche innovante permettrait de minimiser la dégradation aérobie de la matière organique et de produire des boues plus fermentescibles pour la digestion anaérobie (Xu et al., 2015).

Une des possibilités prometteuses de la récupération du phosphore est la précipitation de la struvite provenant des eaux usées. La struvite (phosphate d'ammonium et de magnésium hexahydraté -  $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$ ) est un engrais à libération lente qui pourrait remplacer les engrais industriels conventionnels. La récupération de la struvite à partir des eaux usées permettrait non seulement une diminution de la production d'engrais minéraux et l'épuisement des ressources naturelles de phosphore, mais aussi une diminution du phosphore rejeté. Cependant, pour être réalisables et présenter des avantages réels, la précipitation de la struvite doit être conduite dans des eaux usées riches en nutriments, contenant principalement du phosphate et de l'ammonium. Plusieurs études ont été menées pour la précipitation de la struvite en utilisant, entre autres, le surnageant de digesteur, le lixiviat de décharge et l'urine. Cependant, comme l'ont discuté Maurer et al. (2006), sans ajout de phosphate, seulement 3% de l'azote dans l'urine pourraient être éliminés dans la précipitation de la struvite (avec une précipitation efficace de 98% de phosphore). Par conséquent, davantage de recherches sur les nouveaux procédés de récupération de l'azote sont encore nécessaires.

Comme précédemment mentionné, plusieurs possibilités de valorisation sont disponibles et bien appliquées dans les stations d'épuration. Cependant, l'un des freins pour tirer pleinement parti de la récupération des ressources dans les eaux usées est que dans les eaux usées municipales, les flux riches en éléments nutritifs (par exemple l'urine et les fèces) ne doivent pas être dilués (par exemple par les eaux grises) et donc la séparation à la source devrait être encouragée. Dans le même temps, le choix des systèmes centralisés ou décentralisés n'est pas évident: entre autres, l'approche de gestion dépend de la zone (urbaine ou rurale), de la taille et de la densité de la population, du niveau de développement, de la faisabilité technique, de la qualité de l'eau requise et de l'éducation et de la culture de la population, étant nécessaire de l'évaluer au cas par cas (Corcoran et al., 2010, Libralato et al., 2012).

De nombreux aspects des systèmes centralisés et décentralisés font l'objet de discussions dans la littérature. Selon Libralato et al. (2012), quelques aspects importants à prendre en compte pour les systèmes centralisés sont les coûts concurrentiels des installations existantes, les phénomènes potentiels d'eutrophisation et les problèmes de surcharge en eau de pluie. D'autre part, les systèmes décentralisés peuvent répondre à des situations diverses, à la diminution ou à l'arrêt de la réduction de la qualité de l'eau dans les bassins versants et permettre la récupération et le recyclage des nutriments à partir des eaux usées comme dans le cas de la séparation de l'urine à la source.

De plus, certains inconvénients ont également été présentés dans les systèmes pilotes décentralisés tels que les précipitations et, par conséquent, le colmatage des tuyaux et les odeurs ainsi que les difficultés lors que des changements dans le système centralisé sont nécessaires et le stockage et le transport doivent être ajoutés à la nouvelle structure de gestion (Maurer et Udert et al., 2003). En

ce qui concerne les impacts, certaines études ont montré des impacts plus importants pour l'acidification lors de l'analyse de l'empreinte écologique des systèmes séparés à la source. Cependant, il est également souligné que, contrairement aux systèmes conventionnels déjà optimisés, les systèmes alternatifs doivent être bien évalués afin d'obtenir des résultats optimaux en termes de qualité des effluents et de consommation d'énergie et de produits chimiques (Remy, 2010).

Même lorsque l'on dispose de données pour évaluer les technologies classiques et les nouvelles technologies, on pourrait prétendre que, selon la méthodologie utilisée pour évaluer le processus, les résultats seraient différents. Il est donc nécessaire d'avoir une méthodologie normalisée pour évaluer l'ensemble du processus et de ses besoins. Actuellement, différents outils d'évaluation sont disponibles pour évaluer la durabilité des systèmes tels que l'analyse de l'exergie, l'analyse économique et l'Analyse de Cycle de Vie (ACV) (Balkema et al., 2002).

Dans le but d'analyser l'empreinte écologique des stations d'épuration, plusieurs études suggèrent l'utilisation de l'ACV. Cette méthodologie permet d'évaluer les impacts environnementaux attribués au cycle de vie d'un processus ou d'un produit. Selon l'ISO 14044 (2006), l'ACV est définie comme la compilation et l'évaluation des intrants, des sortants et des impacts environnementaux potentiels d'un système ou d'un produit tout au long de son cycle de vie. Dans ce contexte, il convient de tenir compte de l'impact de la décharge des effluents (approche de fin de cycle), mais également de l'ensemble des processus associés au traitement principal, tels que le traitement et l'élimination des boues, la consommation d'énergie et la production de matériaux auxiliaires.

Lors de l'application d'une ACV sur un procédé, les quatre étapes principales recommandées par l'ISO 14044 (2006) doivent être suivies: i.) La définition de l'objectif et du scope de l'étude; ii) la définition de l'inventaire; iii) la phase d'analyse d'impact et iv.) L'interprétation. La première étape, la définition de l'objectif et du scope, permet de décrire le système en fonction des limites du même, de l'unité fonctionnelle et des méthodes d'allocation. Aussi, la bonne définition de l'unité fonctionnelle permet la comparaison entre différentes alternatives. La deuxième étape, l'inventaire du cycle de vie, est la compilation des toutes les consommations estimées de ressources de l'environnement et des substances émises à l'environnement pendant le cycle de vie. A la fin de cette étape, un inventaire du système est obtenu sur la base d'une unité fonctionnelle bien définie. La troisième étape, l'évaluation de l'impact sur le cycle de vie, fournit la corrélation entre les substances émises et les indicateurs d'impacts sur l'environnement. Enfin, la dernière étape, c'est-à-dire, l'interprétation de l'analyse du cycle de vie, apparaît naturellement lors de l'étape de décision, après la comparaison des scénarios (Rebitze et al., 2004) et de l'identification des *hotspots* dans le système étudié.

Dans le domaine du traitement de l'eau et des eaux usées, l'ACV a déjà été utilisée dans plusieurs études pour évaluer les performances environnementales des technologies proposées. Les différentes applications de l'ACV dans ce domaine publiées jusqu'à présent ont été recensées (Corominas et al., 2013a) pour différentes configurations de stations d'épuration ainsi que pour les technologies de gestion des boues d'épuration (Yoshida et al., 2013) et pour le système complet d'eau urbain (Loubet et al. ). Cependant, comme les résultats sont généralement obtenus par les données collectées sur site, les études ne peuvent pas être utilisées pour analyser automatiquement les tendances générales ni pour optimiser les processus. Par conséquent, la prise en compte d'une ACV avec les outils de modélisation et de simulation est une approche puissante pour permettre la modification des paramètres opérationnels et de l'écoconception. Cependant, il faut souligner que, pour être réaliste et pour fournir une comparaison équitable par rapport aux scénarios étudiés, l'ACV doit être conduite en tenant compte des limites appropriées et d'une méthodologie d'allocation pertinente. Par exemple, lors de l'analyse de la récupération des nutriments, l'évaluation du cycle de vie doit être adaptée pour tenir compte de tous les impacts évités via les sous-produits. De même, les nouvelles fonctions du système doivent être ajoutées car les nouveaux scénarios ne fourniront plus la même unité fonctionnelle.

Une autre caractéristique importante de l'ACV qui permet de l'appliquer à la quantification des impacts et à l'évaluation des scénarios dans le traitement des eaux usées apparaît quand on considère les émissions directes de la station d'épuration. Même si aujourd'hui, les méthodologies d'évaluation de l'impact sur le cycle de vie ne sont pas capables d'intégrer toutes les substances sortant d'une station d'épuration, comme les résidus des produits de soins et les résidus de médicaments, les principales émissions résultantes de la mise en œuvre d'un traitement des eaux usées (tels que le rejet de polluants non traités, le rejet des gaz à effet de serre et la forte consommation d'énergie et de produits chimiques) peuvent être correctement quantifiés et évalués par les catégories d'impact actuellement disponibles (par exemple l'eutrophisation marine et d'eau douce, la toxicité humaine, le changement climatique et l'épuisement des ressources).

Cependant, lorsqu'une nouvelle technologie doit être évaluée en tenant compte de la durabilité mais aussi des aspects techniques et économiques, il est important de conduire une optimisation. De plus, cette optimisation doit considérer, non seulement un point de fonctionnement optimal; Il est nécessaire de faire des compromis entre les différents résultats sans aucun jugement préliminaire.

Comme l'explique Deb (2011), l'optimisation multi-objectif consiste à optimiser simultanément plus d'un objectif. Contrairement à l'optimisation mono-objectif, l'optimisation multi-objectifs minimise toutes les fonctions objectives, généralement contradictoires, simultanément et sans utiliser une équivalence entre les objectifs via des poids. Par conséquent, un ensemble de solutions, appelé un front de Pareto, est généralement obtenu à la fin d'une optimisation multi-objectif. Ensuite,

une étape supplémentaire, le processus décisionnel, est nécessaire pour comprendre les compromis et pour trouver le point de fonctionnement optimal, si besoin. En outre, étant donné que les objectifs contradictoires sont le plus souvent impliqués, aucune des solutions optimales trouvées ne peut être améliorée sans aggraver au moins un des autres objectifs (Hakanen et al., 2011) et ainsi les solutions ne peuvent pas être facilement triées seulement sur la base de leur valeur objective.

Il existe différentes façons de résoudre un problème d'optimisation multi-objectif parmi lesquels les algorithmes génétiques, largement connus en raison de leur robustesse. Dans cette méthode, l'optimisation est réalisée en utilisant une population de solutions, habituellement créées au hasard et donc la robustesse est assurée indépendamment de la qualité de l'initialisation. Ensuite, l'algorithme fournit une opération de génération (itérative) mettant à jour la population actuelle pour créer de nouvelles populations basées sur des opérations génétiques telles que la sélection génétique, le croisement, la mutation et la migration. Cette opération, basée sur la génération, est poursuivie jusqu'à ce qu'un ou plusieurs critères de terminaison prédéterminés soient satisfaits (Deb, 2011).

Du point de vue de l'application, l'optimisation de la conception et de l'exploitation des stations d'épuration a été appliquée depuis les années 1990. En général, les stratégies d'optimisation décrites dans la littérature sont basées sur l'agrégation, c'est-à-dire que l'optimisation est réalisée en agrégeant plusieurs objectifs en une fonction objective unique à travers des facteurs de poids représentant l'importance de chaque objectif (Hakanen et al., 2011; 2013).

Cependant, comme décrit par Hreiz et al. (2015) dans un état de l'art de l'optimisation des stations d'épuration, plusieurs objectifs n'ont pas les mêmes unités (et parfois ils sont même contradictoires) et ne peuvent donc pas être combinés instinctivement pour former une seule fonction objective. D'un point de vue pratique, même si des procédés hautement non linéaires sont présents dans une station d'épuration, par exemple en raison d'une modélisation rigoureuse des réactions biochimiques, il est important d'éviter l'agrégation des objectifs et de préserver la structure intrinsèquement multi-objective du problème d'optimisation. Par exemple, la qualité des eaux usées traitées et les coûts opérationnels sont deux objectifs contradictoires car, pour atteindre des concentrations faibles de matière organique, d'ammonium ou de phosphate dans les effluents, la consommation d'énergie et de produits chimiques dans l'usine doit être élevée.

L'optimisation multi-objectif est reconnue comme étant plus appropriée pour traiter les problèmes dans les stations d'épuration en raison de la nature conflictuelle des objectifs pris en compte. De plus, l'utilisation d'algorithmes d'optimisation qui n'utilisent pas un gradient tels que les algorithmes génétiques peut être priorisé pour éviter les incertitudes dues à l'approximation numérique des gradients dans les systèmes hautement non-linéaires et pour assurer la robustesse de l'algorithme.

Néanmoins, en ce qui concerne ces algorithmes, le principal inconvénient est le budget numérique requis. Aussi, l'étude d'une station d'épuration complète est un exemple d'un problème d'optimisation coûteux, où la résolution sans un outil d'optimisation efficace serait pratiquement impossible.

Dans le but de fixer un budget de calcul qui permet d'obtenir un front de Pareto optimal, Ahmadi et al. (2016) ont proposé un nouvel algorithme appelé AMOEA-MAP pour traiter les problèmes coûteux de simulation et réduire le budget informatique de l'optimisation à environ 300 évaluations de la fonction objective. Les modifications proposés dans cet algorithme reposent principalement sur le maillage adaptatif de l'espace de recherche, pour accélérer la recherche sans perte de précision et sur une approche bi-population (Ahmadi et al., 2016).

Finalement, le choix des systèmes innovants et plus durables de gestion et de traitement des eaux usées nécessite un soutien décisionnel multicritère capable de prendre en compte tous les aspects techniques, économiques et environnementaux. Par conséquent, il est nécessaire d'avoir un outil capable de prédire de manière fiable et interconnectée les avantages et les inconvénients lors de l'application d'une technologie nouvelle.

Les travaux présentés dans ce manuscrit poursuivent une thèse conclue au Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (LISBP) de Méry (2012). Dans le travail précédemment cité, un outil intégré pour la modélisation et l'évaluation du cycle de vie appliqué à l'analyse environnementale des stations de potabilisation de l'eau a été mis au point avec succès. En revanche, ce travail été axé sur le développement de la modélisation et de la simulation des processus unitaires en régime stationnaire (considérées comme satisfaisantes pour ce type de processus) et sur l'application à une installation existante. Suite à l'idée de cette approche antérieure, il semblait évident que la même approche pourrait être appliquée à d'autres champs d'étude comme le traitement des eaux usées. Cependant, comme les processus physico-chimiques et biologiques impliqués dans ce type de procédé sont complexes et dépendent fortement des entrants (composition, variation de débit), il est extrêmement important d'adopter une modélisation rigoureuse et dynamique. Un autre intérêt recherché dans le présent travail est la construction de scénarios de perspective, ce qui signifie que l'outil devrait avoir un aspect prédictif et une capacité d'écoconception. Une approche d'optimisation multi-objectif devrait alors être intégrée pour aborder les objectifs contradictoires impliqués.

**L'objectif principal de cette étude est donc d'obtenir une plateforme couplant la modélisation dynamique rigoureuse, l'analyse de cycle de vie et un outil d'optimisation multi-objectif efficace.**

La plateforme développée, DM-LCA-EMOO, doit être flexible afin de permettre la mise en œuvre des différents scénarios ainsi que des multiples critères en fonction des différents paramètres de décision. Aussi, pour atteindre les objectifs, les outils impliqués dans la plateforme doivent être interconnectés avec leurs paramètres de processus et leurs résultats. Initialement il est donc nécessaire de contrôler automatiquement les simulateurs commerciaux existant ainsi que d'exécuter des simulations et de récupérer les résultats. Lorsque les résultats sont récupérés, ils doivent être convertis en substances et modules corrects pour l'ACV afin de permettre la prise en compte des processus de premier plan et de fond avec les bilans de masse et d'énergie. Des exemples de valeurs importantes récupérées sont la violation des limites de rejet, la quantité d'énergie produite sur la quantité d'énergie consommée, les concentrations moyennes en sortie de la STEP, entre autres. Aussi, les impacts doivent être obtenus d'une sorte à ce qu'à la fin de l'évaluation d'une gamme de scénarios, une analyse de contribution détaillée puisse identifier les *hotspots* les plus importants de chaque scénario à optimiser ultérieurement. Enfin, pour permettre l'optimisation multi objectif des scénarios, la plateforme doit être reliée à un algorithme d'optimisation multi-objectif efficace qui permet l'optimisation de la station d'épuration.

La plateforme développée doit être en mesure d'évaluer et de comparer les options de gestion et de traitement des eaux usées classiques et alternatives. Parmi les alternatives envisagées, on cherche à étudier la séparation à la source de l'urine avec un traitement spécifique (production de la struvite et nitrification / oxydation anaérobie d'ammonium) et / ou la valorisation en agriculture et la clarification primaire renforcée pour augmenter la production de biogaz dans la station d'épuration afin d'atteindre une autarcie énergétique.

L'intérêt d'une telle plateforme combinée peut être compris sous deux angles. Premièrement, il s'agit d'un outil de validation de benchmark, qui consiste donc à évaluer et à comparer des scénarios conventionnels et alternatifs (approche DM-LCA - chapitre 2). Deuxièmement, lorsqu'elle est couplée à l'outil d'optimisation, la plateforme est capable d'optimiser simultanément les variables opérationnelles et de conception (approche DM-LCA-EMOO - chapitres 4 et 5), pouvant aussi valider des nouvelles configurations avec un réajustement des conditions de fonctionnement en raison des modifications éventuelles de la structure de l'installation et des conditions de fonctionnement. De plus, afin de satisfaire aux objectifs de modélisation et de simulation, un générateur d'influents phénoménologique et dynamique doit être adapté pour tenir compte des intrants réalistes dans la station d'épuration et dans le traitement de l'urine (chapitre 3).

Ce manuscrit est structuré en 6 chapitres. Le chapitre I présente le contexte et les objectifs de la thèse en présentant les principaux défis à relever en tenant compte des approches existantes dans la littérature. Dans ce contexte, les objectifs de recherche et les tâches correspondantes sont définis.

Le chapitre II décrit le développement initial de la plateforme qui couple la modélisation dynamique et l'évaluation du cycle de vie avec des limites étendues. De plus, la plateforme développée est utilisée pour évaluer des scénarios conventionnels et alternatifs. En mettant l'accent sur le choix de scénarios alternatifs pour l'avenir, l'attention a été portée à la modélisation et à l'analyse des *hotspots* de chaque scénario visant à les optimiser davantage.

Le chapitre III présente l'adaptation d'un générateur influent phénoménologique et dynamique qui est nécessaire pour obtenir des données d'influents plus réalistes (et par conséquent des résultats de simulation plus précis) pour des scénarios de séparation à la source de l'urine avec le flux d'eaux usées résultant.

Le chapitre IV est une étude préliminaire sur l'optimisation multi-objectif de la station d'épuration qui vise à comprendre la faisabilité d'une telle optimisation, tant du point de vue du calcul que de la fiabilité. Une attention particulière est portée dans ce chapitre à la formulation du problème en tenant compte des variables de décision, des fonctions objectives et des contraintes. Le choix d'un algorithme d'optimisation efficace est également discuté et justifié.

Finalement, le chapitre V présente l'application de la plateforme DM-LCA-EMOO élaborée précédemment à un scénario de référence et à des scénarios alternatifs. De plus, différentes formulations de problèmes sont étudiées en même temps que ses effets sur les résultats du front de Pareto.

Enfin, le chapitre VI présente les principales conclusions de ce travail ainsi que les perspectives qui suivent cette thèse.

## *Chapitre II*

Ce chapitre est publié dans *Water Research*, 84 (99-111), doi: 10.1016 / j.watres.2015.06.048. Il est le résultat du couplage de la modélisation dynamique et de l'analyse de cycle de vie (ACV) avec l'application correspondante à plusieurs scénarios. Les scénarios étudiés comprennent i.) Un scénario de référence; ii) un scénario de clarification primaire renforcée; iii) un scénario de séparation d'urine à la source; iv) un scénario combinant les variantes ii et iii (USS + EPC); v.) Un scénario adapté du scénario iv où le flux résiduel riche en azote issu de la précipitation de la struvite est épandu sur les terres agricoles et valorisé comme engrais (USS + EPC + AGRI); vi.) Un scénario adapté de iv où le flux riche en azote est traité par nitrification / oxydation anaérobie d'ammonium conjointement avec l'effluent de déshydratation provenant de la digestion anaérobie (USS + EPC + ANA).

Le choix des scénarios reflète ce qui a été discuté précédemment dans l'introduction et est inévitable aujourd'hui: Les stations d'épuration devraient se diriger vers les installations de récupération d'énergie et nutriments afin d'obtenir des systèmes de gestion et de traitement des eaux usées plus durables. Toutefois, cette perspective respectueuse de l'environnement ne peut être atteinte et bien évaluée qu'en ayant une vision intégrée de l'ensemble du processus et en considérant la voie complète des eaux usées, de la source à la réutilisation de l'eau traitée dans l'environnement et à la récupération des sous-produits.

Plusieurs questions doivent être adressées lors de la modélisation de ces systèmes. Afin de répondre à cette approche comparative qui permet d'aller vers les systèmes plus durables, la plateforme a été développée en tenant compte des frontières étendues de l'évaluation du cycle de vie, c'est-à-dire que toutes les émissions (directes et indirectes), ainsi que les émissions évitées ont été prises en compte.

### *Chapitre III*

La récupération des nutriments, en particulier de l'azote et du phosphore, pourrait être envisagée si l'urine était récupérée séparément et non diluée. En ce qui concerne les expériences de séparation de l'urine à la source, plusieurs études pilotes ou même des villages écologiques ont été mis en œuvre de nos jours. Cependant, peu de études de modélisation et de simulation ont été trouvées sur la littérature concernant cette séparation. A la connaissance des auteurs, il s'agit d'une conséquence de la variabilité de la concentration et de la génération de l'urine qui n'est pas constante car elle dépend du comportement humain et il est donc difficile de caractériser dynamiquement l'urine de manière réaliste. Par conséquent, il est essentiel d'avoir un outil pour générer un flux d'urine réaliste, dynamique et standardisé ainsi que les autres flux d'eaux usées. Comme montré dans une revue proposée par Martin et Vanrolleghem (2014) sur l'analyse et la génération d'influents, plusieurs approches sont actuellement disponibles pour pallier au manque d'information sur les influents. Cependant, il existe encore un besoin important de mettre en œuvre des générateurs d'influent plus réalistes.

En conséquence, l'objectif de ce chapitre est de proposer un générateur d'influent flexible, dynamique et phénoménologique pour considérer à la fois l'urine et les eaux usées. Ce chapitre est en préparation pour être soumis à une revue en partenariat avec l'Institut Eawag afin d'assurer des aspects réalistes dans la génération d'urine. Ce générateur d'influent a été adapté à partir du générateur d'influent dynamique et phénoménologique de Gernaey et al. (2011). Les données sur la composition des urines et des eaux usées ont été obtenues à partir d'une compilation de la littérature pour respecter

les données réelles. Aussi, le modèle est flexible et permet de simuler des études de cas spécifiques (lorsque l'utilisateur veut considérer, par exemple, d'autres systèmes de séparation à la source, d'autres dynamiques de génération ou d'autres conditions géographiques ou de collecte) ainsi que l'utilisation à posteriori des influents dans les modèles de la famille ASM et les super-modèles.

#### *Chapitre IV*

Lorsqu'un outil automatisé est disponible pour la quantification des performances, des coûts et des impacts environnementaux tels que la plateforme précédemment décrite, on pourrait vouloir analyser un large éventail de scénarios disponibles et d'alternatives opérationnelles. Cependant, étant donné l'aspect rigoureux des simulateurs dynamiques, le problème pourrait facilement devenir coûteux et complexe à résoudre, avec des exigences considérables en termes de temps de calcul.

Une étude de faisabilité de l'optimisation - du point de vue du temps de calcul et des perspectives de fiabilité - a donc été menée dans ce chapitre (récemment accepté pour publication dans *Chemical Engineering Research and Design*) en tenant compte de trois fonctions objectives: le coût opérationnel, la qualité des effluents et les impacts environnementaux. De plus, l'impact de l'addition de contraintes a été analysé sur la base des limites de rejet européennes. Aussi, l'étude de faisabilité a été menée à l'aide d'un scénario alternatif (séparation de la source d'urine et traitement par struvite et nitrification / anammox) pour assurer l'optimisation d'un problème plus complexe que celui de la station d'épuration classique.

#### *Chapitre V*

Lorsqu'un outil rigoureux et intégré est disponible et que la faisabilité de l'approche a déjà été validée, une analyse appropriée des différentes études de cas du monde réel peut être réalisée afin de comprendre, par exemple, comment les objectifs, les contraintes ou la dynamique du processus sont influencés par un point de fonctionnement de la station d'épuration. Par ailleurs, pour la suite, des études comparatives basées sur l'optimisation sur différents scénarios alternatifs par rapport aux procédés conventionnels sont pratiques et fiables à réaliser. En effet, dans ce cas, l'optimisation devient un outil puissant pour aider à l'apprentissage des interactions entre les systèmes et des objectifs interdépendants.

Par conséquent, un des objectifs de ce chapitre est d'étudier les différentes formulations de problèmes ainsi que leurs conséquences sur les résultats optimaux, lorsqu'ils sont appliqués aux

scénarios de référence ou aux scénarios alternatifs. Ensuite, sur la base d'un scénario conventionnel de référence, des études comparatives sur la simulation dynamique par rapport à l'état stationnaire sont fournies. De plus, l'impact de la formulation de contraintes sur la qualité des solutions optimales est discuté. La différence entre la méthode ReCiPe Endpoint et le ReCiPe Midpoint pour l'analyse environnementale est également réalisée en tant qu'étude comparative. Enfin, une comparaison entre la référence et un scénario alternatif (séparation de l'urine à la source suivie d'un traitement de l'azote) est fournie. Ce chapitre sera soumis pour publication dans la revue *Water Research*.

### *Conclusions et perspectives*

De nos jours, les eaux usées peuvent être considérées à la fois comme un problème et comme une occasion de récupération des nutriments et de l'énergie. Si considérée comme un problème, vu qu'on doit assurer la qualité de l'eau dans les bassins versants et éviter d'autres problèmes environnementaux indirects, les eaux usées doivent être correctement traitées. Ce traitement nécessite l'utilisation d'une quantité importante d'énergie (en particulier pour le traitement de l'azote) et de produits chimiques.

Cependant, si l'on considère les eaux usées comme source d'éléments nutritifs et d'énergie, elles sont une alternative prometteuse et, par conséquent, les stations d'épuration sont aujourd'hui considérées principalement comme des installations de récupération des ressources. La récupération pourrait inclure des options différentes et plus ou moins innovantes telles que la récupération d'énergie par la production de biogaz et la séparation à la source de l'urine avec la récupération / traitement de nutriments (principalement l'azote et le phosphore).

Le travail présenté dans ce manuscrit est le résultat d'une approche de couplage comprenant une modélisation dynamique rigoureuse, une évaluation du cycle de vie avec des limites étendues et une optimisation multi-objectif efficace. En ce qui concerne les influents, une plus grande fiabilité a été obtenue puisque cette étude a examiné la caractérisation dynamique de l'urine et des eaux usées suivie de son inclusion dans un générateur d'influents adapté. En ce qui concerne la dernière partie de ce travail - l'optimisation multi-objectifs - différentes formulations de problèmes et études de cas ont été proposées avec l'application de la plateforme aux scénarios de traitement conventionnels et alternatifs.

En outre, il est important d'indiquer que la principale différence entre cette étude et d'autres trouvés dans la littérature est la fiabilité de la plateforme lors de l'utilisation de simulations dynamiques et d'une entrée dynamique plus fiable pour les flux, notamment d'urine. De plus, cette

étude est la première qui comprend l'optimisation multi-objectif de scénarios alternatifs, couplant la modélisation de la totalité de la station et les aspects dynamiques, ainsi qu'une intégration pertinente de l'ACV. On a également étudié les scénarios alternatifs liés à la séparation de l'urine à la source et l'épandage agricole pas encore largement évalués dans la littérature par l'ACV.

Les perspectives pour la suite de cette étude pourraient être divisées en trois principaux aspects de la plateforme: la modélisation de la station d'épuration, l'ACV et l'optimisation multi-objectif. Aussi, il convient de noter que la flexibilité est l'une des principales caractéristiques de la plateforme DM-LCA-EMOO et que cette caractéristique a été particulièrement envisagée tout au long de ce travail. Des efforts particuliers ont été déployés pendant la construction de la plateforme afin d'en assurer l'applicabilité à d'autres cas d'études qui pourraient devenir pertinentes dans le futur.

En ce qui concerne la modélisation et la simulation, la souplesse est particulièrement importante, car les technologies et les configurations changent fréquemment pour atteindre, par exemple, des limites de rejet plus faibles. En outre, la modélisation de certaines parties du processus évolue rapidement de nos jours, comme la modélisation des émissions de N<sub>2</sub>O qui n'ont pas encore atteint un consensus dans les communautés scientifiques et industrielles. Ces derniers, cependant, pourraient changer complètement le choix des paramètres de fonctionnement lorsque des scénarios durables sont ciblés.

Selon les intrants de la station d'épuration, il est également important d'intensifier les efforts pour fournir des informations plus réalistes à différents niveaux (dépendance temporelle, caractéristiques géographiques et de collecte). Cependant, cela dépend aussi fortement de la collecte de données qui permettrait la compréhension de la dynamique, principalement pour la génération de l'urine qui n'est pas profondément étudiée, en particulier en fonction des aspects liés à la dépendance de la concentration de certains composants. Aussi, une perspective intéressante qui pourrait être considérée est la génération d'autres flux d'un ménage lors de l'examen d'autres scénarios de séparation de source.

L'amélioration des propositions dans le domaine de l'ACV comprend principalement l'ajout d'aspects dynamiques dans l'évaluation environnementale ainsi que l'ajout de plus de détails - comme les substances émergentes telles que les micropolluants. Il convient de noter que, actuellement, comme l'ACV repose sur des conditions statiques, les résultats dynamiques de l'exploitation de la station d'épuration sont intégrés et calculés en moyenne. Cependant, certaines améliorations de l'ACV permettraient de tenir compte de la dépendance temporelle des processus de *background* en fonction de l'opération de l'installation ainsi que des changements à long terme des systèmes de collecte.

Un autre effort important à réaliser lorsque l'on considère l'analyse environnementale couplée aux différents scénarios de gestion et de traitement des eaux usées concerne l'infrastructure, car les évaluations basées sur des scénarios alternatifs devraient également inclure des modifications d'infrastructure afin de refléter leurs gains réels. Cependant, de nos jours, une grande incertitude est impliquée dans l'analyse environnementale et par conséquent, de légères modifications dans l'infrastructure peuvent ne pas être quantifiées correctement. Dans ce sens, des efforts doivent être déployés pour considérer la modélisation des infrastructures de manière rigoureuse ou du moins pour valider les incertitudes liées à la taille d'une installation afin de permettre des conclusions plus réalistes pour les scénarios alternatifs. Par conséquent, on pourrait penser à une liste exhaustive de scénarios de perspective (avec des changements d'infrastructure) à évaluer et optimiser tels que l'inclusion de l'oxydation anaérobie de l'ammonium dans la filière principale d'une station d'épuration ainsi qu'une multitude de procédés pour le traitement et la valorisation de l'urine séparée à la source.

Considérant les aspects d'optimisation, la méthodologie évolue rapidement et les progrès récents sur l'apprentissage automatique sont actuellement utilisés dans le domaine de l'optimisation coûteuse. A notre connaissance, l'utilisation de ces outils pour une reconnaissance et une approximation efficace des fonctions objectives, pourrait représenter un gain important dans l'optimisation des stations d'épuration, mais aussi lorsque l'optimisation est sujette à des contraintes rigides multiples. Enfin, il est également possible d'inclure une superstructure dans le problème d'optimisation en utilisant des variables binaires afin de définir les voies à suivre dans le traitement de l'eau, par exemple dans le cas de la séparation à la source de l'urine et surtout quand les problèmes plus complexes, tels que la gestion complète des déchets ménagers ou des pourcentages plus élevés de rétention d'urine sont envisagés.

En conclusion, l'outil DM-LCA-EMOO développé est désormais disponible pour l'évaluation et l'optimisation de tout scénario souhaité dans le domaine du traitement des eaux usées. L'outil est en effet assez souple pour être adapté à toutes les études de cas connexes et peut être intégré à différentes plateformes de modélisation existantes.



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# **Supplementary Information**



## A. Supplementary Information for chapter II

### A.1. Emissions calculation

Dynamic simulation results integration and conversion

$$T_i = \int_{t=0}^{t_f} Q_i \cdot c_i \cdot f_i \cdot dt$$

Where:

$T_i$  is the total mass of species  $i$  in kg (required for LCA calculation)

$c_i$  is the concentration of species  $i$  in concentration units

$Q_i$  is the flow related to species  $i$  in  $m^3 \cdot d^{-1}$  (depending on the species  $i$  it can be a specific flow or influent/effluent flow)

$f_i$  is the conversion factor used for species  $i$  (unit is function of species concentration)

### Effluent discharged

COD:

$$Q_{EFFLUENT} \left[ \frac{m^3}{d} \right] \cdot c_{COD} \left[ \frac{g \text{ COD}}{m^3} \right] \cdot \frac{1}{10^3} \left[ \frac{kg \text{ COD}}{g \text{ COD}} \right]$$

BOD:

$$Q_{EFFLUENT} \left[ \frac{m^3}{d} \right] \cdot c_{BOD} \left[ \frac{g \text{ BOD}}{m^3} \right] \cdot \frac{1}{10^3} \left[ \frac{kg \text{ BOD}}{g \text{ BOD}} \right]$$

Nitrate

$$Q_{EFFLUENT} \left[ \frac{m^3}{d} \right] \cdot c_{NO_3} \left[ \frac{g \text{ N}}{m^3} \right] \cdot \frac{1}{14.007} \left[ \frac{mol \text{ N}}{g \text{ N}} \right] \cdot 1 \left[ \frac{mol \text{ NO}_3}{mol \text{ N}} \right] \cdot 62.004 \left[ \frac{g \text{ NO}_3}{mol \text{ NO}_3} \right] \cdot \frac{1}{10^3} \left[ \frac{kg \text{ NO}_3}{g \text{ NO}_3} \right]$$

Nitrite

$$Q_{EFFLUENT} \left[ \frac{m^3}{d} \right] \cdot c_{NO_2} \left[ \frac{g \text{ N}}{m^3} \right] \cdot \frac{1}{14.007} \left[ \frac{mol \text{ N}}{g \text{ N}} \right] \cdot 1 \left[ \frac{mol \text{ NO}_2}{mol \text{ N}} \right] \cdot 46.005 \left[ \frac{g \text{ NO}_2}{mol \text{ NO}_2} \right] \cdot \frac{1}{10^3} \left[ \frac{kg \text{ NO}_2}{g \text{ NO}_2} \right]$$

## Supplementary Information

Ammonium:

$$Q_{EFFLUENT} \left[ \frac{m^3}{d} \right] \cdot c_{NH_4} \left[ \frac{g N}{m^3} \right] \cdot \frac{1}{14.007} \left[ \frac{mol N}{g N} \right] \cdot 1 \left[ \frac{mol NH_4}{mol N} \right] \cdot 18.039 \left[ \frac{g NH_4}{mol NH_4} \right] \cdot \frac{1}{10^3} \left[ \frac{kg NH_4}{g NH_4} \right]$$

Nitrogen, organic bound:

$$Q_{EFFLUENT} \left[ \frac{m^3}{d} \right] \cdot \left( c_{X_{U,N}} \left[ \frac{g N}{m^3} \right] + c_{X_{B,N}} \left[ \frac{g N}{m^3} \right] + c_{S_{B,N}} \left[ \frac{g N}{m^3} \right] \right) \cdot \frac{1}{10^3} \left[ \frac{kg N}{g N} \right]$$

Nitrogen:

$$Q_{EFFLUENT} \left[ \frac{m^3}{d} \right] \cdot c_{S_{U,N}} \left[ \frac{g N}{m^3} \right] \cdot \frac{1}{10^3} \left[ \frac{kg N}{g N} \right]$$

N in Biomass

$$Q_{SLUDGE} \left[ \frac{m^3}{d} \right] \cdot \left( c_{OHO} \left[ \frac{g COD}{m^3} \right] + c_{MEOLO} \left[ \frac{g COD}{m^3} \right] + c_{AOO} \left[ \frac{g COD}{m^3} \right] + c_{NOO} \left[ \frac{g COD}{m^3} \right] + c_{AMO} \left[ \frac{g COD}{m^3} \right] + c_{PRO} \left[ \frac{g COD}{m^3} \right] + c_{ACO} \left[ \frac{g COD}{m^3} \right] + c_{HMO} \left[ \frac{g COD}{m^3} \right] \right. \\ \left. + c_{PAO} \left[ \frac{g COD}{m^3} \right] + c_E \left[ \frac{g COD}{m^3} \right] \right) \cdot 0.07 \left[ \frac{g N}{g COD} \right] \cdot \frac{1}{10^3} \left[ \frac{kg N}{g N} \right]$$

Phosphorus:

$$Q_{EFFLUENT} \left[ \frac{m^3}{d} \right] \cdot c_{TP} \left[ \frac{g P}{m^3} \right] \cdot \frac{1}{30.974} \left[ \frac{mol P}{g P} \right] \cdot 1 \left[ \frac{mol PO_4}{mol P} \right] \cdot 94.97 \left[ \frac{g PO_4}{mol PO_4} \right] \cdot \frac{1}{10^3} \left[ \frac{kg PO_4}{g PO_4} \right]$$

Magnesium:

$$Q_{EFFLUENT} \left[ \frac{m^3}{d} \right] \cdot c_{Mg} \left[ \frac{g Mg}{m^3} \right] \cdot \frac{1}{10^3} \left[ \frac{kg Mg}{g Mg} \right]$$

Calcium:

$$Q_{EFFLUENT} \left[ \frac{m^3}{d} \right] \cdot c_{Ca} \left[ \frac{g Ca}{m^3} \right] \cdot \frac{1}{10^3} \left[ \frac{kg Ca}{g Ca} \right]$$

TOC

$$Q_{EFFLUENT} \left[ \frac{m^3}{d} \right] \cdot \left( \left( \left( c_{SU} \left[ \frac{g COD}{m^3} \right] + c_{XU} \left[ \frac{g COD}{m^3} \right] \right) \cdot 0.553 \left[ \frac{g C}{g COD} \right] \right) + \left( \left( c_{SB,COMPLEX} \left[ \frac{g COD}{m^3} \right] + c_{XB} \left[ \frac{g COD}{m^3} \right] \right) \cdot 0.594 \left[ \frac{g C}{g COD} \right] \right) \right. \\ \left. + \left( \left( c_{OHO} \left[ \frac{g COD}{m^3} \right] + c_{MEOLO} \left[ \frac{g COD}{m^3} \right] + c_{AOO} \left[ \frac{g COD}{m^3} \right] + c_{NOO} \left[ \frac{g COD}{m^3} \right] + c_{AMO} \left[ \frac{g COD}{m^3} \right] + c_{PRO} \left[ \frac{g COD}{m^3} \right] + c_{ACO} \left[ \frac{g COD}{m^3} \right] + c_{HMO} \left[ \frac{g COD}{m^3} \right] \right. \right. \\ \left. \left. + c_{PAO} \left[ \frac{g COD}{m^3} \right] + c_E \left[ \frac{g COD}{m^3} \right] \right) \cdot 0.531 \left[ \frac{g C}{g COD} \right] \right) \right) \cdot \frac{1}{10^3} \left[ \frac{kg C}{g C} \right]$$

DOC

$$Q_{EFFLUENT} \left[ \frac{m^3}{d} \right] \cdot \left( \left( c_{SU} \left[ \frac{g COD}{m^3} \right] \cdot 0.553 \left[ \frac{g C}{g COD} \right] \right) + \left( c_{SB,COMPLEX} \left[ \frac{g COD}{m^3} \right] \cdot 0.594 \left[ \frac{g C}{g COD} \right] \right) \right) \cdot \frac{1}{10^3} \left[ \frac{kg C}{g C} \right]$$

Carbon dioxide (total):

$$\sum_{i=1}^5 Q_{gas,i} \left[ \frac{m^3}{h} \right] \cdot 24 \left[ \frac{h}{d} \right] \cdot c_{\%CO_2,i} [dimensionless] \cdot 1.830 \cdot 10^{-2}$$

Where i represents each reactor of the process (aerobic and anoxic ones) and  $c_{\%CO_2,i}$  is between 0-100.

Total carbon dioxide is then divided between biogenic (from influent) and fossil (from methanol added) by the ratio of biogenic/fossil carbon:

DCO biogenic:

$$Q_{INFLUENT} \left[ \frac{m^3}{d} \right] \cdot \left( c_{XB} \left[ \frac{g COD}{m^3} \right] + c_{SB,COMPLEX} \left[ \frac{g COD}{m^3} \right] + c_{CB} \left[ \frac{g COD}{m^3} \right] \right) \cdot \frac{29.160}{93.440} \left[ \frac{g C}{g COD} \right] \cdot \frac{1}{10^3} \left[ \frac{kg C}{g C} \right]$$

DCO fossil:

$$Q_{CARBON} \left[ \frac{m^3}{d} \right] \cdot c_{CARBON} \left[ \frac{g COD}{m^3} \right] \cdot \frac{12}{48} \left[ \frac{g C}{g COD} \right] \cdot \frac{1}{10^3} \left[ \frac{kg C}{g C} \right]$$

Methane:

$$\sum_{i=1}^5 Q_{gas,i} \left[ \frac{m^3}{h} \right] \cdot 24 \left[ \frac{h}{d} \right] \cdot c_{\%CH_4,i} [dimensionless] \cdot 6.669 \cdot 10^{-3}$$

Where i represents each reactor of the process (aerobic and anoxic ones) and  $c_{\%CH_4,i}$  is between 0-100.

## Supplementary Information

Ammonia:

$$\sum_{i=1}^5 Q_{gas,i} \left[ \frac{m^3}{h} \right] \cdot 24 \left[ \frac{h}{d} \right] \cdot c_{\%NH_3,i} [dimensionless] \cdot 7.079 \cdot 10^{-3}$$

Where i represents each reactor of the process (aerobic and anoxic ones) and  $c_{\%NH_3,i}$  is between 0-100.

Hydrogen:

$$\sum_{i=1}^5 Q_{gas,i} \left[ \frac{m^3}{h} \right] \cdot 24 \left[ \frac{h}{d} \right] \cdot c_{\%H_2,i} [dimensionless] \cdot 8.380 \cdot 10^{-4}$$

Where i represents each reactor of the process (aerobic and anoxic ones) and  $c_{\%H_2,i}$  is between 0-100.

For details in gas calculations please refer to Section 7

Dinitrogen monoxide:

$$\sum_{i=1}^5 dNit_i \left[ \frac{mg N}{L \cdot h} \right] \cdot \frac{0.5}{100} [dimensionless] \cdot \frac{1}{14.007} \left[ \frac{mmol N}{mg N} \right] \cdot \frac{1}{2} \left[ \frac{mmol N_2O}{mmol N} \right] \cdot 44.013 \left[ \frac{mg N_2O}{mmol N_2O} \right] \cdot 1000 \left[ \frac{L}{m^3} \right] \cdot 24 \left[ \frac{h}{d} \right] V_{liquid,i} [m^3] \cdot \frac{1}{10^6} \left[ \frac{kg N_2O}{mg N_2O} \right]$$

Where i represents each reactor of the process (aerobic and anoxic ones) and  $V_{liquid,i}$  is the liquid volume.

### Sludge to agriculture

Total N:

$$Q_{SLUDGE} \left[ \frac{m^3}{d} \right] \cdot c_{TN} \left[ \frac{g N}{m^3} \right] \cdot \frac{1}{10^3} \left[ \frac{kg N}{g N} \right]$$

Ammonia:

$$TN \left[ \frac{kg N}{d} \right] \cdot 0.2581 \left[ \frac{kg NH_3 - N}{kg N} \right] \cdot \frac{17.031}{14.007} \left[ \frac{kg NH_3}{kg NH_3 - N} \right]$$

Dinitrogen monoxide:

$$TN \left[ \frac{kg N}{d} \right] \cdot 0.0118 \left[ \frac{kg N_2O - N}{kg N} \right] \cdot \frac{44.013}{14.007} \left[ \frac{kg N_2O}{kg N_2O - N} \right]$$

Total P:

$$Q_{SLUDGE} \left[ \frac{m^3}{d} \right] \cdot c_{TP} \left[ \frac{g P}{m^3} \right] \cdot \frac{1}{10^3} \left[ \frac{kg P}{g P} \right]$$

Phosphate to ground water:

$$TP \left[ \frac{kg P}{d} \right] \cdot 0.0057 \left[ \frac{kg PO_4 - P}{kg P} \right] \cdot \frac{94.97}{30.974} \left[ \frac{kg PO_4}{kg PO_4 - P} \right]$$

Phosphate to surface water:

$$TP \left[ \frac{kg P}{d} \right] \cdot 0.02005 \left[ \frac{kg PO_4 - P}{kg P} \right] \cdot \frac{94.97}{30.974} \left[ \frac{kg PO_4}{kg PO_4 - P} \right]$$

Total C:

$$\begin{aligned} Q_{SLUDGE} \left[ \frac{m^3}{d} \right] \cdot & \left( \left( c_{SU} \left[ \frac{g COD}{m^3} \right] + c_{XU} \left[ \frac{g COD}{m^3} \right] \right) \cdot 0.553 \left[ \frac{g C}{g COD} \right] + \left( c_{SB,COMPLEX} \left[ \frac{g COD}{m^3} \right] + c_{XB} \left[ \frac{g COD}{m^3} \right] \right) \cdot 0.594 \left[ \frac{g C}{g COD} \right] \right) \\ & + \left( c_{OHO} \left[ \frac{g COD}{m^3} \right] + c_{MEOLO} \left[ \frac{g COD}{m^3} \right] + c_{AOO} \left[ \frac{g COD}{m^3} \right] + c_{NOO} \left[ \frac{g COD}{m^3} \right] + c_{AMO} \left[ \frac{g COD}{m^3} \right] + c_{PRO} \left[ \frac{g COD}{m^3} \right] + c_{ACO} \left[ \frac{g COD}{m^3} \right] + c_{HMO} \left[ \frac{g COD}{m^3} \right] \right. \\ & + c_{PAO} \left[ \frac{g COD}{m^3} \right] + c_E \left[ \frac{g COD}{m^3} \right] \left. \right) \cdot 0.531 \left[ \frac{g C}{g COD} \right] + \left( c_{CO_3^{2-}} \left[ \frac{mol CO_3^{2-}}{m^3} \right] \cdot 1 \left[ \frac{mol C}{mol CO_3^{2-}} \right] \cdot 12.011 \left[ \frac{g C}{mol C} \right] \right) \\ & + \left( c_{HCO_3^-} \left[ \frac{mol HCO_3^-}{m^3} \right] \cdot 1 \left[ \frac{mol C}{mol HCO_3^-} \right] \cdot 12.011 \left[ \frac{g C}{mol C} \right] \right) \cdot \frac{1}{10^3} \left[ \frac{kg C}{g C} \right] \end{aligned}$$

Magnesium:

$$Q_{SLUDGE} \left[ \frac{m^3}{d} \right] \cdot c_{Mg} \left[ \frac{g Mg}{m^3} \right] \cdot \frac{1}{10^3} \left[ \frac{kg Mg}{g Mg} \right]$$

Calcium:

$$Q_{SLUDGE} \left[ \frac{m^3}{d} \right] \cdot c_{Ca} \left[ \frac{g Ca}{m^3} \right] \cdot \frac{1}{10^3} \left[ \frac{kg Ca}{g Ca} \right]$$

**Effluent and sludge (divided in function):**

**Chloride**

From coagulant:

$$Q_{METAL} \left[ \frac{m^3}{d} \right] \cdot 10^3 \left[ \frac{L}{m^3} \right] \cdot c_{METAL,ION} \left[ \frac{mmol Fe^{3+}}{L} \right] \cdot 3 \left[ \frac{mmol Cl^-}{mmol Fe^{3+}} \right] \cdot 35.453 \left[ \frac{mg Cl^-}{mmol Cl^-} \right] \cdot \frac{1}{10^6} \left[ \frac{kg Cl^-}{mg Cl^-} \right]$$

Supplementary Information

## Supplementary Information

From H<sub>2</sub>S treatment:

$$Q_{INFLUENT} \left[ \frac{m^3}{d} \right] \cdot c_{FeCl_3} \left[ \frac{g FeCl_3}{m^3} \right] \cdot \frac{1}{162.206} \left[ \frac{mol FeCl_3}{g FeCl_3} \right] \cdot 3 \left[ \frac{mol Cl^-}{mol FeCl_3} \right] \cdot 35.453 \left[ \frac{g Cl^-}{mol Cl^-} \right] \cdot \frac{1}{10^3} \left[ \frac{kg Cl^-}{g Cl^-} \right]$$

**Iron**

From coagulant:

$$Q_{METAL} \left[ \frac{m^3}{d} \right] \cdot 10^3 \left[ \frac{L}{m^3} \right] \cdot c_{METAL} \left[ \frac{mg Fe^{3+}}{L} \right] \cdot \frac{1}{10^6} \left[ \frac{kg Fe^{3+}}{mg Fe^{3+}} \right]$$

From H<sub>2</sub>S treatment:

$$Q_{INFLUENT} \left[ \frac{m^3}{d} \right] \cdot c_{FeCl_3} \left[ \frac{g FeCl_3}{m^3} \right] \cdot \frac{1}{162.206} \left[ \frac{mol FeCl_3}{g FeCl_3} \right] \cdot 1 \left[ \frac{mol Fe^{3+}}{mol FeCl_3} \right] \cdot 55.847 \left[ \frac{g Fe^{3+}}{mol Fe^{3+}} \right] \cdot \frac{1}{10^3} \left[ \frac{kg Fe^{3+}}{g Fe^{3+}} \right]$$

**Background processes****Infrastructure:**

$$\frac{1[\text{unit}]}{t_{Plant\ lifetime} [y] \cdot Q_{average\ annual\ sewage\ in} \left[ \frac{m^3}{y} \right]}$$

**FeCl<sub>3</sub>**

From coagulant:

$$Q_{METAL} \left[ \frac{m^3}{d} \right] \cdot 10^3 \left[ \frac{L}{m^3} \right] \cdot c_{METAL} \left[ \frac{mg Fe^{3+}}{L} \right] \cdot \frac{1}{55.847} \left[ \frac{mmol Fe^{3+}}{mg Fe^{3+}} \right] \cdot 1 \left[ \frac{mmol FeCl_3}{mmol Fe^{3+}} \right] \cdot 162.206 \left[ \frac{mg FeCl_3}{mmol FeCl_3} \right] \cdot \frac{1}{10^6} \left[ \frac{kg FeCl_3}{mg FeCl_3} \right]$$

From H<sub>2</sub>S treatment:

$$Q_{INFLUENT} \left[ \frac{m^3}{d} \right] \cdot c_{FeCl_3} \left[ \frac{g FeCl_3}{m^3} \right] \cdot \frac{1}{10^3} \left[ \frac{kg FeCl_3}{g FeCl_3} \right]$$

**Methanol**

$$Q_{CARBON} \left[ \frac{m^3}{d} \right] \cdot c_{CARBON} \left[ \frac{g DCO}{m^3} \right] \cdot \frac{32.042}{48} \left[ \frac{g MeOH}{g DCO} \right] \cdot \frac{1}{10^3} \left[ \frac{kg MeOH}{g MeOH} \right]$$

**NaOH**

$$Q_{ALKALINITY} \left[ \frac{m^3}{d} \right] \cdot c_{STRONG\ BASES} \left[ \frac{mol NaOH}{m^3} \right] \cdot 39.997 \left[ \frac{g NaOH}{mol NaOH} \right] \cdot \frac{1}{10^3} \left[ \frac{kg NaOH}{g NaOH} \right]$$

### Struvite production and emissions

Magnesium oxide:

$$Q_{URINE} \left[ \frac{m^3}{d} \right] \cdot c_{Mg} \left[ \frac{g \text{ Mg}}{m^3} \right] \cdot \frac{1}{24.305} \left[ \frac{mol \text{ Mg}}{g \text{ Mg}} \right] \cdot 1 \left[ \frac{mol \text{ MgO}}{mol \text{ Mg}} \right] \cdot 40.304 \left[ \frac{g \text{ MgO}}{mol \text{ MgO}} \right] \cdot \frac{1}{10^3} \left[ \frac{kg \text{ MgO}}{g \text{ MgO}} \right]$$

Struvite production:

$$Q_{STRUVITE} \left[ \frac{m^3}{d} \right] \cdot c_{TSS} \left[ \frac{g \text{ Struvite}}{m^3} \right] \cdot \frac{1}{10^3} \left[ \frac{kg \text{ Struvite}}{g \text{ Struvite}} \right]$$

### A.2. Inventory

UF: 1 m<sup>3</sup> of raw wastewater to be treated

Process	Operational data		Ecoinvent process	Unit	REF	EPC	USS	USS+E PC	USS+E PC+AG RI	USS+ EPC+ ANA
WWTP	Infrastructure		wastewater treatment plant, class 2, CH, [unit] (#2284)	unit	4.42E-9	4.42E-9	4.42E-9	4.42E-9	4.42E-9	4.42E-9
	Effluent discharge	NH <sub>4</sub>	Ammonium, ion, water, river, [kg] (#4259)	kg	1.21E-3	6.10E-4	8.14E-4	4.43E-4	9.15E-4	1.33E-3
		NO <sub>2</sub>	Nitrite, water, river, [kg] (#5075)	kg	6.08E-4	2.56E-4	3.69E-4	1.86E-4	4.24E-4	8.52E-4
		NO <sub>3</sub>	Nitrate, water, river, [kg] (#5067)	kg	1.91E-2	1.35E-2	1.53E-2	1.46E-2	1.33E-2	1.35E-2
		N <sub>org</sub>	Nitrogen, organic bound, water, river, [kg] (#5091)	kg	1.63E-3	1.73E-3	1.63E-3	1.71E-3	1.59E-3	1.54E-3
		PO <sub>4</sub>	Phosphate, water, river, [kg] (#5139)	kg	2.05E-3	1.33E-3	1.79E-3	1.15E-3	1.16E-3	1.52E-3
		BOD5	BOD5, Biological Oxygen Demand, water, river, [kg] (#4371)	kg	4.47E-3	6.31E-3	4.62E-3	5.83E-3	4.32E-3	3.78E-3
		COD	COD, Chemical Oxygen Demand, water, river, [kg] (#4603)	kg	4.09E-2	4.41E-2	4.15E-2	4.36E-2	3.79E-2	4.05E-2
		TOC	TOC, Total Organic Carbon, water, river, [kg] (#5563)	kg	2.18E-2	2.32E-2	2.20E-2	2.30E-2	2.02E-2	2.16E-2
		DOC	DOC, Dissolved Organic Carbon, water, river, [kg]	kg	1.53E-2	1.55E-2	1.55E-2	1.56E-2	1.35E-2	1.52E-2

Supplementary Information



	Zn	Zinc, ion, water, river, [kg] (#5667)	kg	5.99E-5	5.99E-5	5.99E-5	5.99E-5	5.99E-5	5.99E-5	
	Si	Silicon, water, river, [kg] (#5339)	kg	1.56E-4	1.56E-4	1.56E-4	1.56E-4	1.56E-4	1.56E-4	
	Al	Aluminium, water, river, [kg] (#4243)	kg	3.25E-5	3.25E-5	3.25E-5	3.25E-5	3.25E-5	3.25E-5	
	SO <sub>4</sub>	Sulfate, water, river, [kg] (#5427)	kg	4.40E-4	4.40E-4	4.40E-4	4.40E-4	4.40E-2	4.40E-2	
	Cl	Chloride, water, river, [kg] (#4515)	kg	5.09E-2	4.36E-2	4.24E-2	3.73E-2	3.98E-2	3.48E-2	
	F	Fluoride, water, river, [kg] (#4731)	kg	3.27E-5	3.27E-5	3.27E-5	3.27E-5	3.27E-5	3.27E-5	
	K	Potassium, ion, water, river, [kg] (#5211)	kg	3.98E-4	3.98E-4	3.98E-4	3.98E-4	3.98E-4	3.98E-4	
	Na	Sodium, ion, water, river, [kg] (#5363)	kg	2.18E-3	2.18E-3	2.18E-3	2.18E-3	2.18E-3	2.18E-3	
Electricity		electricity, production mix RER, RER, [kWh] (#7209) <sup>1</sup>	kWh	1.08E-1	3.42E-1	1.02E-1	-	-	-	
Heat		heat, natural gas, at boiler modulating >100kW, RER, [MJ] (#1350) <sup>1</sup>	MJ	-	-	-	-	-	-	
Grits collection	Transport	transport, lorry 20-28t, fleet average, CH, [tkm] (#1942)	tkm	3.10E-4	3.10E-4	3.10E-4	3.10E-4	3.10E-4	3.10E-4	
	Disposal	disposal, paper, 11.2% water, to municipal incineration, CH, [kg] (#2108)	kg	1.55E-2	1.55E-2	1.55E-2	1.55E-2	1.55E-2	1.55E-2	
		disposal, plastics, mixture, 15.3% water, to municipal incineration, CH, [kg] (#2112)	kg	1.55E-2	1.55E-2	1.55E-2	1.55E-2	1.55E-2	1.55E-2	
Cogeneration unit	Infrastructure	cogen unit 160kWe, common components for heat+electricity, RER, [unit] (#1201)	unit	1.04E-8	1.32E-8	1.08E-8	1.37E-8	1.32E-8	1.32E-8	
	Oil for maintenance	Production	lubricating oil, at plant, RER, [kg] (#416)	kg	6.25E-5	7.93E-5	6.47E-5	8.20E-5	7.91E-5	7.90E-5
		Disposal	disposal, used mineral oil, 10% water, to hazardous waste incineration, CH, [kg] (#2064)	kg	6.25E-5	7.93E-5	6.47E-5	8.20E-5	7.91E-5	7.90E-5
	Operation emissions <sup>2</sup>		biogas, burned in cogen with gas engine, CH, [MJ] (#135)	MJ	2.08E0	2.64E0	2.16E0	2.73E0	2.64E0	2.63E0
			electricity, at cogen with biogas engine, allocation exergy, CH, [kWh] (#6221)	kWh	2.03E-1	2.57E-1	2.10E-1	2.66E-1	2.56E-1	2.56E-1
			heat, at cogen with biogas engine, allocation exergy, CH, [MJ] (#6219)	MJ	1.01E0	1.28E0	1.05E0	1.33E0	1.28E0	1.28E0
		Dinitrogen monoxide, air, high population density, [kg] (#2814)	kg	5.21E-6	6.61E-6	5.39E-6	6.83E-6	6.59E-6	6.59E-6	

Supplementary Information

## Supplementary Information

				Methane, biogenic, air, high population density, [kg] (#3149)	kg	4.79E-5	6.08E-5	4.96E-5	6.29E-5	6.06E-5	6.06E-5
				Carbon dioxide, biogenic, air, high population density, [kg] (#2694)	kg	1.51E-1	1.87E-1	1.56E-1	1.98E-1	2.08E-1	2.20E-1
				Carbon dioxide, fossil, air, high population density, [kg] (#2699)	kg	2.32E-2	3.35E-2	2.40E-2	3.04E-2	1.24E-2	-
				Carbon monoxide, biogenic, air, high population density, [kg] (#2709)	kg	8.67E-5	1.08E-4	8.98E-5	1.14E-4	1.19E-4	1.26E-4
				Carbon monoxide, fossil, air, high population density, [kg] (#2714)	kg	1.33E-5	1.93E-5	1.38E-5	1.75E-5	7.10E-6	-
				NM VOC, non-methane volatile organic compounds, unspecified origin, air, high population density, [kg] (#3274)	kg	4.17E-6	5.29E-6	4.32E-6	5.47E-6	5.27E-6	5.27E-6
				Nitrogen oxides, air, high population density, [kg] (#3269)	kg	3.12E-5	3.97E-5	3.24E-5	4.10E-5	3.95E-5	3.95E-5
				Sulfur dioxide, air, high population density, [kg] (#3529)	kg	4.38E-5	5.55E-5	4.53E-5	5.74E-5	5.54E-5	5.53E-5
				Heat, waste, air, high population density, [MJ] (#2979)	MJ	3.44E-1	4.36E-1	3.56E-1	4.51E-1	4.35E-1	4.35E-1
			Chemicals	Methanol	Production	methanol, at plant, GLO, [kg] (#422)	kg	5.27E-2	6.15E-2	5.44E-2	5.44E-2
Transport	transport, freight, rail, RER, [tkm] (#1983)	tkm			3.16E-2	3.69E-2	3.26E-2	3.26E-2	1.20E-2	-	
	transport, lorry 20-28t, fleet average, CH, [tkm] (#1942)	tkm			2.64E-3	3.07E-3	2.72E-3	2.72E-3	9.96E-4	-	
FeCl <sub>3</sub>	Production	iron (III) chloride, 40% in H <sub>2</sub> O, at plant, CH, [kg] (#292)		kg	7.78E-2	6.66E-2	6.47E-2	5.70E-2	6.08E-2	5.31E-2	
	Transport	transport, freight, rail, RER, [tkm] (#1983)		tkm	1.17E-1	9.98E-2	9.70E-2	8.55E-2	9.13E-2	7.97E-2	
		transport, lorry 20-28t, fleet average, CH, [tkm] (#1942)		tkm	9.72E-3	8.32E-3	8.08E-3	7.12E-3	7.60E-3	6.64E-3	
Urine separation	Storage		glass fibre, at plant, RER, [kg] (#808)	kg	-	-	8.40E-5	8.40E-5	8.40E-5	8.40E-5	
	Transport		transport, lorry 20-28t, fleet average, CH, [tkm] (#1942)	tkm	-	-	1.56E-2	1.56E-2	1.56E-2	1.56E-2	
Struvite precipitation and utilization	Chemicals	MgO	Production	magnesium oxide, at plant, RER, [kg] (#296)	kg	-	-	2.12E-3	2.12E-3	2.12E-3	2.12E-3
			Transport	transport, freight, rail, RER, [tkm] (#1983)	tkm	-	-	1.27E-3	1.27E-3	1.27E-3	1.27E-3
				transport, lorry 20-28t, fleet average, CH, [tkm] (#1942)	tkm	-	-	1.06E-4	1.06E-4	1.06E-4	1.06E-4

	NaOH	Production	sodium hydroxide, 50% in H2O, production mix, at plant, RER, [kg] (#336)	kg	-	-	-	-	-	1.19E-2		
		Transport		transport, freight, rail, RER, [tkm] (#1983)	tkm	-	-	-	-	-	1.43E-2	
				transport, lorry 20-28t, fleet average, CH, [tkm] (#1942)	tkm	-	-	-	-	-	1.19E-3	
	Transport			transport, lorry 20-28t, fleet average, CH, [tkm] (#1942)	tkm	-	-	1.14E-4	1.14E-4	1.14E-4	1.14E-4	
	Spreading			fertilising, by broadcaster, CH, [ha] (#156)	ha	-	-	3.26E-6	3.26E-6	3.26E-6	3.26E-6	
	Post emissions		NH <sub>3</sub>	Ammonia, air, high population density, [kg] (#2579)	kg	-	-	2.38E-5	2.38E-5	2.38E-5	2.38E-5	
			N <sub>2</sub> O	Dinitrogen monoxide, air, high population density, [kg] (#2814)	kg	-	-	9.23E-6	9.23E-6	9.23E-6	9.23E-6	
			NO <sub>x</sub>	Nitrogen oxides, air, high population density, [kg] (#3269)	kg	-	-	8.39E-6	8.39E-6	8.39E-6	8.39E-6	
			PO <sub>4</sub>		Phosphate, water, river, [kg] (#5139)	kg	-	-	1.19E-4	1.19E-4	1.19E-4	1.19E-4
					Phosphate, water, ground-, [kg] (#5135)	kg	-	-	4.34E-5	4.34E-5	4.34E-5	4.34E-5
		Cd	Cadmium, soil, agricultural, [kg] (#3951)	kg	-	-	7.42E-8	7.42E-8	7.42E-8	7.42E-8		
		Cu	Copper, soil, agricultural, [kg] (#3991)	kg	-	-	1.85E-7	1.85E-7	1.85E-7	1.85E-7		
		Zn	Zinc, soil, agricultural, [kg] (#4186)	kg	-	-	1.16E-6	1.16E-6	1.16E-6	1.16E-6		
		Pb	Lead, soil, agricultural, [kg] (#4047)	kg	-	-	7.49E-8	7.49E-8	7.49E-8	7.49E-8		
	Ni	Nickel, soil, agricultural, [kg] (#4088)	kg	-	-	1.56E-7	1.56E-7	1.56E-7	1.56E-7			
	Cr	Chromium, soil, agricultural, [kg] (#3976)	kg	-	-	8.56E-7	8.56E-7	8.56E-7	8.56E-7			
Sludge utilization	Transport			transport, lorry 20-28t, fleet average, CH, [tkm] (#1942)	tkm	2.17E-2	2.32E-2	2.19E-2	2.29E-2	2.24E-2	2.11E-2	
	Spreading			slurry spreading, by vacuum tanker, CH, [m <sup>3</sup> ] (#176)	m <sup>3</sup>	1.06E-3	1.14E-3	1.07E-3	1.12E-3	1.10E-3	1.04E-3	
	Post emissions		NH <sub>3</sub>	Ammonia, air, high population density, [kg] (#2579)	kg	3.58E-3	4.62E-3	3.69E-3	4.66E-3	4.38E-3	4.19E-3	
			N <sub>2</sub> O	Dinitrogen monoxide, air, high population density, [kg] (#2814)	kg	2.12E-4	2.73E-4	2.18E-4	2.75E-4	2.59E-4	2.48E-4	
			C	Carbon, soil, agricultural, [kg] (#3962)	kg	1.04E-1	1.25E-1	1.06E-1	1.27E-1	1.21E-1	1.16E-1	

Supplementary Information

## Supplementary Information

PO <sub>4</sub>	Phosphate, water, river, [kg] (#5139)	kg	6.80E-4	6.99E-4	6.21E-4	6.38E-4	6.36E-4	5.82E-4
	Phosphate, water, ground-, [kg] (#5135)	kg	1.93E-4	1.99E-4	1.76E-4	1.81E-4	1.81E-4	1.65E-4
Ca	Calcium, soil, agricultural, [kg] (#3955)	kg	1.59E-5	1.71E-5	1.66E-5	1.73E-5	1.70E-5	1.65E-5
Mg	Magnesium, soil, agricultural, [kg] (#4053)	kg	7.95E-5	1.34E-5	6.54E-5	9.87E-6	2.63E-5	4.54E-6
Fe	Iron, soil, agricultural, [kg] (#4041)	kg	2.73E-2	2.34E-2	2.28E-2	2.01E-2	2.14E-2	1.88E-2
As	Arsenic, soil, agricultural, [kg] (#3924)	kg	6.62E-7	6.63E-7	6.63E-7	6.63E-7	6.63E-7	6.62E-7
Cd	Cadmium, soil, agricultural, [kg] (#3951)	kg	1.00E-6	1.00E-6	1.00E-6	1.00E-6	1.00E-6	1.00E-6
Co	Cobalt, soil, agricultural, [kg] (#3987)	kg	5.01E-7	5.01E-7	5.01E-7	5.01E-7	5.01E-7	5.01E-7
Cr	Chromium, soil, agricultural, [kg] (#3976)	kg	1.25E-5	1.25E-5	1.25E-5	1.25E-5	1.25E-5	1.25E-5
Cu	Copper, soil, agricultural, [kg] (#3991)	kg	5.25E-5	5.25E-5	5.25E-5	5.25E-5	5.25E-5	5.25E-5
Hg	Mercury, soil, agricultural, [kg] (#4068)	kg	1.40E-6	1.40E-6	1.40E-6	1.40E-6	1.40E-6	1.40E-6
Mn	Manganese, soil, agricultural, [kg] (#4059)	kg	5.01E-5	5.01E-5	5.01E-5	5.01E-5	5.01E-5	5.01E-5
Mo	Molybdenum, soil, agricultural, [kg] (#4082)	kg	4.79E-7	4.79E-7	4.79E-7	4.79E-7	4.79E-7	4.79E-7
Ni	Nickel, soil, agricultural, [kg] (#4088)	kg	1.00E-5	1.00E-5	1.00E-5	1.00E-5	1.00E-5	1.00E-5
Pb	Lead, soil, agricultural, [kg] (#4047)	kg	5.85E-5	5.85E-5	5.85E-5	5.85E-5	5.85E-5	5.85E-5
Ag	Silver, ion, water, river, [kg] (#5347)	kg	5.25E-6	5.25E-6	5.25E-6	5.25E-6	5.25E-6	5.25E-6
Sn	Tin, soil, agricultural, [kg] (#4165)	kg	2.01E-6	2.01E-6	2.01E-6	2.01E-6	2.01E-6	2.01E-6
Zn	Zinc, soil, agricultural, [kg] (#4186)	kg	1.40E-4	1.40E-4	1.40E-4	1.40E-4	1.40E-4	1.40E-4
Si	Silicon, soil, agricultural, [kg] (#4133)	kg	2.97E-3	2.97E-3	2.97E-3	2.97E-3	2.97E-3	2.97E-3
Al	Aluminium, soil, agricultural, [kg] (#3915)	kg	6.18E-4	6.18E-4	6.18E-4	6.18E-4	6.18E-4	6.18E-4
S	Sulfur, soil, agricultural, [kg] (#4151)	kg	2.00E-3	2.00E-3	2.00E-3	2.00E-3	2.00E-3	2.00E-3
SO <sub>4</sub>	Sulfate, water, ground-, [kg] (#5423)	kg	4.68E-5	5.01E-5	4.72E-5	4.94E-5	4.84E-5	4.56E-5
Cl	Chloride, soil, agricultural, [kg] (#3967)	kg	5.43E-5	4.97E-5	4.55E-5	4.19E-5	4.39E-5	3.61E-5
F	Fluoride, soil, agricultural, [kg] (#4021)	kg	3.49E-8	3.73E-8	3.52E-8	3.68E-8	3.61E-8	3.39E-8
K	Potassium, soil, agricultural, [kg] (#4114)	kg	4.24E-7	4.54E-7	4.28E-7	4.47E-7	4.39E-7	4.13E-7

		Na	Sodium, soil, agricultural, [kg] (#4142)	kg	2.33E-6	2.49E-6	2.34E-6	2.45E-6	2.41E-6	2.26E-6
<b>N-rich utilization</b>	Transport		transport, lorry 20-28t, fleet average, CH, [tkm] (#1942)	tkm	-	-	-	-	1.32E-2	-
	Spreading		fertilising, by broadcaster, CH, [ha] (#156)	ha	-	-	-	-	1.32E-3	-
	Post emissions	NH <sub>3</sub>	Ammonia, air, high population density, [kg] (#2579)	kg	-	-	-	-	4.37E-4	-
		N <sub>2</sub> O	Dinitrogen monoxide, air, high population density, [kg] (#2814)	kg	-	-	-	-	2.26E-4	-
		NO <sub>x</sub>	Nitrogen oxides, air, high population density, [kg] (#3269)	kg	-	-	-	-	2.15E-4	-
		PO <sub>4</sub>	Phosphate, water, river, [kg] (#5139)	kg	-	-	-	-	2.77E-6	-
Phosphate, water, ground-, [kg] (#5135)	kg		-	-	-	-	1.01E-6	-		
<b>Fertilizers avoided</b>	Production	P-fertilizer	triple superphosphate, as P <sub>2</sub> O <sub>5</sub> , at regional storehouse, RER, [kg] (#57)	kg	1.77E-2	1.82E-2	1.95E-2	2.00E-2	2.00E-2	1.85E-2
		N-fertilizer	ammonium nitrate, as N, at regional storehouse, RER, [kg] (#40)	kg	4.57E-3	5.89E-3	5.36E-3	6.59E-3	2.06E-2	6.00E-3
	Transport	transport, freight, rail, RER, [tkm] (#1983)		tkm	2.23E-3	2.41E-3	2.49E-3	2.65E-3	4.06E-3	2.45E-3
		transport, lorry 20-28t, fleet average, CH, [tkm] (#1942)		tkm	2.23E-3	2.41E-3	2.49E-3	2.65E-3	4.06E-3	2.45E-3
		transport, barge, RER, [tkm] (#1966)		tkm	1.12E-2	1.26E-2	1.26E-2	1.39E-2	2.65E-2	1.28E-2
	Spreading		fertilising, by broadcaster, CH, [ha] (#156)	ha	2.28E-5	2.94E-5	2.68E-5	3.29E-5	1.03E-4	3.00E-5
	Post emissions	NH <sub>3</sub>	Ammonia, air, high population density, [kg] (#2579)	kg	9.14E-5	1.18E-4	1.07E-4	1.32E-4	4.12E-4	1.20E-4
		N <sub>2</sub> O	Dinitrogen monoxide, air, high population density, [kg] (#2814)	kg	3.66E-5	4.71E-5	4.29E-5	5.27E-5	1.65E-4	4.80E-5
		NO <sub>x</sub>	Nitrogen oxides, air, high population density, [kg] (#3269)	kg	2.74E-5	3.53E-5	3.22E-5	3.95E-5	1.24E-4	3.60E-5
		PO <sub>4</sub>	Phosphate, water, river, [kg] (#5139)	kg	1.04E-4	1.07E-4	1.14E-4	1.17E-4	1.17E-4	1.08E-4
			Phosphate, water, ground-, [kg] (#5135)	kg	3.79E-5	3.90E-5	4.17E-5	4.26E-5	4.27E-5	3.95E-5
As		Arsenic, soil, agricultural, [kg] (#3924)	kg	3.00E-7	3.19E-7	3.33E-7	3.51E-7	4.81E-7	3.24E-7	
Cd	Cadmium, soil, agricultural, [kg] (#3951)	kg	7.28E-7	7.56E-7	8.03E-7	8.28E-7	9.12E-7	7.66E-7		

Supplementary Information

## Supplementary Information

		Cu	Copper, soil, agricultural, [kg] (#3991)	kg	1.72E-6	1.80E-6	1.90E-6	1.98E-6	2.34E-5	1.83E-6
		Zn	Zinc, soil, agricultural, [kg] (#4186)	kg	1.58E-5	1.65E-5	1.75E-5	1.81E-5	2.09E-5	1.67E-5
		Pb	Lead, soil, agricultural, [kg] (#4047)	kg	1.44E-6	1.54E-6	1.60E-6	1.70E-6	2.47E-6	1.57E-6
		Ni	Nickel, soil, agricultural, [kg] (#4088)	kg	1.66E-6	1.73E-6	1.83E-6	1.90E-6	2.19E-6	1.76E-6
		Hg	Mercury, soil, agricultural, [kg] (#4068)	kg	5.64E-9	5.88E-9	6.23E-9	6.44E-9	7.43E-9	5.97E-9
		Cr	Chromium, soil, agricultural, [kg] (#3976)	kg	9.99E-6	1.04E-5	1.10E-5	1.14E-5	1.25E-5	1.05E-5
<b>Electricity avoided</b>	Electricity		electricity, production mix RER, RER, [kWh] (#7209)	kWh	-	-	-	8.22E-3	4.11E-2	2.22E-2

<sup>1</sup> In the case of no auto-sufficiency

<sup>2</sup> Modified with efficiencies of 35% electrical and 48.5% thermal (16.5% losses).

### A.3. Energy parameters

#### Aeration

$$P_{aeration} = \frac{w_{air}RT_1}{M_w n e} \left[ \left( \frac{p_2}{p_1} \right)^n - 1 \right]$$

$$p_2 = P_{atm} + h_L + H$$

$$h_L = 9.82 \times 10^{-8} \left( \frac{fLTQ_{air}}{PD} \right)$$

Where:

$P_{aeration}$  is the power requirement of the blower used for aeration (kW)

$w_{air}$  is the mass flow of air ( $\text{kg} \cdot \text{s}^{-1}$ )

$T_1$  is the inlet temperature ( $^{\circ}\text{C}$ )

$p_2$  is the outlet pressure (atm)

$p_1$  is the inlet pressure (atm)

$h_L$  is the head loss due to air friction

Symbol	Parameter	Unit	Value	Reference
$d_{air}$	Air density	$\text{kg} \cdot \text{m}^{-3}$	1.2	Tchobanoglous et al. (2004)
R	Gas constante R	$\text{kJ} \cdot (\text{kmol K})^{-1}$	8.314	Tchobanoglous et al. (2004)
$M_w$	Molecular mass of air	$\text{g} \cdot \text{mol}^{-1}$	29.7	Tchobanoglous et al. (2004)
n	$(k-1)/k$	dimensionless	0.283	Tchobanoglous et al. (2004)
e	efficiency	dimensionless	0.7	Tchobanoglous et al. (2004)
$P_{atm}$	Atmosferic pression	atm	1	Tchobanoglous et al. (2004)
$d_{water}$	Water density	$\text{kg} \cdot \text{m}^{-3}$	1000	Tchobanoglous et al. (2004)
g	Standart gravity	$\text{m} \cdot \text{s}^{-2}$	9.80665	Tchobanoglous et al. (2004)
D	Pipe diameter	m	0.4	[Estimation]
L	Length of pipe	m	100	[Estimation]
H	Height of the reactor	m	4	[BSM2]
f	Friction factor	dimensionless	0.016	Tchobanoglous et al. (2004)

Supplementary Information

## Supplementary Information

DAmp	Daily amplitude of sin function for ambient temperature	dimensionless	9	[Estimation]
DFreq	Daily frequency of sin function for ambient temperature	dimensionless	6.2832	[Estimation]
DBiais	Daily biases of sin function for ambient temperature	dimensionless	0	[Estimation]
DPhase	Daily phase of sin function for ambient temperature	dimensionless	4.7124	[Estimation]
SAMP	Seasonal amplitude of sin function for ambient temperature	dimensionless	14	[Estimation]
SFreq	Seasonal frequency of sin function for ambient temperature	dimensionless	0.0172615	[Estimation]
SBiais	Seasonal biases of sin function for ambient temperature	dimensionless	5.5	[Estimation]
SPhase	Seasonal phase of sin function for ambient temperature	dimensionless	1.1126474	[Estimation]

*Pumping*

$$P_{pumping} = \frac{\rho g Q_{pumped} \Delta h}{e}$$

$$\Delta h_f = f \left( \frac{L}{D} \right) \left( \frac{u^2}{2g} \right)$$

Where:

$P_{pumping}$  is the required power for pumping

$Q_{pumped}$  is the flow (dynamic variable) to be pumped

Symbol	Parameter	Unit	Value	Reference
g	Standard gravity	m . s <sup>-2</sup>	9.80665	Tchobanoglous et al. (2004)
$\rho_1$	AER3 to ANOX1 density	kg . m <sup>-3</sup>	1000	Tchobanoglous et al. (2004)
$\rho_2$	SEC to ANOX1 density	kg . m <sup>-3</sup>	1005	Tchobanoglous et al. (2004)
$\rho_3$	SEC to THK density	kg . m <sup>-3</sup>	1005	Tchobanoglous et al. (2004)
$\rho_4$	PRIM to AD density	kg . m <sup>-3</sup>	1020	Tchobanoglous et al. (2004)
$\rho_5$	THK to AD density	kg . m <sup>-3</sup>	1020	Tchobanoglous et al. (2004)
$\rho_6$	DW to PRIM density	kg . m <sup>-3</sup>	1000	Tchobanoglous et al. (2004)
$\rho_7$	INFLUENT density	kg . m <sup>-3</sup>	1000	[Estimated]

$\rho_8$	EFFLUENT density	$\text{kg} \cdot \text{m}^{-3}$	1000	[Estimated]
$\rho_9$	CARBON density	$\text{kg} \cdot \text{m}^{-3}$	1000	[Estimated]
$\rho_{10}$	METAL density	$\text{kg} \cdot \text{m}^{-3}$	1000	[Estimated]
$\rho_{11}$	URINE density	$\text{kg} \cdot \text{m}^{-3}$	1000	[Estimated]
$\rho_{12}$	ALKALINITY density	$\text{kg} \cdot \text{m}^{-3}$	1000	[Estimated]
$\rho_{\text{water}}$	water density	$\text{kg} \cdot \text{m}^{-3}$	1000	Tchobanoglous et al. (2004)
$D_1$	AER3 to ANOX1 pipe diameter	m	1.2	Gernaey et al., 2005
$D_2$	SEC to ANOX1 pipe diameter	m	0.6	Gernaey et al., 2005
$D_3$	SEC to THK pipe diameter	m	0.1	Gernaey et al., 2005
$D_4$	PRIM to AD pipe diameter	m	0.1	Gernaey et al., 2005
$D_5$	THK to AD pipe diameter	m	0.1	Gernaey et al., 2005
$D_6$	DW to PRIM pipe diameter	m	0.1	Gernaey et al., 2005
$D_7$	INFLUENT input pipe diameter	m	0.6	[Estimated]
$D_8$	EFFLUENT output pipe diameter	m	0.6	[Estimated]
$D_9$	CARBON pipe diameter	m	0.1	[Estimated]
$D_{10}$	METAL pipe diameter	m	0.1	[Estimated]
$D_{11}$	URINE pipe diameter	m	0.1	[Estimated]
$D_{12}$	ALKALINITY pipe diameter	m	0.1	[Estimated]
$L_1$	AER3 to ANOX1 pipe length	m	100	Gernaey et al., 2005
$L_2$	SEC to ANOX1 pipe length	m	100	Gernaey et al., 2005
$L_3$	SEC to THK pipe length	m	100	Gernaey et al., 2005
$L_4$	PRIM to AD pipe length	m	200	Gernaey et al., 2005
$L_5$	THK to AD pipe length	m	100	Gernaey et al., 2005
$L_6$	DW to PRIM pipe length	m	200	Gernaey et al., 2005
$L_7$	INFLUENT input length	m	100	[Estimated]
$L_8$	EFFLUENT output length	m	100	[Estimated]
$L_9$	CARBON input length	m	50	[Estimated]

Supplementary Information

## Supplementary Information

L <sub>10</sub>	METAL input length	m	50	[Estimated]
L <sub>11</sub>	URINE length	m	50	[Estimated]
L <sub>12</sub>	ALKALINITY length	m	50	[Estimated]
f <sub>1</sub>	AER3 to ANOX1 friction factor	dimensionless	0.03	Gernaey et al., 2005
f <sub>2</sub>	SEC to ANOX1 friction factor	dimensionless	0.03	Gernaey et al., 2005
f <sub>3</sub>	SEC to THK friction factor	dimensionless	0.03	Gernaey et al., 2005
f <sub>4</sub>	PRIM to AD friction factor	dimensionless	0.06	[Based on Tchobanoglous et al. (2004)]
f <sub>5</sub>	THK to AD friction factor	dimensionless	0.1	[Based on Tchobanoglous et al. (2004)]
f <sub>6</sub>	DW to PRIM friction factor	dimensionless	0.03	Gernaey et al., 2005
f <sub>7</sub>	INFLUENT input friction factor	dimensionless	0.03	[Based on Tchobanoglous et al. (2004)]
f <sub>7</sub>	EFFLUENT output friction factor	dimensionless	0.03	[Based on Tchobanoglous et al. (2004)]
f <sub>7</sub>	CARBON friction factor	dimensionless	0.03	[Based on Tchobanoglous et al. (2004)]
f <sub>7</sub>	METAL friction factor	dimensionless	0.03	[Based on Tchobanoglous et al. (2004)]
f <sub>7</sub>	URINE friction factor	dimensionless	0.03	[Based on Tchobanoglous et al. (2004)]
f <sub>7</sub>	ALKALINITY friction factor	dimensionless	0.03	[Based on Tchobanoglous et al. (2004)]
u <sub>1</sub>	AER3 to ANOX1 liquid velocity	m . s <sup>-1</sup>	0.98	Gernaey et al., 2005
u <sub>2</sub>	SEC to ANOX1 liquid velocity	m . s <sup>-1</sup>	0.98	Gernaey et al., 2005
u <sub>3</sub>	SEC to THK liquid velocity	m . s <sup>-1</sup>	0.44	Gernaey et al., 2005
u <sub>4</sub>	PRIM to AD liquid velocity	m . s <sup>-1</sup>	0.23	Gernaey et al., 2005
u <sub>5</sub>	THK to AD liquid velocity	m . s <sup>-1</sup>	0.06	Gernaey et al., 2005
u <sub>6</sub>	DW to PRIM liquid velocity	m . s <sup>-1</sup>	0.35	Gernaey et al., 2005
u <sub>7</sub>	INFLUENT input velocity	m . s <sup>-1</sup>	0.98	[Estimated]
u <sub>8</sub>	EFFLUENT output velocity	m . s <sup>-1</sup>	0.98	[Estimated]
u <sub>9</sub>	CARBON velocity	m . s <sup>-1</sup>	0.98	[Estimated]
u <sub>10</sub>	METAL velocity	m . s <sup>-1</sup>	0.98	[Estimated]
u <sub>11</sub>	URINE velocity	m . s <sup>-1</sup>	0.98	[Estimated]
u <sub>12</sub>	ALKALINITY velocity	m . s <sup>-1</sup>	0.98	[Estimated]

Z <sub>1</sub>	AER3 to ANOX1 height	m	0	Gernaey et al., 2005
Z <sub>2</sub>	SEC to ANOX1 height	m	4	Gernaey et al., 2005
Z <sub>3</sub>	SEC to THK height	m	8	Gernaey et al., 2005
Z <sub>4</sub>	PRIM to AD height	m	21	Gernaey et al., 2005
Z <sub>5</sub>	THK to AD height	m	17	Gernaey et al., 2005
Z <sub>6</sub>	DW to PRIM height	m	0	Gernaey et al., 2005
Z <sub>7</sub>	INFLUENT input height	m	0	[Estimated]
Z <sub>8</sub>	EFFLUEN output height	m	0	[Estimated]
Z <sub>9</sub>	CARBON height	m	4	[Estimated]
Z <sub>10</sub>	METAL height	m	4	[Estimated]
Z <sub>11</sub>	URINE height	m	0	[Estimated]
Z <sub>12</sub>	ALKALINITY height	m	4	[Estimated]
e	Efficiency	dimensionless	0.65	Descoins et al., 2012

### Mixing

$$P_{mixing} = P \cdot V$$

Where:

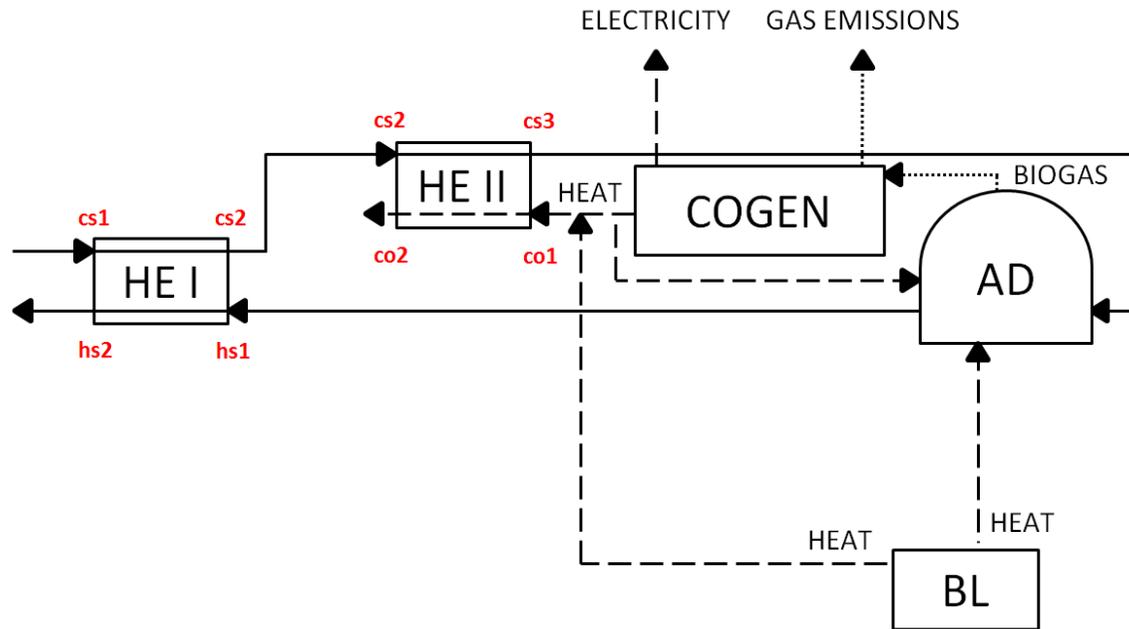
$P_{mixing}$  is the power consumed for mixing

V is the volume of liquid in the reactor to be mixed

Symbol	Parameter	Unit	Value	Reference
P <sub>ANOX</sub>	Mix power for anaerobic reactors	kW . m <sup>-3</sup>	0.008	Tchobanoglous et al. (2004)
P <sub>AD</sub>	Mix power for anaerobic digester	kW . m <sup>-3</sup>	0.005	Tchobanoglous et al. (2004)

Supplementary Information

## Cogeneration



Energy balance:  $\sum \dot{m}_{output} h_{output} - \sum \dot{m}_{input} h_{input} = 0$

HE I (Heat exchanger I):  $\dot{m}_{cs2} h_{cs2} + \dot{m}_{hs2} h_{hs2} - \dot{m}_{cs1} h_{cs1} - \dot{m}_{hs1} h_{hs1} = 0$

As  $\dot{m}_{cs1} = \dot{m}_{cs2}$ , they are called  $\dot{m}_{cs}$ . The same for  $\dot{m}_{hs1}$  and  $\dot{m}_{hs2}$ , which become  $\dot{m}_{hs}$

$$\dot{m}_{cs}(h_{cs2} - h_{cs1}) + \dot{m}_{hs}(h_{hs2} - h_{hs1}) = 0$$

$\dot{m}_{cs}$ ,  $\dot{m}_{hs}$ ,  $h_{cs1}$  and  $h_{hs1}$  are known by simulation results and  $h_{cs2}$  and  $h_{hs2}$  are still unknown

The hypothesis is that there is a gradient of temperature of 10°C in HEI and then  $h_{hs2}$  become known. The balance is solved for  $h_{cs2}$ .

$$\text{HE II (Heat exchanger II): } \dot{m}_{cs3}h_{cs3} + \dot{m}_{co2}h_{co2} - \dot{m}_{cs2}h_{cs2} - \dot{m}_{co1}h_{co1} = 0$$

As  $\dot{m}_{cs1} = \dot{m}_{cs2}$  they are called  $\dot{m}_{cs}$  and  $\dot{m}_{co2}h_{co2} - \dot{m}_{co1}h_{co1}$  is the heat provided by cogeneration unit which need to be used in HEII and so is called  $q_{COGEN, HEII}$ .

$$\dot{m}_{cs}(h_{cs3} - h_{cs2}) + q_{COGEN, HEII} = 0$$

$\dot{m}_{cs}$ ,  $h_{cs3}$  are known by simulation results and  $h_{cs2}$  is known by HE I energy balance. HE II balance is then solved for  $q_{COGEN, HEII}$ .

Requirements for sludge heating and heat loss by digester walls:

$$q_{sludge} = w_{sludge}c_{p, sludge}\Delta T_{sludge}$$

$$q_{digester} = U_{wall}A_{wall}\Delta T_{wall} + U_{roof}A_{roof}\Delta T_{roof} + U_{floor}A_{floor}\Delta T_{floor}$$

With A being the surface to be heated.

$$\text{COGEN: } q_{COGEN, TOTAL} = q_{COGEN, HEII} + q_{AD} \pm q_{DIFF}$$

Where  $q_{AD}$  is the sum of all requirements for sludge heating and heat loss by digester walls

Symbol	Parameter	Unit	Value	References
$d_{water}$	Water density	$kg \cdot m^{-3}$	1000	Tchobanoglous et al. (2004)
$LHV_{Methane}$	Biogas lower heating value (20°C; 1 atm)	$MJ \cdot m^{-3}$	35.8	Tchobanoglous et al. (2004)
$d_{sludge}$	Sludge (digester input) density	$kg \cdot m^{-3}$	1020	Tchobanoglous et al. (2004)
$U_{floor}$	Heat transfer coefficient for digester floor	$W \cdot (m^2 \cdot ^\circ C)^{-1}$	0.85	Tchobanoglous et al. (2004)
$U_{roof}$	Heat transfer coefficient for digester floor	$W \cdot (m^2 \cdot ^\circ C)^{-1}$	0.91	Tchobanoglous et al. (2004)
$U_{wall}$	Heat transfer coefficient for digester floor	$W \cdot (m^2 \cdot ^\circ C)^{-1}$	0.68	Tchobanoglous et al. (2004)
D	Digester diameter	m	25	[Estimated]
$H_1$	Digester side depth	m	7	[Estimated]

Supplementary Information

## Supplementary Information

$H_2$	Digester middepth	m	9	[Estimated]
$e_{\text{heat}}$	Heat efficiency of cogeneration	dimensionless	0.485	[Adapted from Doka (2009)]
$\text{Grad}_T$	Temperature gradient in HEI	$^{\circ}\text{C}$	10	[Estimated]

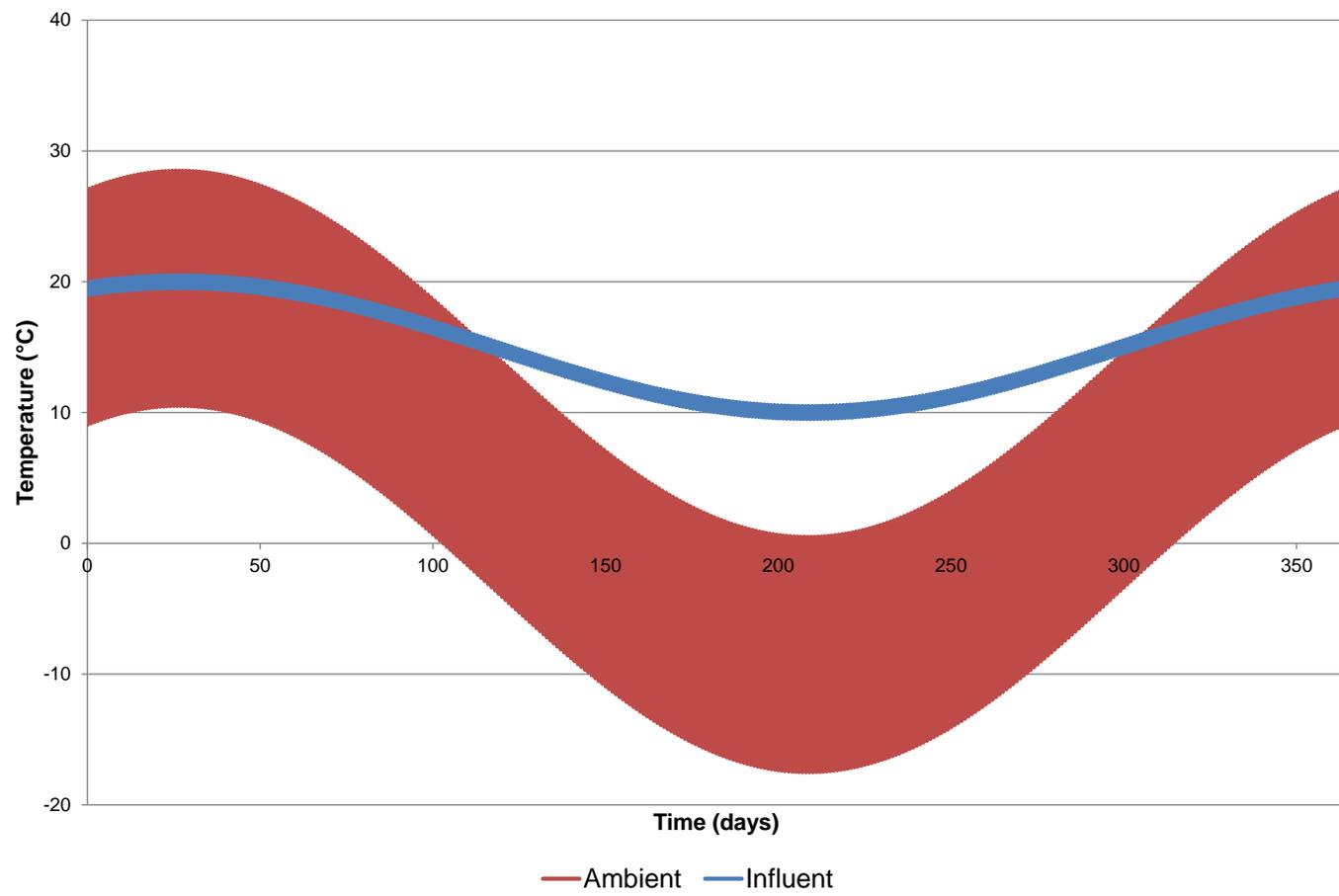
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Ambient temperature considerations for AD are the same as for aeration calculation.

Finally, if  $q_{\text{DIFF}}$  is positive there is a surplus of heat production. Otherwise, energy should be provided by another source.

#### A.4. *Effluent and ambient temperature*

Influent temperature was obtained from influent data (Gernaey et al., 2011) and ambient temperature was modelled considering regional characteristics to achieve reliable energy results (used in aeration and cogeneration modelling).



Supplementary Information

## Supplementary Information

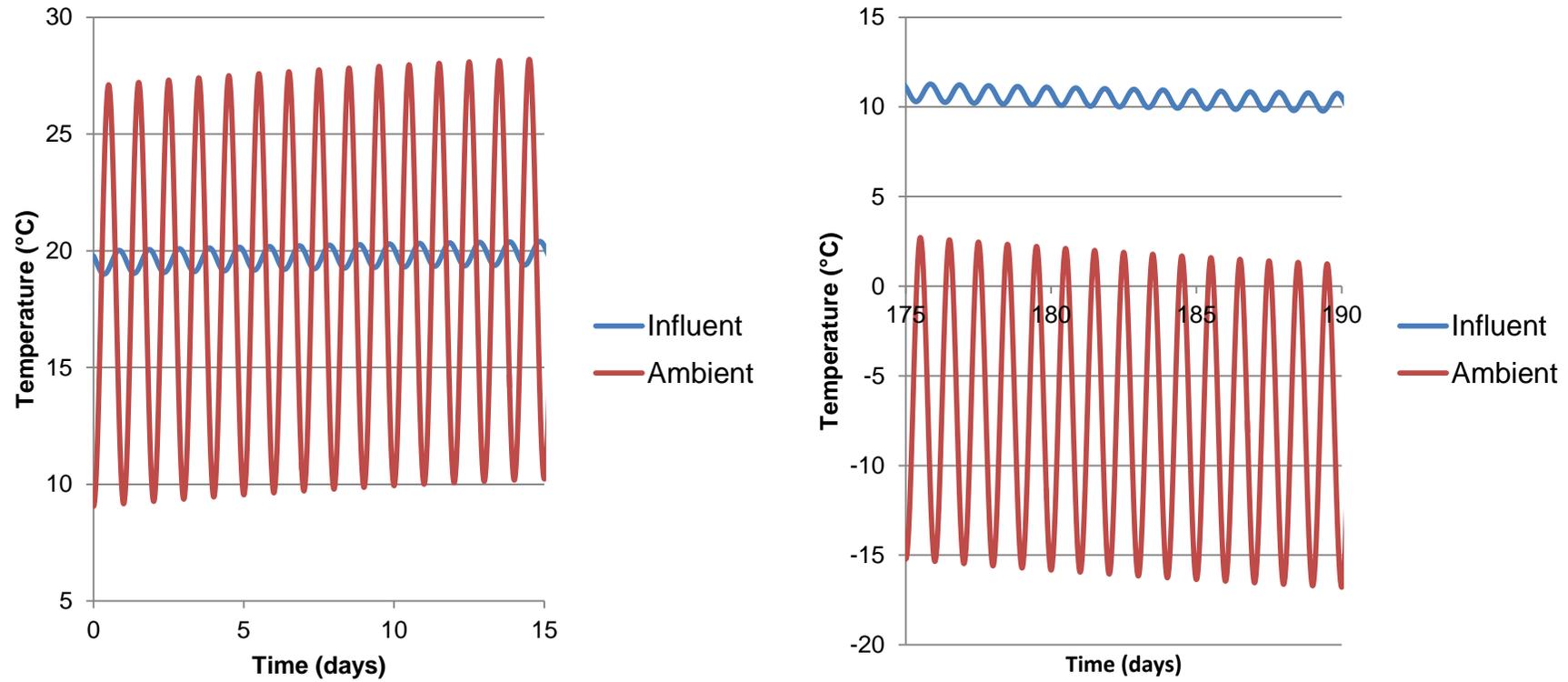


Figure 1: Influent and ambient temperature: General overview of 1 year; Summer overview; Winter overview.

### A.5. *Agricultural spreading*

Post-spreading emissions based on Doka (2009), Bouwman et al. (1997), Bouwman et al. (2002) and Nemecek and Kägi (2007)

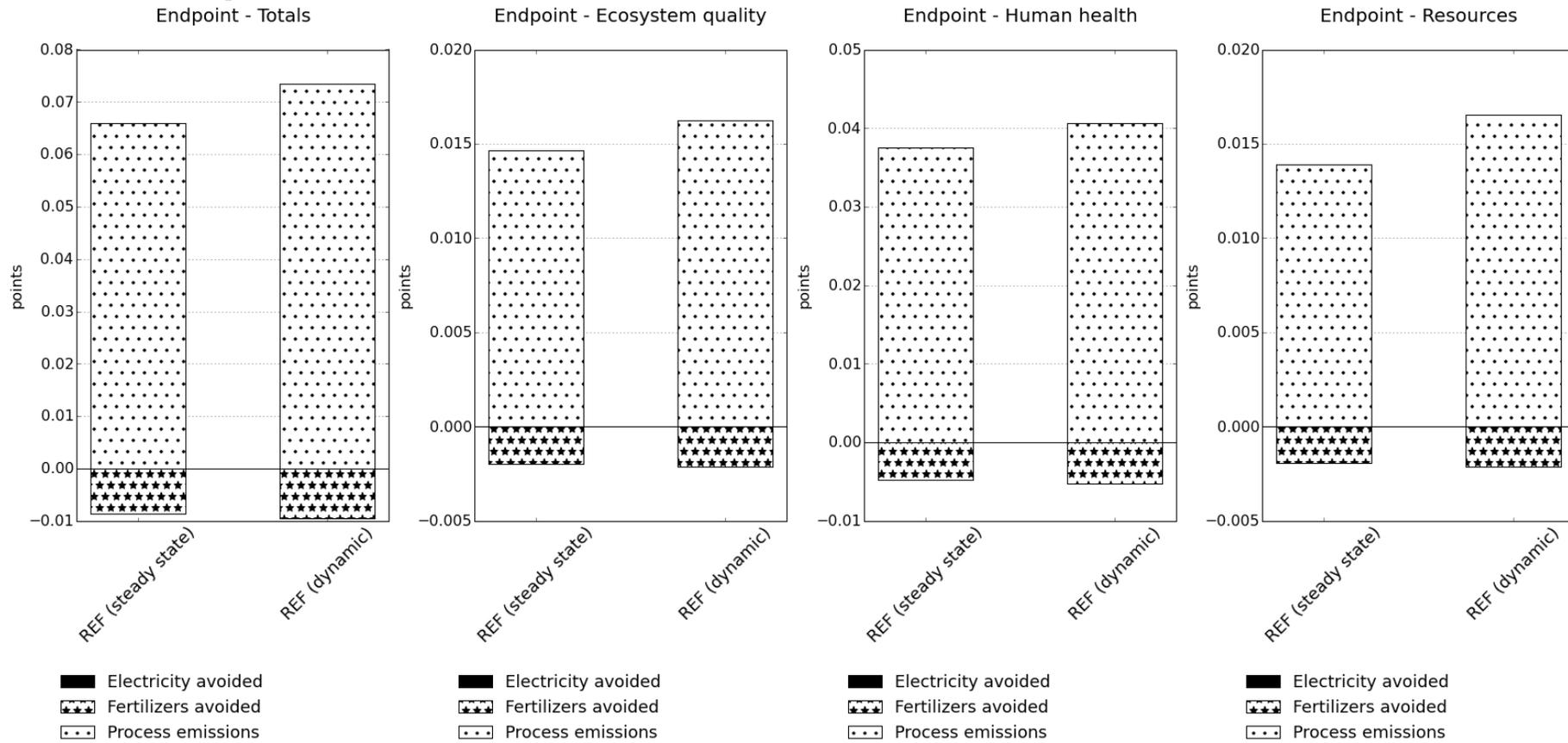
<b>N and P sources</b>	<b>N<sub>2</sub>O-N (% of N content)</b>	<b>NO<sub>x</sub>-N (% of N content)</b>	<b>NH<sub>3</sub>-N (% of N content)</b>	<b>PO<sub>4</sub>-P to ground water (% of P content)</b>	<b>PO<sub>4</sub>-P to surface water (% of P content)</b>
<b>Sludge</b>	1.2	NA	25.6	0.6	2.0
<b>Struvite</b>	0.9	0.6	3.0	1.0	2.7
<b>N-rich effluent</b>	1.0	0.7	2.5	1.0	2.7
<b>Mineral fertilizers</b>	0.8	0.6	2.0	1.0	2.7

## Supplementary Information

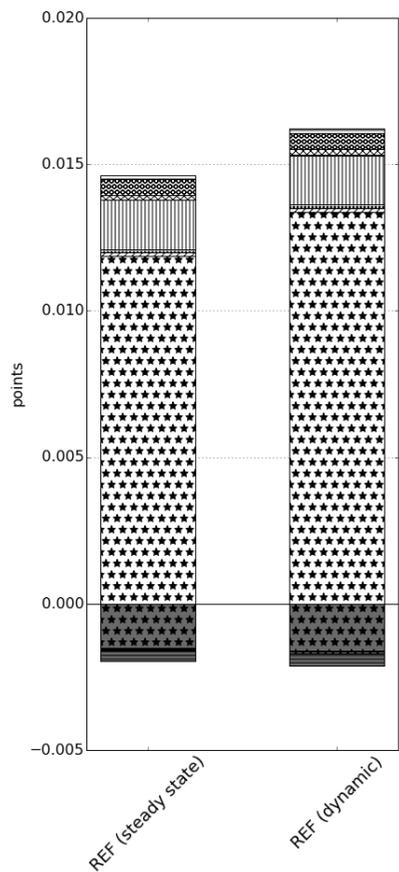
## A.6. Other midpoint and endpoint results

## A.6.1 Environmental impact results for steady state and dynamic results

## A.6.1.1 ReCiPe Endpoint(H,A)



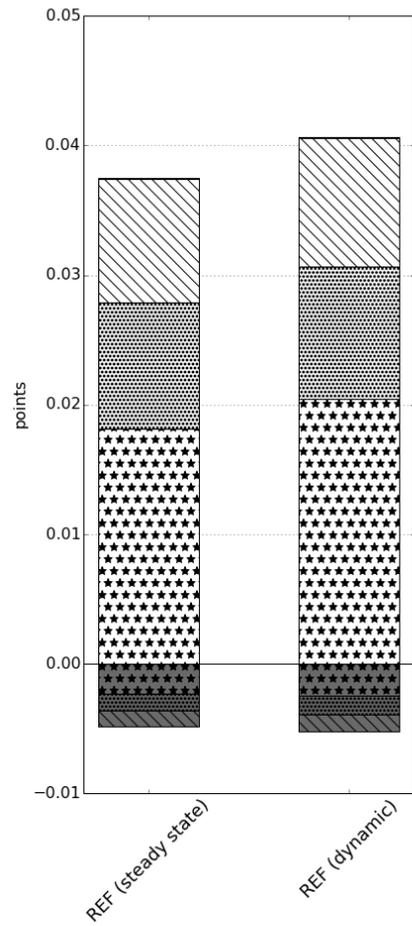
Endpoint categories - Ecosystem quality



- |  |  |  |
|--|--|--|
| ★ ★ ★ Process emissions - climate change, ecosystems | ★ ★ ★ Fertilizers avoided - climate change, ecosystems | ★ ★ ★ Electricity avoided - climate change, ecosystems |
| ▨ Process emissions - terrestrial acidification      | ▨ Fertilizers avoided - terrestrial acidification      | ▨ Electricity avoided - terrestrial acidification      |
| ▨ Process emissions - freshwater eutrophication      | ▨ Fertilizers avoided - freshwater eutrophication      | ▨ Electricity avoided - freshwater eutrophication      |
| ▨ Process emissions - terrestrial ecotoxicity        | ▨ Fertilizers avoided - terrestrial ecotoxicity        | ▨ Electricity avoided - terrestrial ecotoxicity        |
| ▨ Process emissions - freshwater ecotoxicity         | ▨ Fertilizers avoided - freshwater ecotoxicity         | ▨ Electricity avoided - freshwater ecotoxicity         |
| ▨ Process emissions - marine ecotoxicity             | ▨ Fertilizers avoided - marine ecotoxicity             | ▨ Electricity avoided - marine ecotoxicity             |
| ▨ Process emissions - agricultural land occupation   | ▨ Fertilizers avoided - agricultural land occupation   | ▨ Electricity avoided - agricultural land occupation   |
| ▨ Process emissions - urban land occupation          | ▨ Fertilizers avoided - urban land occupation          | ▨ Electricity avoided - urban land occupation          |
| ▨ Process emissions - natural land transformation    | ▨ Fertilizers avoided - natural land transformation    | ▨ Electricity avoided - natural land transformation    |

## Supplementary Information

Endpoint categories - Human health

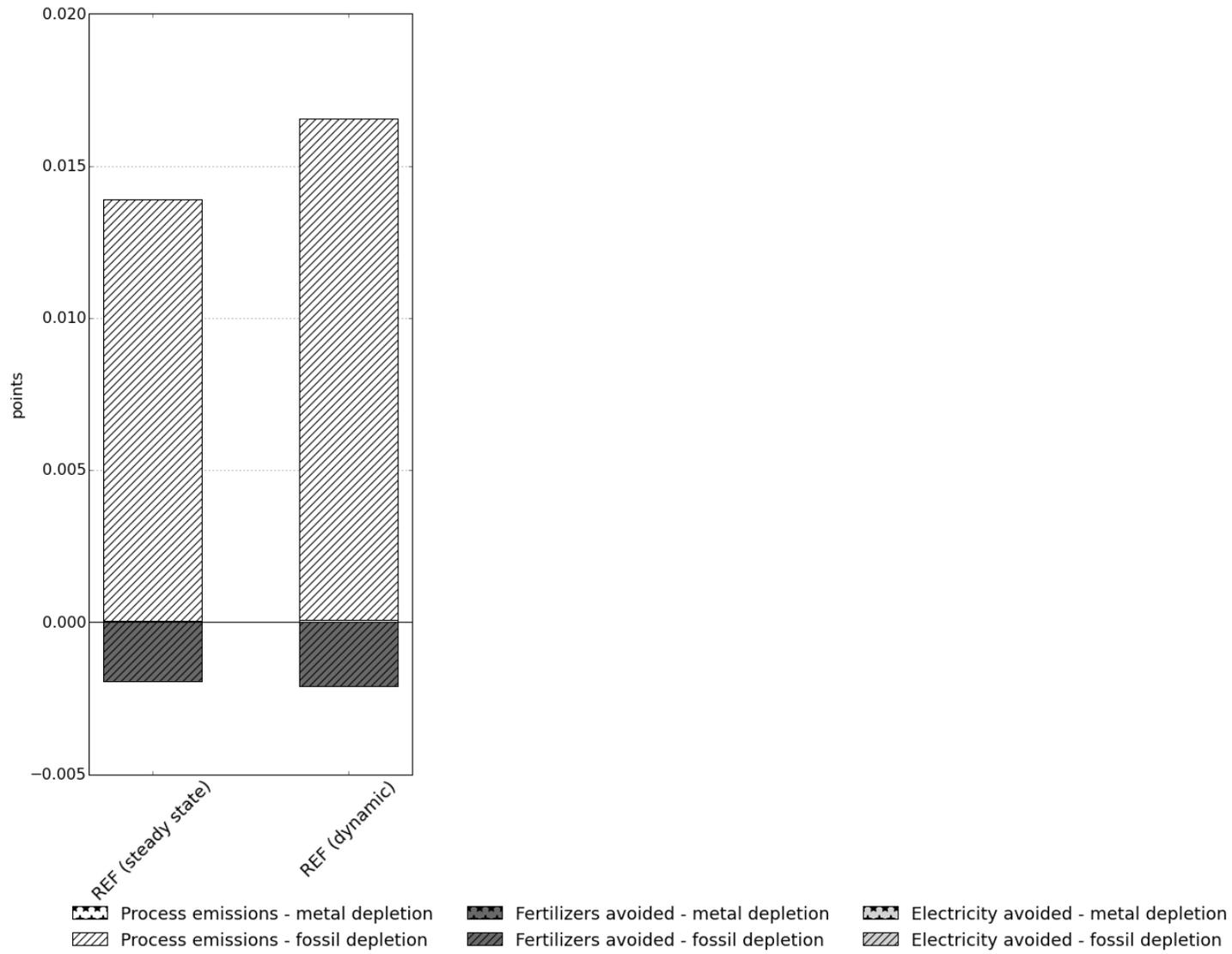


■ Process emissions - climate change, human health  
 ▨ Process emissions - ozone depletion  
 ▩ Process emissions - human toxicity  
 ▪ Process emissions - photochem. oxidant form.  
 ▫ Process emissions - particulate matter formation  
 ▬ Process emissions - ionising radiation

■ Fertilizers avoided - climate change, human health  
 ▨ Fertilizers avoided - ozone depletion  
 ▩ Fertilizers avoided - human toxicity  
 ▪ Fertilizers avoided - photochem. oxidant form.  
 ▫ Fertilizers avoided - particulate matter formation  
 ▬ Fertilizers avoided - ionising radiation

■ Electricity avoided - climate change, human health  
 ▨ Electricity avoided - ozone depletion  
 ▩ Electricity avoided - human toxicity  
 ▪ Electricity avoided - photochem. oxidant form.  
 ▫ Electricity avoided - particulate matter formation  
 ▬ Electricity avoided - ionising radiation

Endpoint categories - Resources

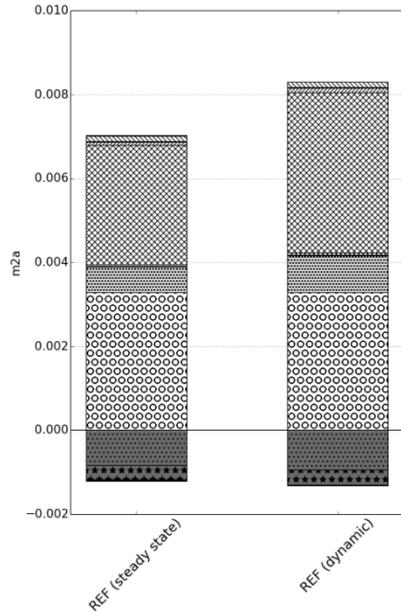


Supplementary Information

Supplementary Information

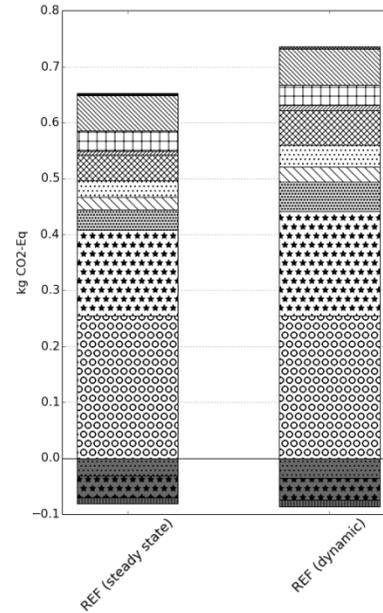
A.6.1.2 ReCiPe Midpoint (H)

Midpoint Contribution Analysis - agricultural land occupation



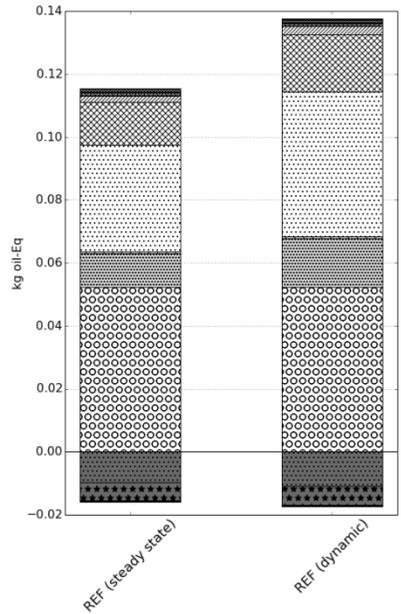
- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

Midpoint Contribution Analysis - climate change



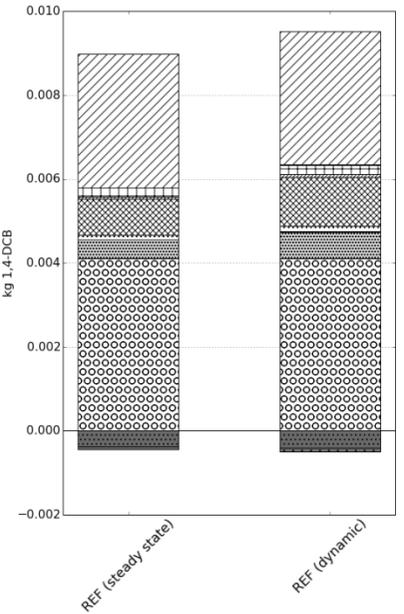
- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

Midpoint Contribution Analysis - fossil depletion



- Infrastructure
- Direct emissions
- Electricity
- Heat
- Cogeneration
- Methanol production
- FeCl3 production
- MgO production
- NaOH production
- Chemicals transport
- Sludge spreading
- Metals (water and sludge)
- Struvite spreading
- TSP avoided Production
- AN avoided production
- N-rich spreading
- Sludge transport
- Mineral fertilizers avoided spreading
- Mineral fertilizers avoided transport
- N-rich transport
- Avoided electricity

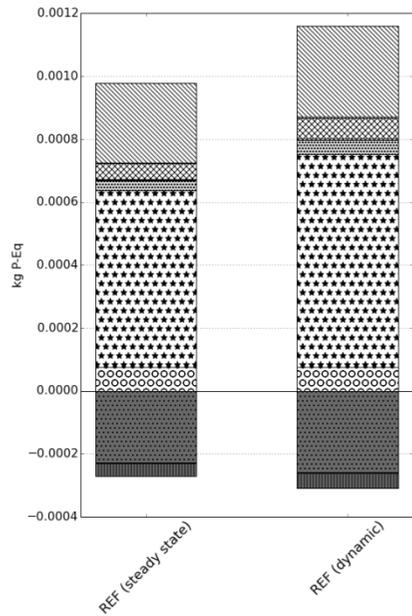
Midpoint Contribution Analysis - freshwater ecotoxicity



- Infrastructure
- Direct emissions
- Electricity
- Heat
- Cogeneration
- Methanol production
- FeCl3 production
- MgO production
- NaOH production
- Chemicals transport
- Sludge spreading
- Metals (water and sludge)
- Struvite spreading
- TSP avoided Production
- AN avoided production
- N-rich spreading
- Sludge transport
- Mineral fertilizers avoided spreading
- Mineral fertilizers avoided transport
- N-rich transport
- Avoided electricity

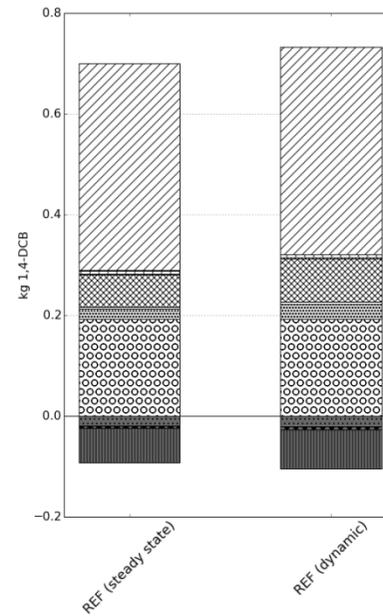
Supplementary Information

Midpoint Contribution Analysis - freshwater eutrophication



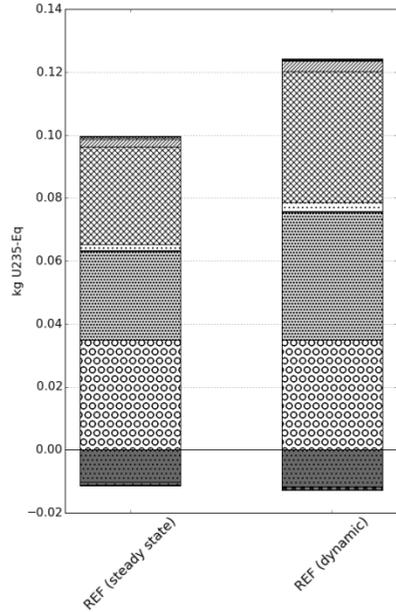
- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

Midpoint Contribution Analysis - human toxicity



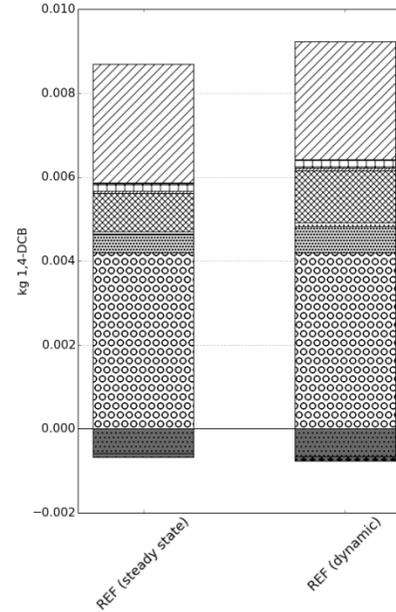
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|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

Midpoint Contribution Analysis - ionising radiation



- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

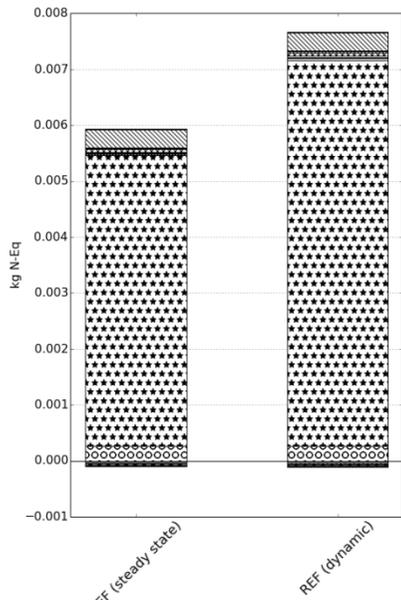
Midpoint Contribution Analysis - marine ecotoxicity



- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

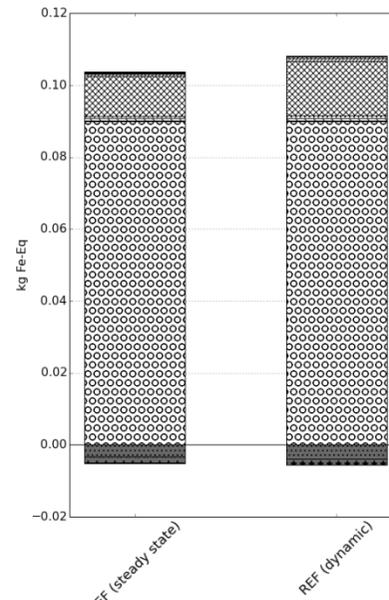
Supplementary Information

Midpoint Contribution Analysis - marine eutrophication



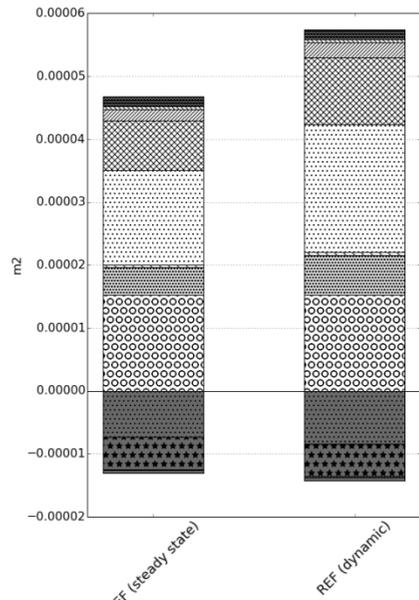
- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

Midpoint Contribution Analysis - metal depletion



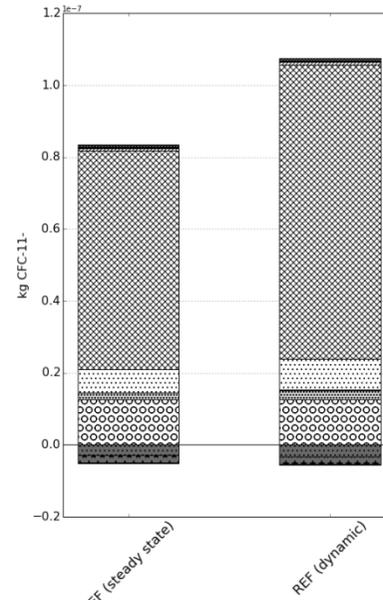
- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

Midpoint Contribution Analysis - natural land transformation



- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

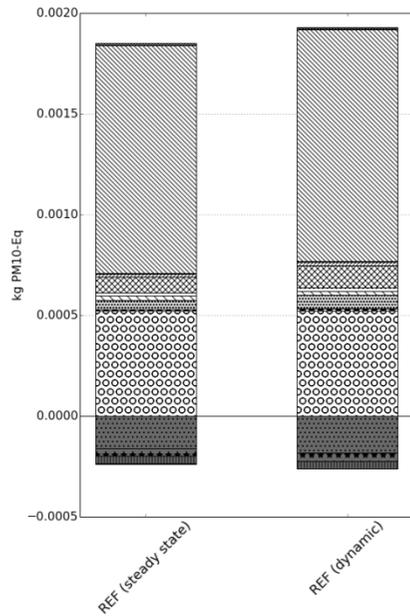
Midpoint Contribution Analysis - ozone depletion



- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

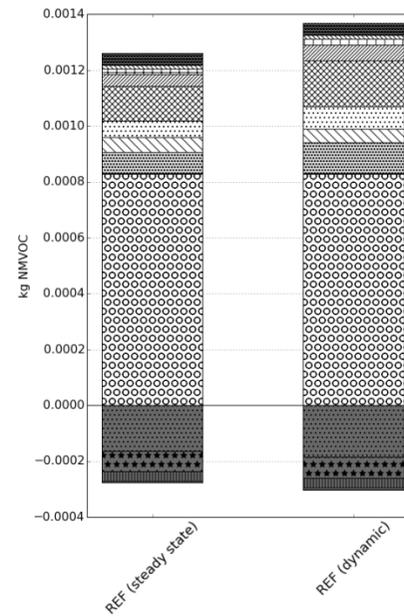
Supplementary Information

Midpoint Contribution Analysis - particulate matter formation



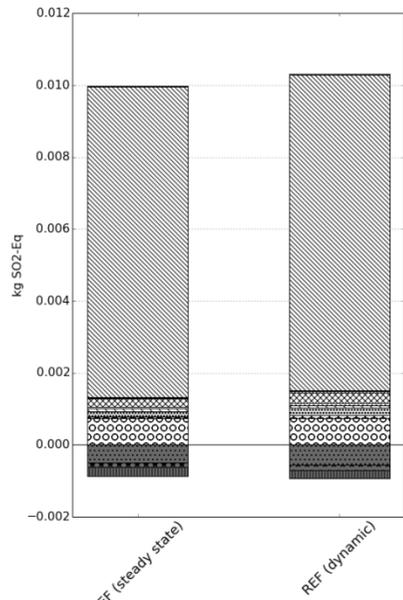
- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

Midpoint Contribution Analysis - photochem. oxidant form.



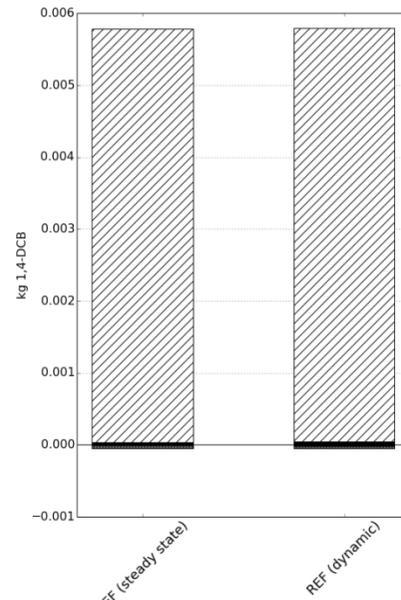
- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

Midpoint Contribution Analysis - terrestrial acidification



- Infrastructure
- Direct emissions
- Electricity
- Heat
- Cogeneration
- Methanol production
- FeCl3 production
- MgO production
- NaOH production
- Chemicals transport
- Grits disposal
- Urine storage
- Urine transport
- Sludge spreading
- Struvite spreading
- N-rich spreading
- Sludge transport
- Struvite transport
- N-rich transport
- Metals (water and sludge)
- TSP avoided Production
- AN avoided production
- Mineral fertilizers avoided spreading
- Mineral fertilizers avoided transport
- Avoided electricity

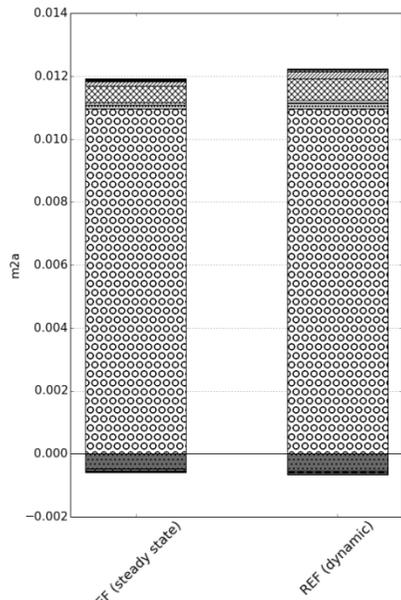
Midpoint Contribution Analysis - terrestrial ecotoxicity



- Infrastructure
- Direct emissions
- Electricity
- Heat
- Cogeneration
- Methanol production
- FeCl3 production
- MgO production
- NaOH production
- Chemicals transport
- Grits disposal
- Urine storage
- Urine transport
- Sludge spreading
- Struvite spreading
- N-rich spreading
- Sludge transport
- Struvite transport
- N-rich transport
- Metals (water and sludge)
- TSP avoided Production
- AN avoided production
- Mineral fertilizers avoided spreading
- Mineral fertilizers avoided transport
- Avoided electricity

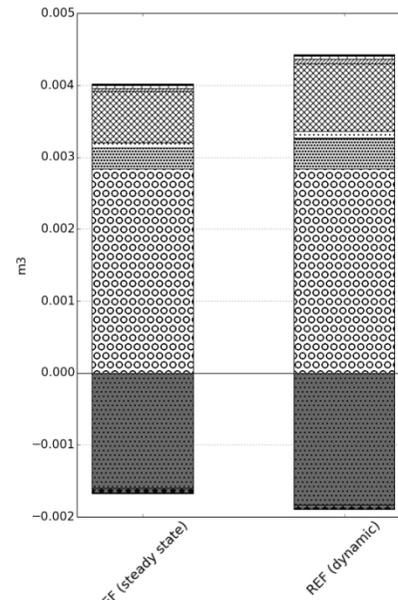
Supplementary Information

Midpoint Contribution Analysis - urban land occupation



- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

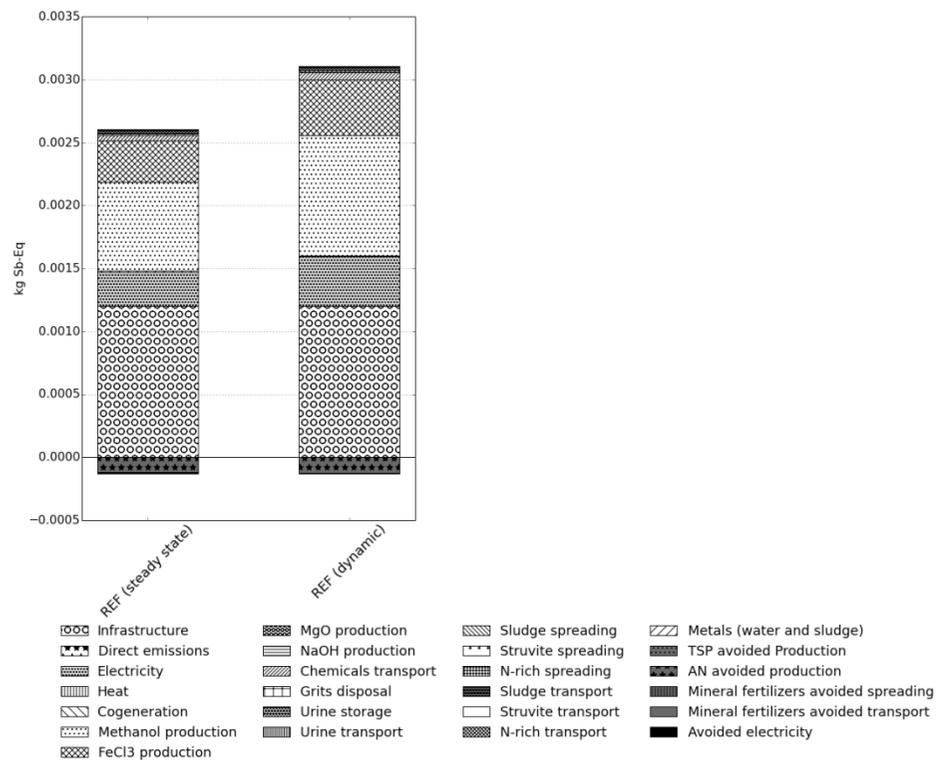
Midpoint Contribution Analysis - water depletion



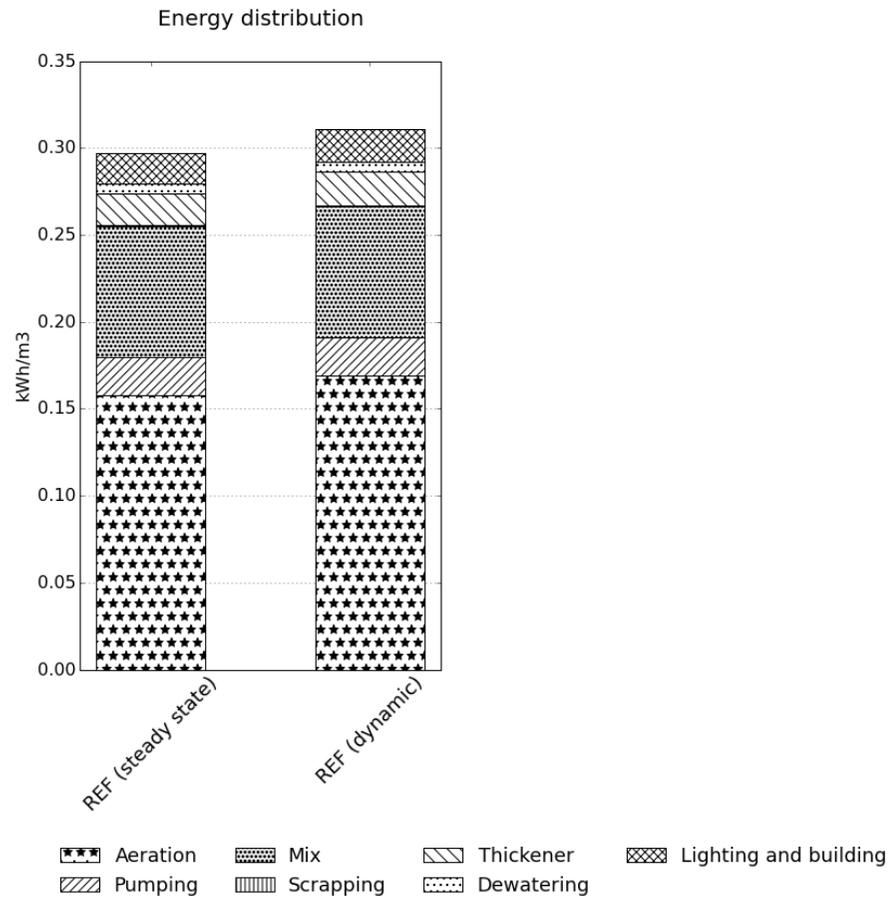
- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

### A.6.1.3 CML 2001

Midpoint Contribution Analysis - depletion of abiotic resources

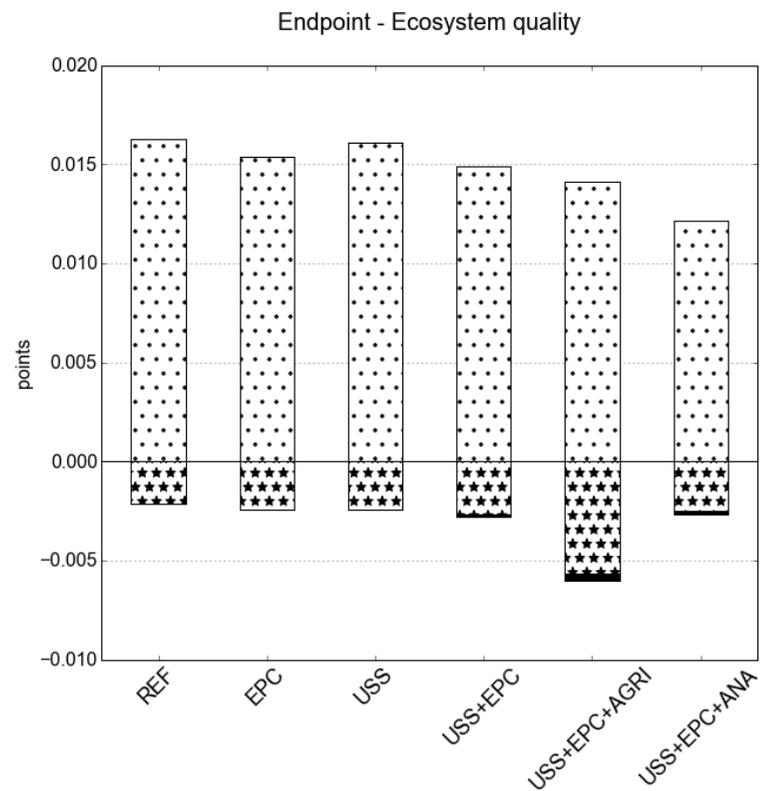
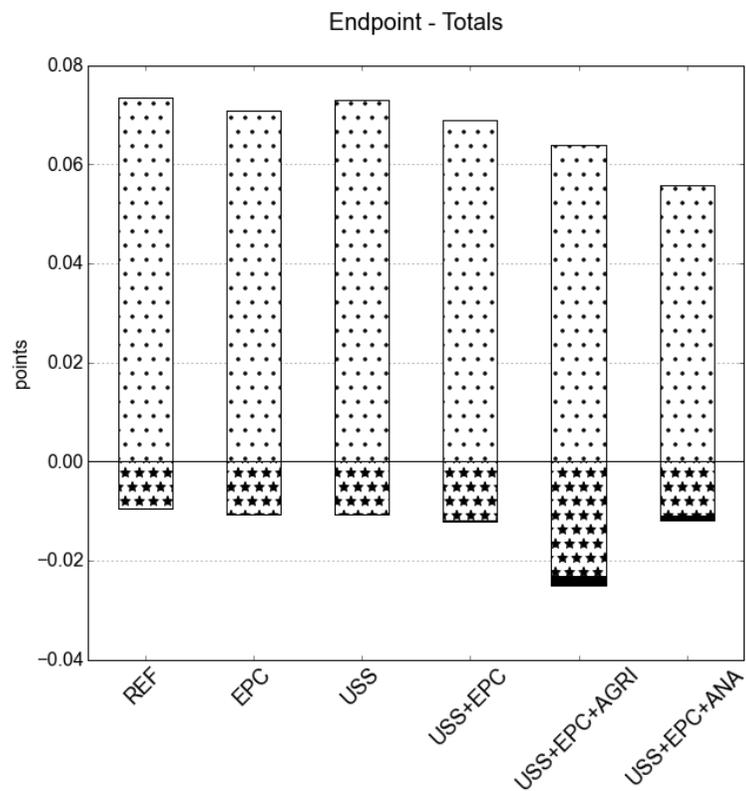


## A.6.1.4 Energy distribution



## A.6.2 Environmental impact results for alternative scenarios

### A.6.2.1 ReCiPe Endpoint (H,A)

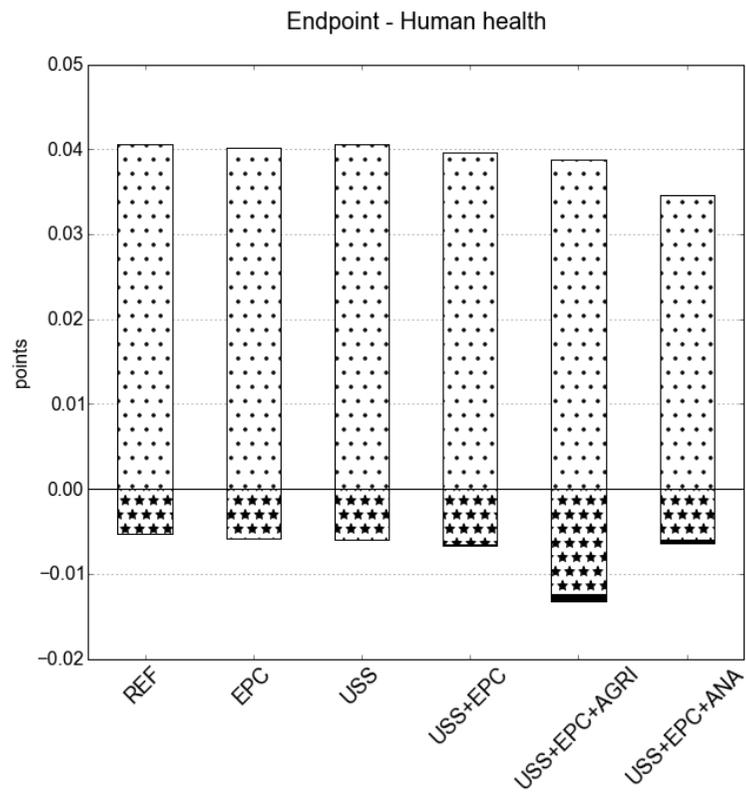


Electricity avoided  
 Fertilizers avoided  
 Process emissions

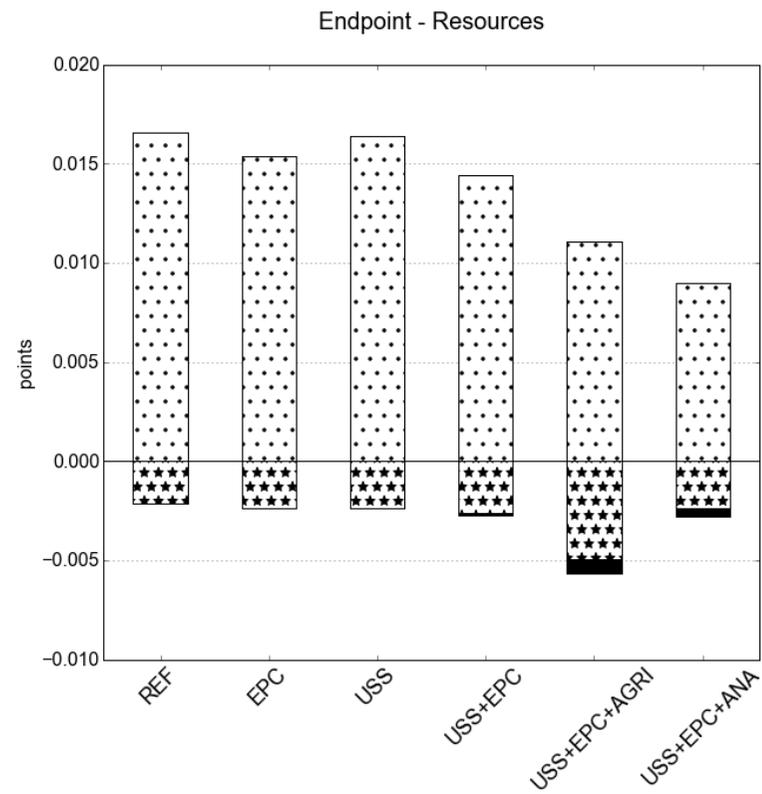
Electricity avoided  
 Fertilizers avoided  
 Process emissions

Supplementary Information

## Supplementary Information

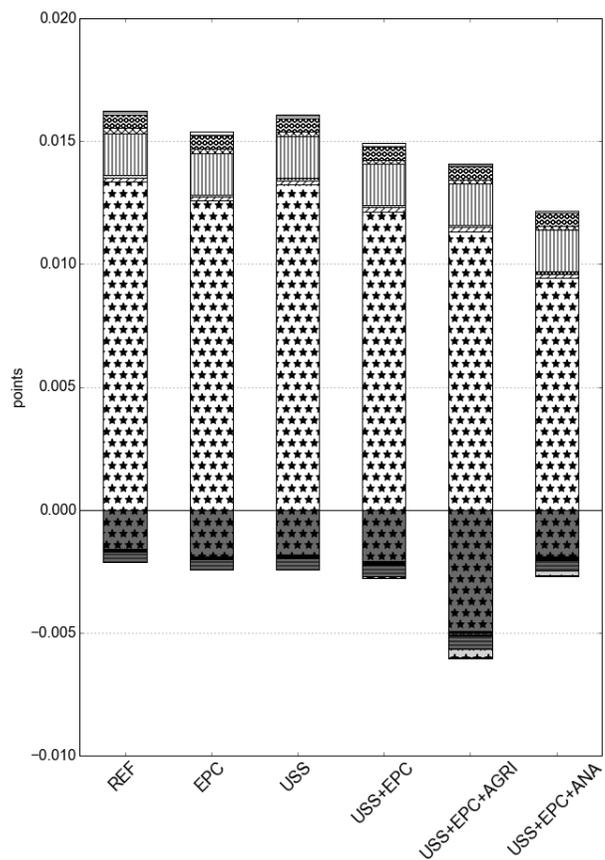


■ Electricity avoided  
 ★ Fertilizers avoided  
 □ Process emissions



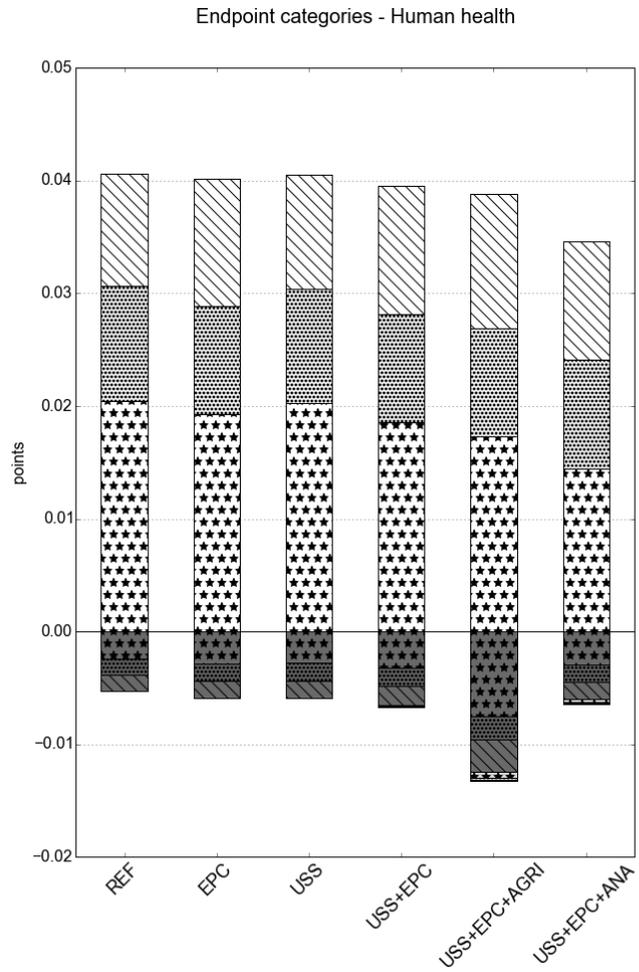
■ Electricity avoided  
 ★ Fertilizers avoided  
 □ Process emissions

Endpoint categories - Ecosystem quality



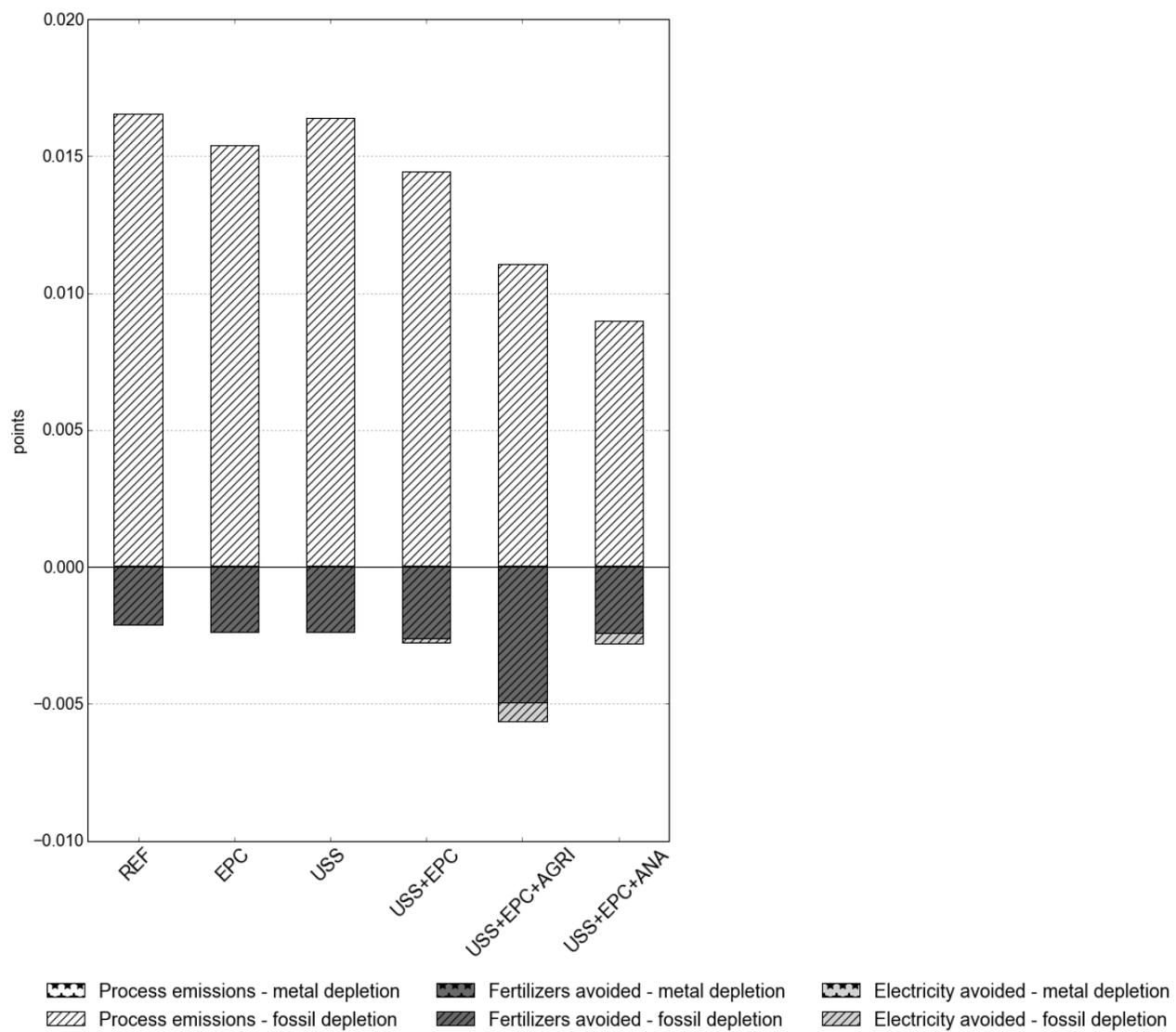
- |  |  |  |
|--|--|--|
| Process emissions - climate change, ecosystems   | Fertilizers avoided - climate change, ecosystems   | Electricity avoided - climate change, ecosystems   |
| Process emissions - terrestrial acidification    | Fertilizers avoided - terrestrial acidification    | Electricity avoided - terrestrial acidification    |
| Process emissions - freshwater eutrophication    | Fertilizers avoided - freshwater eutrophication    | Electricity avoided - freshwater eutrophication    |
| Process emissions - terrestrial ecotoxicity      | Fertilizers avoided - terrestrial ecotoxicity      | Electricity avoided - terrestrial ecotoxicity      |
| Process emissions - freshwater ecotoxicity       | Fertilizers avoided - freshwater ecotoxicity       | Electricity avoided - freshwater ecotoxicity       |
| Process emissions - marine ecotoxicity           | Fertilizers avoided - marine ecotoxicity           | Electricity avoided - marine ecotoxicity           |
| Process emissions - agricultural land occupation | Fertilizers avoided - agricultural land occupation | Electricity avoided - agricultural land occupation |
| Process emissions - urban land occupation        | Fertilizers avoided - urban land occupation        | Electricity avoided - urban land occupation        |
| Process emissions - natural land transformation  | Fertilizers avoided - natural land transformation  | Electricity avoided - natural land transformation  |

Supplementary Information



- |   |   |   |
|---|---|---|
| <ul style="list-style-type: none"> <li>Process emissions - climate change, human health</li> <li>Process emissions - ozone depletion</li> <li>Process emissions - human toxicity</li> <li>Process emissions - photochem. oxidant form.</li> <li>Process emissions - particulate matter formation</li> <li>Process emissions - ionising radiation</li> </ul> | <ul style="list-style-type: none"> <li>Fertilizers avoided - climate change, human health</li> <li>Fertilizers avoided - ozone depletion</li> <li>Fertilizers avoided - human toxicity</li> <li>Fertilizers avoided - photochem. oxidant form.</li> <li>Fertilizers avoided - particulate matter formation</li> <li>Fertilizers avoided - ionising radiation</li> </ul> | <ul style="list-style-type: none"> <li>Electricity avoided - climate change, human health</li> <li>Electricity avoided - ozone depletion</li> <li>Electricity avoided - human toxicity</li> <li>Electricity avoided - photochem. oxidant form.</li> <li>Electricity avoided - particulate matter formation</li> <li>Electricity avoided - ionising radiation</li> </ul> |
|---|---|---|

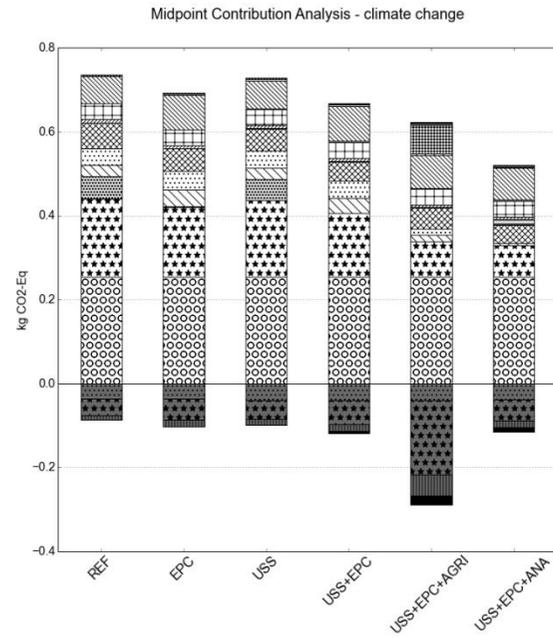
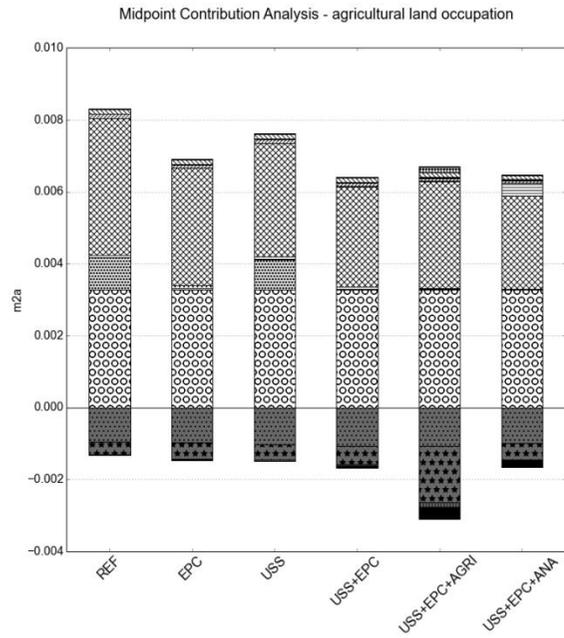
Endpoint categories - Resources



Supplementary Information

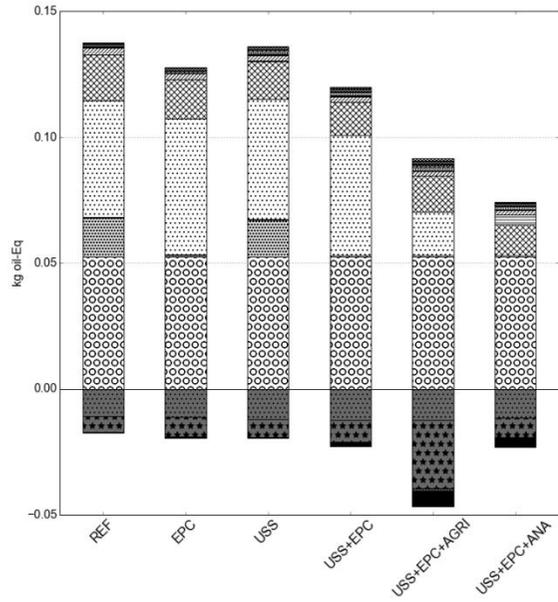
Supplementary Information

6.2.2 ReCiPe Midpoint (H)

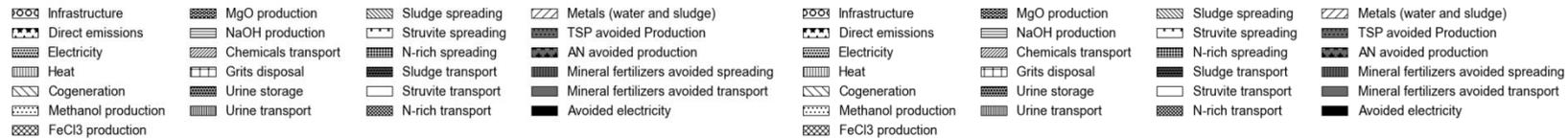
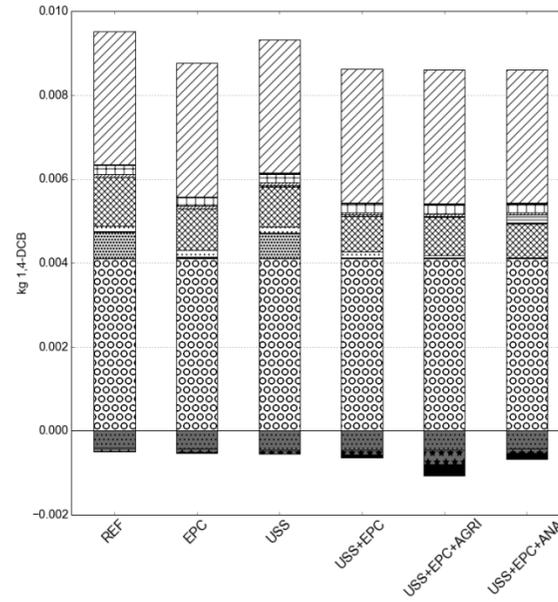


- |                     |                     |                    |                                       |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             | Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                | Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 | Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading | Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport | Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   | Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       | FeCl3 production    |                     |                    |                                       |

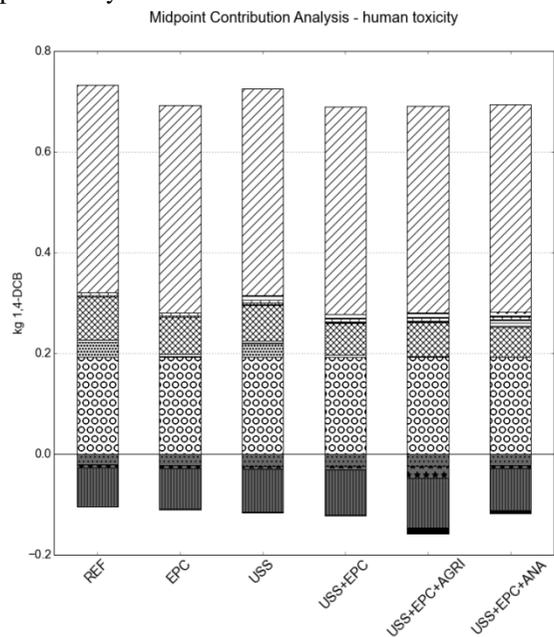
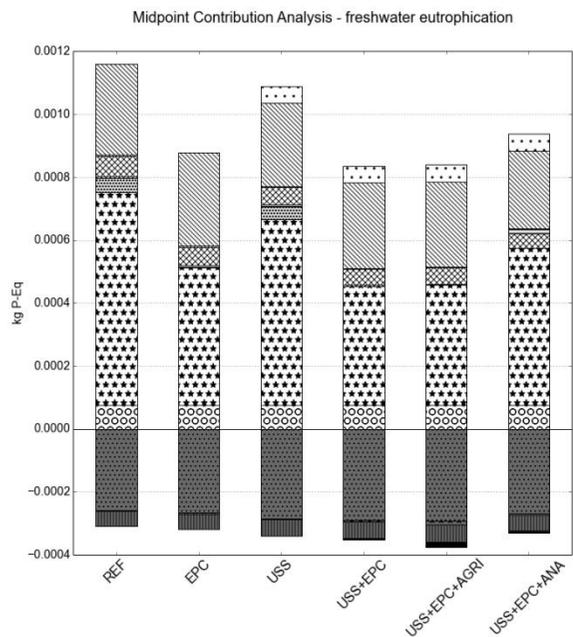
Midpoint Contribution Analysis - fossil depletion



Midpoint Contribution Analysis - freshwater ecotoxicity



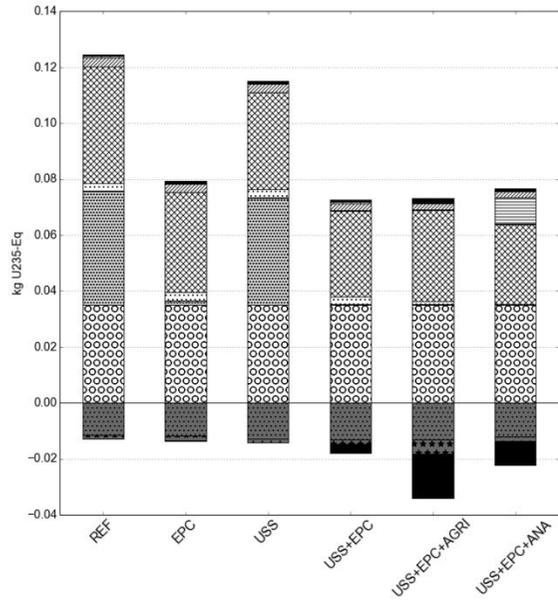
Supplementary Information



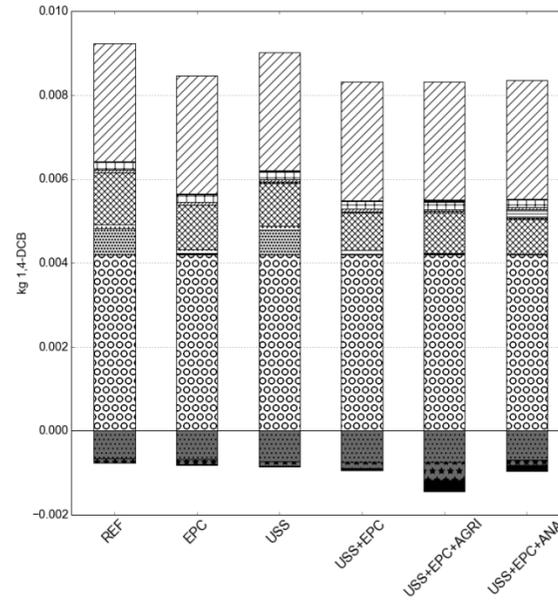
- Infrastructure
- Direct emissions
- Electricity
- Heat
- Cogeneration
- Methanol production
- FeCl3 production
- MgO production
- NaOH production
- Chemicals transport
- Grits disposal
- Urine storage
- Urine transport
- Sludge spreading
- Struvite spreading
- N-rich spreading
- Sludge transport
- Struvite transport
- N-rich transport
- Metals (water and sludge)
- TSP avoided Production
- AN avoided production
- Mineral fertilizers avoided spreading
- Mineral fertilizers avoided transport
- Avoided electricity

- Infrastructure
- Direct emissions
- Electricity
- Heat
- Cogeneration
- Methanol production
- FeCl3 production
- MgO production
- NaOH production
- Chemicals transport
- Grits disposal
- Urine storage
- Urine transport
- Sludge spreading
- Struvite spreading
- N-rich spreading
- Sludge transport
- Struvite transport
- N-rich transport
- Metals (water and sludge)
- TSP avoided Production
- AN avoided production
- Mineral fertilizers avoided spreading
- Mineral fertilizers avoided transport
- Avoided electricity

Midpoint Contribution Analysis - ionising radiation



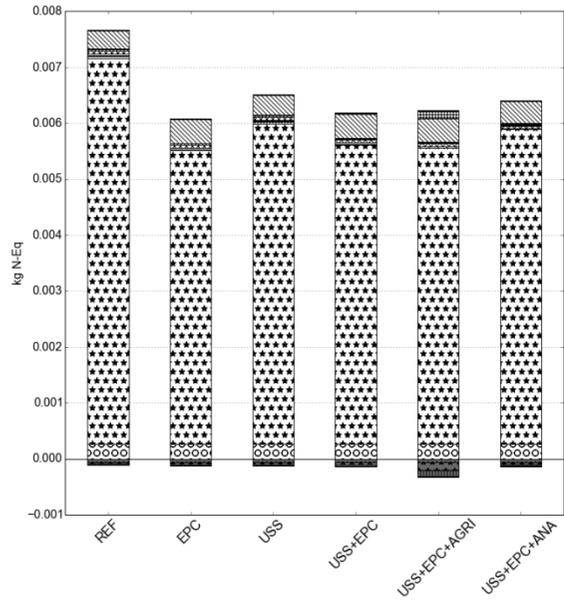
Midpoint Contribution Analysis - marine ecotoxicity



- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

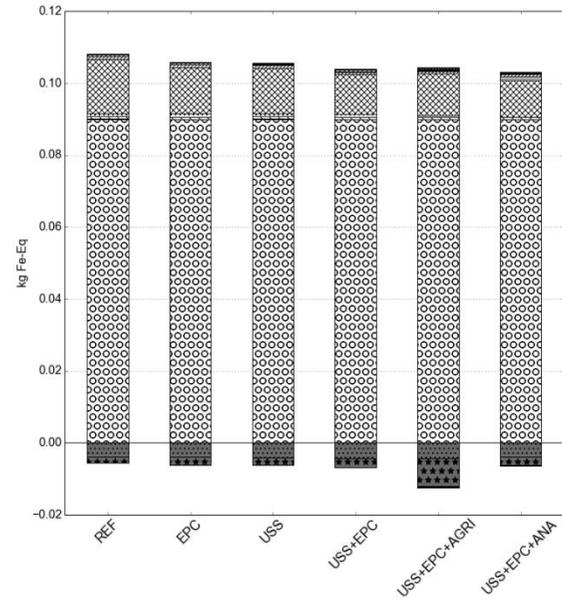
Supplementary Information

Midpoint Contribution Analysis - marine eutrophication

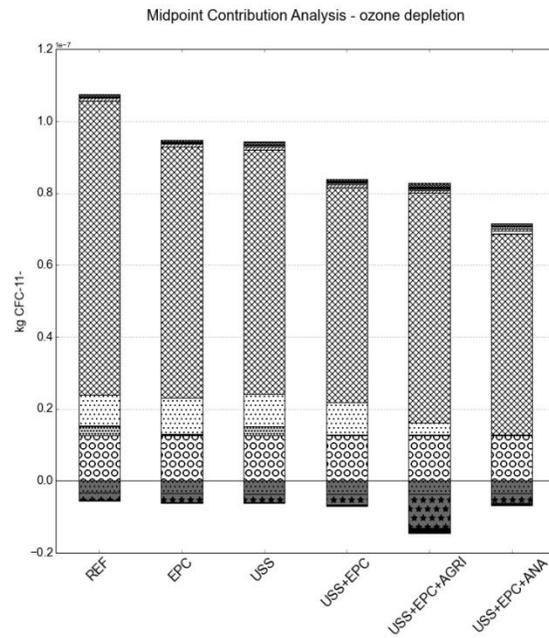
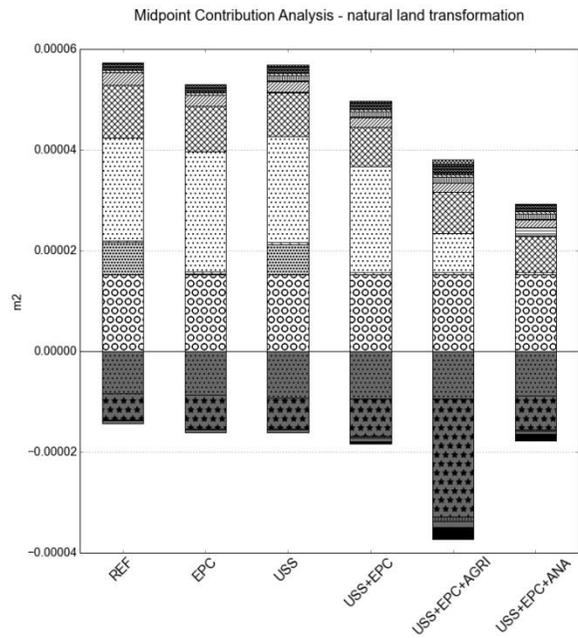


- Infrastructure
- Direct emissions
- Electricity
- Heat
- Cogeneration
- Methanol production
- FeCl3 production
- MgO production
- NaOH production
- Chemicals transport
- Grits disposal
- Urine storage
- Urine transport
- Sludge spreading
- Struvite spreading
- N-rich spreading
- Sludge transport
- Struvite transport
- N-rich transport
- Metals (water and sludge)
- TSP avoided Production
- AN avoided production
- Mineral fertilizers avoided spreading
- Mineral fertilizers avoided transport
- Avoided electricity

Midpoint Contribution Analysis - metal depletion

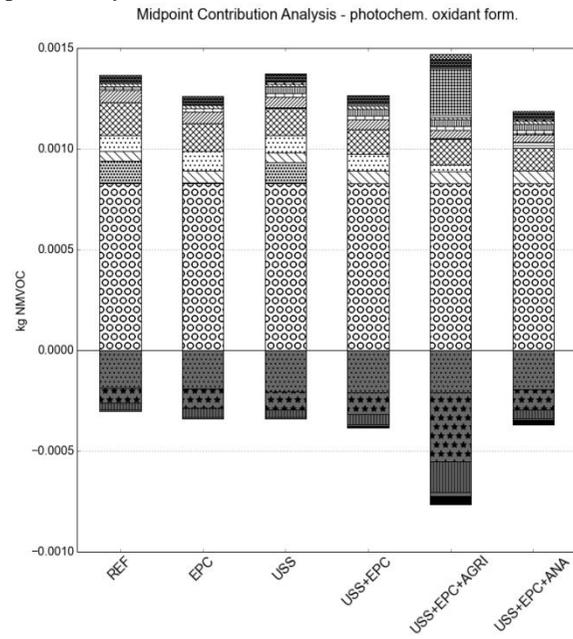
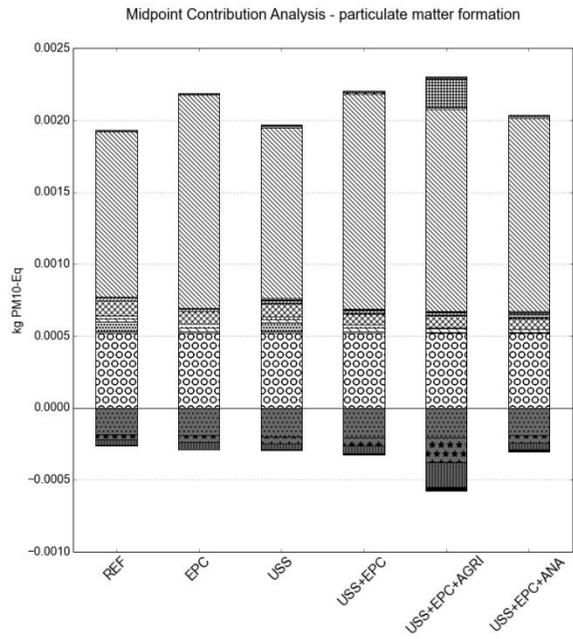


- Infrastructure
- Direct emissions
- Electricity
- Heat
- Cogeneration
- Methanol production
- FeCl3 production
- MgO production
- NaOH production
- Chemicals transport
- Grits disposal
- Urine storage
- Urine transport
- Sludge spreading
- Struvite spreading
- N-rich spreading
- Sludge transport
- Struvite transport
- N-rich transport
- Metals (water and sludge)
- TSP avoided Production
- AN avoided production
- Mineral fertilizers avoided spreading
- Mineral fertilizers avoided transport
- Avoided electricity



- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

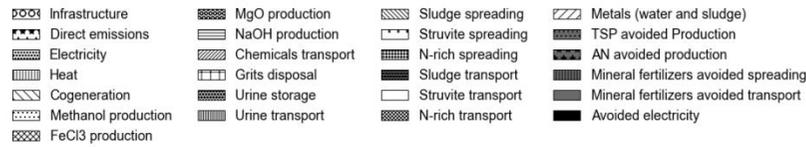
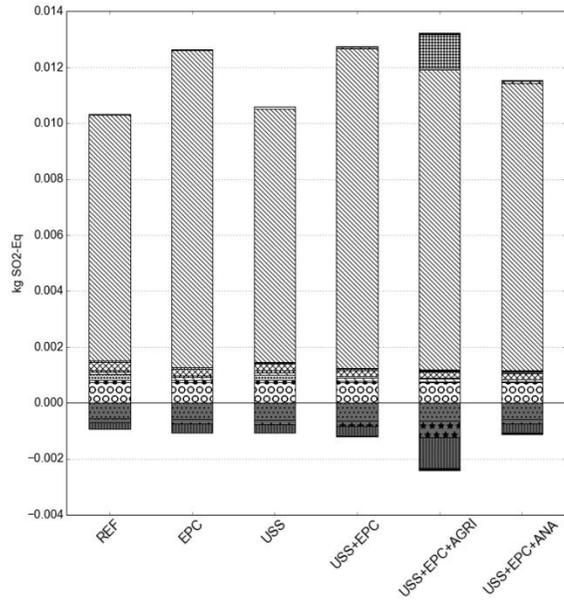
Supplementary Information



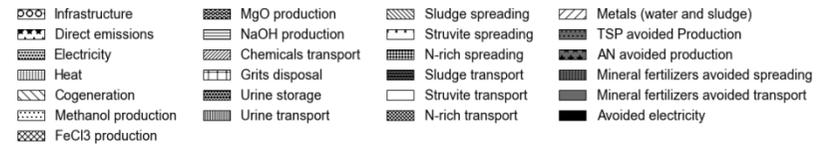
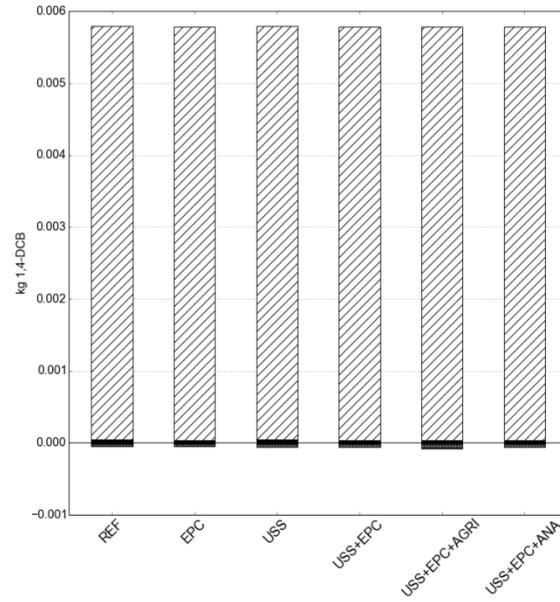
- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

- |                     |                     |                    |                                       |
|---------------------|---------------------|--------------------|---------------------------------------|
| Infrastructure      | MgO production      | Sludge spreading   | Metals (water and sludge)             |
| Direct emissions    | NaOH production     | Struvite spreading | TSP avoided Production                |
| Electricity         | Chemicals transport | N-rich spreading   | AN avoided production                 |
| Heat                | Grits disposal      | Sludge transport   | Mineral fertilizers avoided spreading |
| Cogeneration        | Urine storage       | Struvite transport | Mineral fertilizers avoided transport |
| Methanol production | Urine transport     | N-rich transport   | Avoided electricity                   |
| FeCl3 production    |                     |                    |                                       |

Midpoint Contribution Analysis - terrestrial acidification

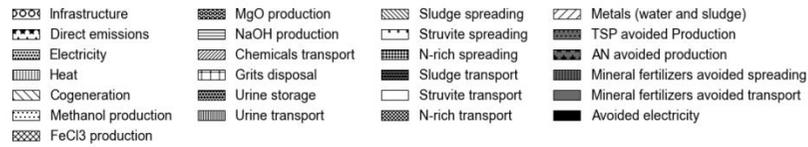
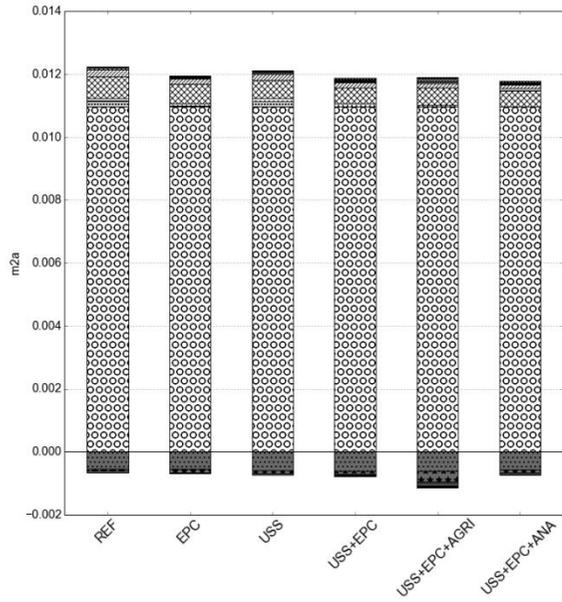


Midpoint Contribution Analysis - terrestrial ecotoxicity

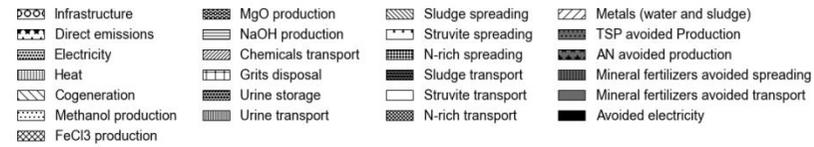
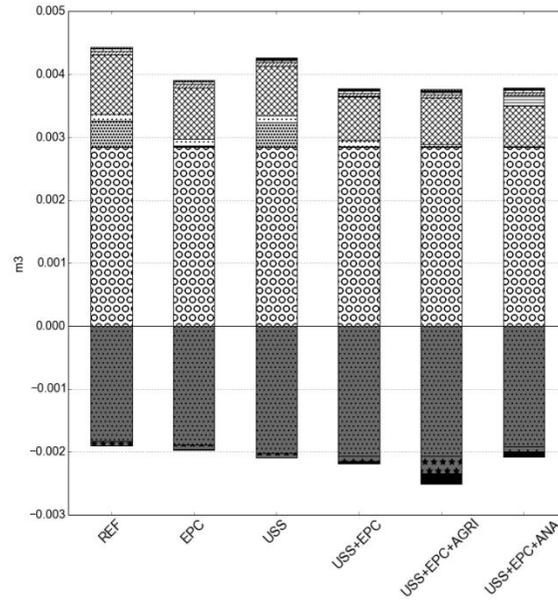


Supplementary Information

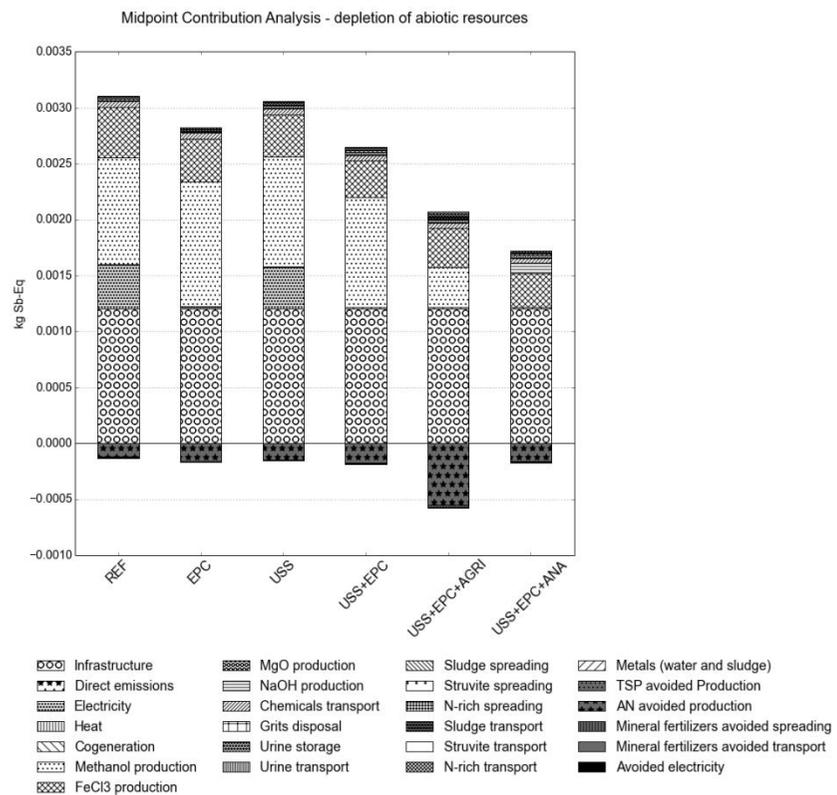
Midpoint Contribution Analysis - urban land occupation



Midpoint Contribution Analysis - water depletion

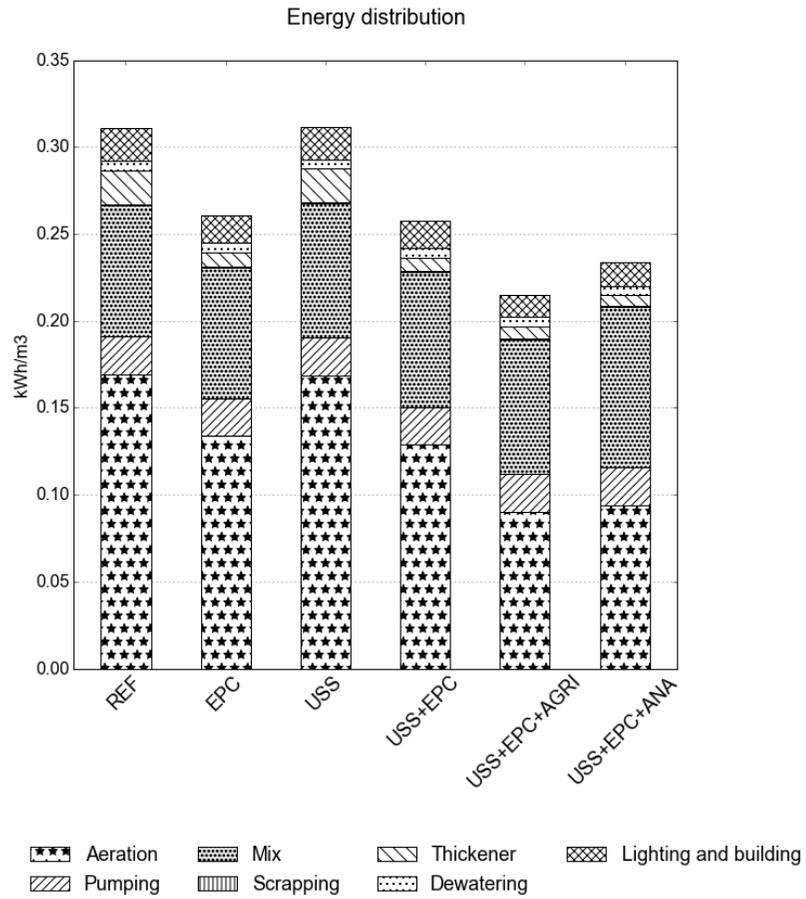


### A.6.2.3 CML 2001

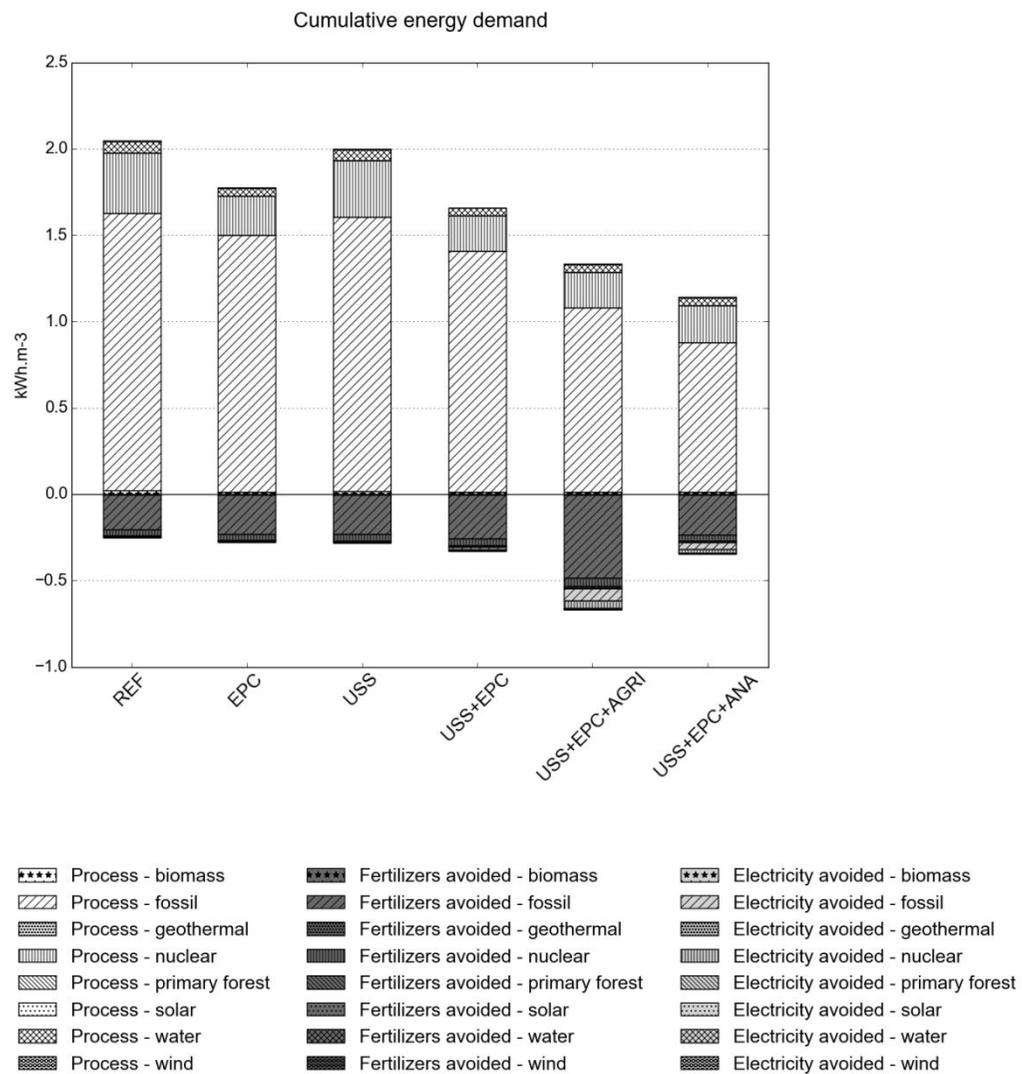


Supplementary Information

## A.6.2.4 Energy distribution



### A.6.3 Cumulative energy demand for reference and alternative scenarios



Supplementary Information

## Supplementary Information

## A.7. General information

## A.7.1 Potable water avoidance

The present study also considers an over production of potable water in scenarios 1 and 2 (scenarios without urine separation). For urine source separation scenarios, low flushing toilets are used. According to STOWA (2002), to flush urine in separation toilets 0.12-0.15 L of water is used in comparison to 6L used for conventional systems. The impacts of the avoidance of this overproduction are not considered, as the activity of “producing wastewater” is not included. However, it should be emphasized that approximately  $600 \text{ m}^3 \cdot \text{d}^{-1}$  are avoided (which represents approximately 3% of total produced wastewater).

## A.7.2 Gas emission calculations

$$\begin{aligned}
 PV &= nRT \\
 n &= \frac{PV}{RT} = \frac{m}{M_w} \\
 m &= \frac{P \cdot V \cdot M_w}{R \cdot T} \\
 m_{i,j} &= \frac{101325 \left[ \frac{\text{N}}{\text{m}^2} \right] \cdot \%gas_j \cdot V_{offgas,i} \left[ \frac{\text{m}^3}{\text{h}} \right] \cdot M_{w,j} \left[ \frac{\text{g}}{\text{mol}} \right] \cdot \frac{1}{1000} \left[ \frac{\text{kg}}{\text{g}} \right] \cdot 24 \left[ \frac{\text{h}}{\text{d}} \right]}{8.3144 \left[ \frac{\text{N} \cdot \text{m}}{\text{mol} \cdot \text{K}} \right] \cdot 293.15 [\text{K}]}
 \end{aligned}$$

Where i represents each reactor and j each considered gas.

## A.7.3 Urine influent calculation

Urine influent was based on original file proposed by Gernaey et al. (2011). A few steps were accomplished in order to separate urine from other flows: 1) Ammonia and soluble biodegradable N were considered to completely come from urine so decreases in volume of used water was calculated based on these flows. 2) With volume reduction, new concentrations were calculated for the effluent without urine (calculated considering 50% of urine separation). 3) For P calculations, a ratio of N/P = 12 was considered and all P is in the form of phosphate. 4) For COD calculations, it was considered the ratio COD/TKN = 1.49 and COD is 85% readily biodegradable and 15%

soluble inert.5) Finally, for alkalinity in urine, a ratio of total CO<sub>2</sub> in relation to total N was calculated based on Udert et al. (2006) and applied to influent calculation. 6) Additionally, magnesium addition for struvite precipitation was calculated considering a molar excess of 10%.

#### A.7.4 General tables

Table 1: Initial concentration and transfer coefficients for metals

Concentration in sewage			Transfer Coefficients <sup>1</sup>		Source
Ecoinvent notation	Short name	Concentration (kg.m <sup>-3</sup> )	To sludge <sup>2</sup>	To effluent <sup>3</sup>	
Arsenic, ion	As	3E-06	0.22	0.78	Henze and Ledin (2001)
Cadmium, ion	Cd	2E-06	0.50	0.50	Henze and Ledin (2001)
Cobalt	Co	1E-06	0.50	0.50	Henze and Ledin (2001)
Copper, ion	Cu	7E-05	0.75	0.25	Henze and Ledin (2001)
Lead	Pb	6.5E-05	0.90	0.10	Henze and Ledin (2001)
Manganese	Mn	1E-04	0.50	0.50	Henze and Ledin (2001)
Mercury	Hg	2E-06	0.70	0.30	Henze and Ledin (2001)
Nickel, ion	Ni	2.5E-05	0.40	0.60	Henze and Ledin (2001)
Silver, ion	Ag	7E-06	0.75	0.25	Henze and Ledin (2001)
Tin, ion	Sn	3.4E-06	0.59	0.41	Doka (2009)
Zinc, ion	Zn	2E-04	0.70	0.30	Henze and Ledin (2001)
Silicon	Si	3.1E-03	0.95	0.05	Doka (2009)
Fluoride	F	3.3E-05	0.00	1.00	Doka (2009)
Potassium, ion	K	4E-04	0.00	1.00	Doka (2009)
Sodium, ion	Na	2.2E-03	0.00	1.00	Doka (2009)
Molybdenum	Mo	9.6E-07	0.50	0.50	Doka (2009)
Chromium VI	Cr	2.5E-05	0.50	0.50	Henze and Ledin (2001)
S particulate	S	2E-03	1.00	0.00	Doka (2009)
Magnesium	Mg	5.7E-03	0.10	0.90	Doka (2009)

Supplementary Information

## Supplementary Information

Calcium, ion	Ca	5.1E-02	0.10	0.90	Doka (2009)
Aluminum	Al	6.5E-04	0.95	0.05	Henze and Ledin (2001)
Sulfate (dissolved)	SO <sub>4</sub>	4.4E-02	0.00	1.00	Doka (2009)
Iron, ion	Fe	1E-03	0.50	0.50	Henze and Ledin (2001)
Chloride	Cl	3E-02	0.00	1.00	Doka (2009)

<sup>1</sup> Doka (2009)<sup>2</sup> Share in particulate matter<sup>3</sup> Dissolved share

Table 2: Direct emissions impacts contribution for ReCiPe Midpoint (H) for Ecoinvent module “treatment, sewage, to wastewater treatment, class 2, CH, [m3] (#2276)” compared to this study.

Category	% Contribution	
	This study <sup>1</sup>	ReCiPe Midpoint (H)
<b>Climate change</b>	33.93%	12.26%
<b>Freshwater ecotoxicity</b>	33.40%	18.84%
<b>Freshwater eutrophication</b>	83.18%	90.08%
<b>Human toxicity</b>	56.11%	33.60%
<b>Marine ecotoxicity</b>	30.53%	17.48%
<b>Marine eutrophication</b>	94.19%	98.57%
<b>Particulate matter formation</b>	59.97%	44.47%
<b>Terrestrial acidification</b>	85.90%	70.31%
<b>Terrestrial ecotoxicity</b>	99.28%	82.17%

<sup>1</sup> For the comparison, direct emissions in this study are here, considered to be all emissions from WWTP (both directly to water body and from sludge)

Table 3: Endpoint impacts for alternative scenarios.

Scenarios	Ecosystem quality		Human health		Resources		Total	
	Impact (points)	Reduction in impact %	Impact (points)	Reduction in impact %	Impacts (points)	Reduction in impact %	Impacts (points)	Reduction in impact %
<b>REF</b>	1.41E-02	-	3.54E-02	-	1.44E-02	-	6.39E-02	-
<b>USS</b>	1.37E-02	3.00%	3.46E-02	2.10%	1.40E-02	3.10%	6.23E-02	2.50%
<b>EPC</b>	1.30E-02	8.20%	3.43E-02	3.10%	1.30E-02	9.90%	6.02E-02	5.80%

<b>USS+EPC</b>	1.21E-02	13.90%	3.29E-02	7.10%	1.17E-02	19.20%	5.67E-02	11.40%
<b>USS+EPC+ AGRI</b>	8.06E-03	42.90%	2.56E-02	27.80%	5.41E-03	62.60%	3.90E-02	39.00%
<b>USS+EPC+ ANA</b>	9.48E-03	32.80%	2.82E-02	20.30%	6.20E-03	57.10%	4.38E-02	31.40%

Table 4: Contribution of each species to Greenhouse Gases (GHGs) directly emitted in each scenario.

		<b>Fossil CO<sub>2</sub></b>	<b>N<sub>2</sub>O</b>	<b>CH<sub>4</sub></b>	<b>Biogenic CO<sub>2</sub></b>
<b>REF</b>	kg CO <sub>2</sub> -Eq	0.068	0.113	0.006	0.442
	% Contribution	36.40%	60.50%	3.10%	-
<b>EPC</b>	kg CO <sub>2</sub> -Eq	0.064	0.1	0.004	0.355
	% Contribution	38.10%	59.80%	2.10%	-
<b>USS</b>	kg CO <sub>2</sub> -Eq	0.067	0.109	0.006	0.437
	% Contribution	36.80%	59.90%	3.20%	-
<b>USS+EPC</b>	kg CO <sub>2</sub> -Eq	0.054	0.095	0.003	0.351
	% Contribution	35.30%	62.40%	2.30%	-
<b>USS+EPC+AGRI</b>	kg CO <sub>2</sub> -Eq	0.018	0.062	0.003	0.304
	% Contribution	21.80%	74.30%	4.00%	-
<b>USS+EPC+ANA</b>	kg CO <sub>2</sub> -Eq	0	0.072	0.004	0.265
	% Contribution	0.00%	95.25%	4.75%	-

## Supplementary Information

Table 5: Characteristics of considered influent.

		<b>Average</b>	<b>Min</b>	<b>Max</b>
<b>Q (m<sup>3</sup>.d<sup>-1</sup>)</b>	Influent flow	20668.44	5146.12	76944.07
<b>S<sub>I</sub> (gCOD.m<sup>-3</sup>)</b>	Soluble inert	27.21	1.99	42.18
<b>S<sub>S</sub> (gCOD.m<sup>-3</sup>)</b>	Readily biodegradable	58.15	0.93	141.56
<b>X<sub>I</sub> (gCOD.m<sup>-3</sup>)</b>	Particulate inert	92.46	1.75	199.53
<b>X<sub>S</sub> (gCOD.m<sup>-3</sup>)</b>	Slowly biodegradable	363.77	16.08	770.23
<b>X<sub>BH</sub> (gCOD.m<sup>-3</sup>)</b>	Heterotrophic biomass	50.66	2.46	106.39
<b>X<sub>BA</sub> (gCOD.m<sup>-3</sup>)</b>	Autotrophic biomass	0	0	0
<b>X<sub>P</sub> (gCOD.m<sup>-3</sup>)</b>	Particulate products from biomass decay	0	0	0
<b>S<sub>O</sub> (gCOD.m<sup>-3</sup>)</b>	Soluble oxygen	0	0	0
<b>S<sub>NO</sub> (gCOD.m<sup>-3</sup>)</b>	Nitrate and nitrite	0	0	0
<b>S<sub>NH</sub> (gCOD.m<sup>-3</sup>)</b>	Soluble ammonia	27.91	1.75	64.01
<b>S<sub>ND</sub> (gCOD.m<sup>-3</sup>)</b>	Soluble biodegradable organic nitrogen	6.66	0.21	17.01
<b>X<sub>ND</sub> (gCOD.m<sup>-3</sup>)</b>	Particulate biodegradable organic nitrogen	19.35	0.91	41.87

## B. Supplementary Information for chapter III

### B.1 Adapted Influent Generator Matlab code

```
% This is an adapted file from the original BSM2 influent generation model
% from Xavier Flores-Alsina, IEA, LTH, Sweden, June 2010
% Adapted in order to include urine source separation (2016)
% Bisinella de Faria et al., 2016. LISBP, INSA Toulouse
```

```
% Loading total profiles (without urine separation)
% These profiles will be used latter to recalculate new profiles in
% function of urine retention in households
% Industry profiles were not changed in this version
```

```
% Load influent flow rate data files, households (HH)
```

```
load Q_day_HS
load Q_week_HS
load Q_year_HS
```

```
% Load influent flow rate data files, Industry (IndS)
```

```
load Q_week_IndS
load Q_year_IndS
```

```
% Load influent pollution load, households (HH)
```

```
load CODsol_day_HS
load CODpart_day_HS
load SNH_day_HS
load TKN_day_HS
load TP_day_HS
load PO4_day_HS
```

```
load pol_week_HS
```

```
% Load influent pollution load, Industry (IndS)
```

```
load CODsol_week_IndS
```

```
load CODpart_week_IndS
load SNH_week_IndS
load TKN_week_IndS
load TP_week_IndS
load PO4_week_IndS
```

```
all_noises = 1;
```

```
%% 1.Households model block (flow rate)
```

```
QperPE_Urine = 1.36;           % in L/d
NFlushes = 5;                  % Number of urine flushes per PE and per day
QOldFlush = 5;                % in L/flush
QNewFlush = 0.15;             % in L/flush
UrineRetention = 0.5;         % Percentage of urine source separated
```

```
Contrib_Ind = 0.2;
PE = 100000;                  % Number of PE connected to the WWTP -
Including HH and Ind
sampling = 24*4;              % Sampling should be set in order to have the
number of points needed per day (e.g: 24h per day * 4 points per hour = sampling
each 15 minutes)
```

```
QperPE_Household = 150;      % This flow only include total domestic
water
```

```
QperPE_WoUrine = (QperPE_Household - (UrineRetention * (QperPE_Urine +
(NFlushes * QOldFlush))))*(1-Contrib_Ind);
QperPE_SeparatedUrine = UrineRetention * (QperPE_Urine + (NFlushes *
QNewFlush))*(1-Contrib_Ind);
```

Supplementary Information

## Supplementary Information

```

QHHsatmin = 1E-50;
QHHsatmax = QperPE_WoUrine*50;
QHHsatmin_Urine = 1E-50;
QHHsatmax_Urine = QperPE_SeparatedUrine*50;

factor_Q = 0.15;
factor_Q_Urine = 0.05;

Q_HH_ns = 3800; % Seed for noise
Q_HH_nv = (factor_Q*QperPE_WoUrine)^2; % Variance
for noise
Q_HH_st = 1/sampling; % Sampling time

Q_HH_ns_Urine = 3801;
Q_HH_nv_Urine = (factor_Q_Urine*QperPE_SeparatedUrine)^2;
Q_HH_st_Urine = 1/sampling;

HHpopswitch = 100; % Switch the household contribution on
(100%) or off (0%)
HHnoiseswitch = all_noises; % Switch the noise term in
household flow rate on (1) or off (0)

%% 2.Industry model block (flow rate)

QInd_weekday = QperPE_Household*PE*Contrib_Ind/1000; %
Average wastewater production industry, for normal week-days (m3)
QIndsatmin=0.001;
QIndsatmax=QInd_weekday*10;

factor_Q_Ind = 0.05;
Q_Ind_ns=2000;
Q_Ind_nv=(QInd_weekday*factor_Q_Ind)^2;
Q_Ind_st=1/sampling;

Indpopswitch = 100;
Indnoiseswitch = all_noises;

%% 3. Seasonal correction factor (flow rate)

InfAmp = 1200; % Sine wave amplitude (m3/d)
InfBias = 7100; % Sine wave bias (m3/d) (= average
infiltration flow rate)
InfFreq = 2*pi/364; % Sine wave frequency (rad/d)
InfPhase = -pi*15/24; % Sine wave phase shift
InfCst = 7100; % Constant flow rate (m3/d), used when the
sine wave is not selected (manual selection possible in 'Groundwater' model block)

QSCIsatmin=0.0;
QSCIsatmax=2*(InfBias+InfAmp);

Q_SCI_ns=1000;
Q_SCI_nv=0.1*InfBias;
Q_SCI_st=1;

SCIpopswitch=100;
SCInoiseswitch=0;

%% 4. rain generation model block (flow-rate)

LLrain=3.5; % Limit for rain (this value is subtracted from
the values generated by the random number generator)
Qpermm=1500; % Flow rate due to rain (m3/mm)
aHpercent=75; % Assumed percentage of the extra flow due
to rain that originates from impervious areas, where water is directly collected in
the sewer system. In the model, the conversion aH = aHpercent/100 is made.
rainmax = 1000; % Max signal after the transfer function
rainmin = 0; % Min signal after the transfer function

rain_ns=3000;
rain_nm=1;
rain_nv=800; % Originally 400
rain_st=1/sampling;

rainpopswitch=100;

%% 5 soil model accumulation block (flow rate)

XINITSOIL=2.2; % Initial h1 value.

```

```

subareas = 4;                % Subareas the catchment is divided
HINV=2;                    % Invert level in tank, i.e. water level
corresponding to bottom of sewer pipes
HMAX=HINV+0.8;            % Maximum water level in tank
A=36000;                  % Surface area
K=1.0;                    % Parameter, permeability of soil for water
penetration
Kinf=2500.0*subareas;    % Infiltration gain, can be an indication of
the quality of the sewer system pipes
Kdown=1000.0;            % Gain to adjust for flow rate to
downstream aquifer

PARS_SOIL=[HMAX HINV A K Kinf Kdown];    % Parameter vector, an
input to the unisoilmodel.c S-function

%% 6.Households model block (pollutants)

% Ratios between soluble and particulate considers that sewers will not consider
hydrolysis

% Total domestic (WITH urine)
Total_COD = 120;          % in g/(PE.d)
TN_TP = 6;                % Ratio between TN and TP
TCOD_TN = 9;              % Ratio between TCOD and TN
TCOD_TP = TCOD_TN * TN_TP; % Ratio between TCOD and TP

CODsol_TCOD = 0.21;      % Ratio between soluble COD and
total COD
SNH_TKN = 0.75;          % Ratio between ammonium and total
nitrogen
PO4_TP = 0.54;           % Ratio between PO4 and total
phosphorus
NOx_TKN = 1E-50;         % Ratio between NOx and total
nitrogen

TotalCOD_HH = Total_COD*(1-Contrib_Ind);
CODsol_gperPEperd = Total_COD * CODsol_TCOD * (1-Contrib_Ind); %
Soluble COD load in g COD/d per PE

```

```

CODpart_gperPEperd = Total_COD * (1-CODsol_TCOD) * (1-Contrib_Ind); %
Particulate COD load in g COD/d per (includes also colloidal part)
TKN_gperPEperd = Total_COD / TCOD_TN * (1-Contrib_Ind);          % TKN
load in g N/d per PE
SNH_gperPEperd = SNH_TKN * TKN_gperPEperd;          % Ammonium load in
g N/d per PE
NOx_gperPEperd = NOx_TKN * TKN_gperPEperd;
TP_gperPEperd = Total_COD / TCOD_TP * (1-Contrib_Ind);          % TP load
in g P/d per PE
PO4_gperPEperd = PO4_TP * TP_gperPEperd;          % PO4 load in g P/d per
PE

% Total urine (100% retention)
% Directly excreted values per PE per day are used for urine (instead of ratios) -
concentration and values are well know
CODsol_gperPEperd_Urine = 10.40;          % Soluble COD load in g
COD/d per PE in Urine
CODpart_gperPEperd_Urine = 0.78;          % Particulate COD load in g
COD/d per PE in Urine
Total_COD_Urine = CODsol_gperPEperd_Urine + CODpart_gperPEperd_Urine;
TKN_gperPEperd_Urine = 9.78;              % TKN load in g N/d per PE in
Urine
SNH_gperPEperd_Urine = 8.80;              % Ammonium load in g N/d per
PE in Urine
NOx_gperPEperd_Urine = 1E-50;             % NOx load in g N/d per PE in
Urine
TP_gperPEperd_Urine = 0.74;              % Total phosphorus load in g P/d
per PE in Urine
PO4_gperPEperd_Urine = 0.70;             % PO4 load in g P/d per PE in
Urine

% Urine separated
CODsol_gperPEperd_SepUrine = UrineRetention*(1-
Contrib_Ind)*(CODsol_gperPEperd_Urine);
CODpart_gperPEperd_SepUrine = UrineRetention*(1-
Contrib_Ind)*(CODpart_gperPEperd_Urine);
Total_COD_SepUrine = CODsol_gperPEperd_SepUrine +
CODpart_gperPEperd_SepUrine;

```

Supplementary Information

## Supplementary Information

```

TKN_gperPEperd_SepUrine = UrineRetention*(1-
Contrib_Ind)*(TKN_gperPEperd_Urine);
SNH_gperPEperd_SepUrine = UrineRetention*(1-
Contrib_Ind)*(SNH_gperPEperd_Urine);
NOx_gperPEperd_SepUrine = UrineRetention*(1-
Contrib_Ind)*(NOx_gperPEperd_Urine);
TP_gperPEperd_SepUrine = UrineRetention*(1-
Contrib_Ind)*(TP_gperPEperd_Urine);
PO4_gperPEperd_SepUrine = UrineRetention*(1-
Contrib_Ind)*(PO4_gperPEperd_Urine);

% Domestic without urine
CODsol_gperPEperd_woUrine = CODsol_gperPEperd -
CODsol_gperPEperd_SepUrine;
CODpart_gperPEperd_woUrine = CODpart_gperPEperd -
CODpart_gperPEperd_SepUrine;
Total_COD_woUrine = CODsol_gperPEperd_woUrine +
CODpart_gperPEperd_woUrine;
TKN_gperPEperd_woUrine = TKN_gperPEperd - TKN_gperPEperd_SepUrine;
SNH_gperPEperd_woUrine = SNH_gperPEperd - SNH_gperPEperd_SepUrine;
NOx_gperPEperd_woUrine = NOx_gperPEperd - NOx_gperPEperd_SepUrine;
TP_gperPEperd_woUrine = TP_gperPEperd - TP_gperPEperd_SepUrine;
PO4_gperPEperd_woUrine = PO4_gperPEperd - PO4_gperPEperd_SepUrine;

CODsol_HH_min = 0.001*CODsol_gperPEperd_woUrine*PE/1000;
CODsol_HH_max = 20*CODsol_gperPEperd_woUrine*PE/1000;
CODpart_HH_min = 0.001*CODpart_gperPEperd_woUrine*PE/1000;
CODpart_HH_max = 20*CODpart_gperPEperd_woUrine*PE/1000;
SNH_HH_min = 0.001*SNH_gperPEperd_woUrine*PE/1000;
SNH_HH_max = 20*SNH_gperPEperd_woUrine*PE/1000;
TKN_HH_min = 0.001*TKN_gperPEperd_woUrine*PE/1000;
TKN_HH_max = 20*TKN_gperPEperd_woUrine*PE/1000;
TP_HH_min = 0.001*TP_gperPEperd_woUrine*PE/1000;
TP_HH_max = 20*TP_gperPEperd_woUrine*PE/1000;
PO4_HH_min = 0.001*PO4_gperPEperd_woUrine*PE/1000;
PO4_HH_max = 20*PO4_gperPEperd_woUrine*PE/1000;

CODsol_HH_min_Urine = 0.001*CODsol_gperPEperd_SepUrine*PE/1000;
CODsol_HH_max_Urine = 20*CODsol_gperPEperd_SepUrine*PE/1000;

```

```

CODpart_HH_min_Urine = 0.001*CODpart_gperPEperd_SepUrine*PE/1000;
CODpart_HH_max_Urine = 20*CODpart_gperPEperd_SepUrine*PE/1000;
SNH_HH_min_Urine = 0.001*SNH_gperPEperd_SepUrine*PE/1000;
SNH_HH_max_Urine = 20*SNH_gperPEperd_SepUrine*PE/1000;
TKN_HH_min_Urine = 0.001*TKN_gperPEperd_SepUrine*PE/1000;
TKN_HH_max_Urine = 20*TKN_gperPEperd_SepUrine*PE/1000;
TP_HH_min_Urine = 0.001*TP_gperPEperd_SepUrine*PE/1000;
TP_HH_max_Urine = 20*TP_gperPEperd_SepUrine*PE/1000;
PO4_HH_min_Urine = 0.001*PO4_gperPEperd_SepUrine*PE/1000;
PO4_HH_max_Urine = 20*PO4_gperPEperd_SepUrine*PE/1000;

```

```

factor1 = 0.1; % Proportionality factor random noise
generators
factor1_Urine = 0.05;

```

```

CODsol_HH_ns = 25000;
CODsol_HH_nv = (factor1*CODsol_gperPEperd_woUrine*PE/1000)^2;
CODsol_HH_st = 1/sampling;
CODpart_HH_ns = 35000;
CODpart_HH_nv = (factor1*CODpart_gperPEperd_woUrine*PE/1000)^2;
CODpart_HH_st = 1/sampling;
SNH_HH_ns = 45000;
SNH_HH_nv = (factor1*SNH_gperPEperd_woUrine*PE/1000)^2;
SNH_HH_st = 1/sampling;
TKN_HH_ns = 55000;
TKN_HH_nv = (factor1*TKN_gperPEperd_woUrine*PE/1000)^2;
TKN_HH_st = 1/sampling;
TP_HH_ns = 65000;
TP_HH_nv = (factor1*TP_gperPEperd_woUrine*PE/1000)^2;
TP_HH_st = 1/sampling;
PO4_HH_ns = 75000;
PO4_HH_nv = (factor1*PO4_gperPEperd_woUrine*PE/1000)^2;
PO4_HH_st = 1/sampling;

```

```

CODsol_HH_ns_Urine = 26000;
CODsol_HH_nv_Urine =
(factor1_Urine*CODsol_gperPEperd_SepUrine*PE/1000)^2;
CODsol_HH_st_Urine = 1/sampling;
CODpart_HH_ns_Urine = 36000;

```

```

CODpart_HH_nv_Urine =
(factor1_Urine*CODpart_gperPEperd_SepUrine*PE/1000)^2;
CODpart_HH_st_Urine = 1/sampling;
SNH_HH_ns_Urine = 46000;
SNH_HH_nv_Urine = (factor1_Urine*SNH_gperPEperd_SepUrine*PE/1000)^2;
SNH_HH_st_Urine = 1/sampling;
TKN_HH_ns_Urine = 56000;
TKN_HH_nv_Urine = (factor1_Urine*TKN_gperPEperd_SepUrine*PE/1000)^2;
TKN_HH_st_Urine = 1/sampling;
TP_HH_ns_Urine = 66000;
TP_HH_nv_Urine = (factor1_Urine*TP_gperPEperd_SepUrine*PE/1000)^2;
TP_HH_st_Urine = 1/sampling;
PO4_HH_ns_Urine = 76000;
PO4_HH_nv_Urine = (factor1_Urine*PO4_gperPEperd_SepUrine*PE/1000)^2;
PO4_HH_st_Urine = 1/sampling;

```

```
HHpolnoiseswitch = all_noises;
```

```
%% 7. Industry model block (pollutants)
```

```

CODsol_Ind_kgperd = CODsol_gperPEperd*Contrib_Ind/(1-
Contrib_Ind)*PE/1000; % Soluble COD load in kg COD/d
CODpart_Ind_kgperd = CODpart_gperPEperd*Contrib_Ind/(1-
Contrib_Ind)*PE/1000; % Particulate COD load in kg COD/d
TKN_Ind_kgperd = TKN_gperPEperd*Contrib_Ind/(1-Contrib_Ind)*PE/1000;
% TKN load in kg N/d
SNH_Ind_kgperd = SNH_gperPEperd*Contrib_Ind/(1-Contrib_Ind)*PE/1000;
% SNH load in kg N/d
TP_Ind_kgperd = TP_gperPEperd*Contrib_Ind/(1-Contrib_Ind)*PE/1000;
% TP load in kg P/d
PO4_Ind_kgperd = PO4_gperPEperd*Contrib_Ind/(1-Contrib_Ind)*PE/1000;
% PO4 load in kg P/d
NOx_Ind_kgperd = NOx_gperPEperd*Contrib_Ind/(1-Contrib_Ind)*PE/1000;

```

```

CODsol_gperPEperd_Ind = CODsol_Ind_kgperd*1000/PE; %
Soluble COD load in kg COD/d
CODpart_gperPEperd_Ind = CODpart_Ind_kgperd*1000/PE; %
Particulate COD load in kg COD/d

```

```

TKN_gperPEperd_Ind = TKN_Ind_kgperd*1000/PE; % TKN
load in kg N/d
SNH_gperPEperd_Ind = SNH_Ind_kgperd*1000/PE; % SNH
load in kg N/d
TP_gperPEperd_Ind = TP_Ind_kgperd*1000/PE; % TP load in
kg P/d
PO4_gperPEperd_Ind = PO4_Ind_kgperd*1000/PE; % PO4 load
in kg P/d
TotalCOD_Ind = CODsol_gperPEperd_Ind + CODpart_gperPEperd_Ind;
NOx_gperPEperd_Ind = NOx_Ind_kgperd*1000/PE;

```

```

CODsol_Ind_max = 20*CODsol_Ind_kgperd;
CODsol_Ind_min = 0.1;
CODpart_Ind_max = 20*CODpart_Ind_kgperd;
CODpart_Ind_min = 0.1;
SNH_Ind_max = 20*SNH_Ind_kgperd;
SNH_Ind_min = 0.1;
TKN_Ind_max = 20*TKN_Ind_kgperd;
TKN_Ind_min = 0.1;
TP_Ind_max = 20*TP_Ind_kgperd;
TP_Ind_min = 0.1;
PO4_Ind_max = 20*PO4_Ind_kgperd;
PO4_Ind_min = 0.1;

```

```
factor2 = 0.1;
```

```

CODsol_Ind_ns = 11000;
CODsol_Ind_nv = (factor2*CODsol_Ind_kgperd)^2;
CODsol_Ind_st = 1/sampling;
CODpart_Ind_ns = 21000;
CODpart_Ind_nv = (factor2*CODpart_Ind_kgperd)^2;
CODpart_Ind_st = 1/sampling;
SNH_Ind_ns = 31000;
SNH_Ind_nv = (factor2*SNH_Ind_kgperd)^2;
SNH_Ind_st = 1/sampling;
TKN_Ind_ns = 41000;
TKN_Ind_nv = (factor2*TKN_Ind_kgperd)^2;
TKN_Ind_st = 1/sampling;
TP_Ind_ns = 51000;

```

Supplementary Information

## Supplementary Information

```

TP_Ind_nv = (factor2*TP_Ind_kgperd)^2;
TP_Ind_st = 1/sampling;
PO4_Ind_ns = 61000;
PO4_Ind_nv = (factor2*PO4_Ind_kgperd)^2;
PO4_Ind_st = 1/sampling;

```

```

Indpolnoiseswitch=all_noises;

```

```

%% 8. Influent fractionation model

```

```

% General parameters

```

```

COD_TSS = 0.75;

```

```

Biomass_COD_VSS = 1.42;
XU_COD_VSS = 1.3;
XB_COD_VSS = 1.8;
XE_COD_VSS = 1.42;

```

```

% Parameters for total influent

```

```

Total_XU_CODpart = 0.124;
Total_XOHO_CODpart = 0.025;
Total_XOtherBiomass_CODpart = 1E-50;
Total_XE_CODpart = 1E-50;
Total_SVFA_CODsol = 0.26;
Total_CB_CODpart = 0.203;
Total_CU_CODpart = 0.0405;
Total_SMEOL_CODsol = 1E-50;
Total_TCODinert_TCOD = 0.18;

```

```

Total_TKNinert_TKN = 0.0245;
Total_Organic_TKN = 1 - (SNH_TKN);
Total_XNU_TKN = 0.0034;
Total_XNB_TKN = 0.0904;
Total_CNU_TKN = 0.0011;
Total_CNB_TKN = 0.0301;
Total_SNO3_NOx = 0.5;

```

```

Total_TPinert_TP = 0.0075;
Total_Organic_TP = 1 - (PO4_TP);

```

```

Total_XPU_TP = 0.0011;
Total_XPB_TP = 0.1714;
Total_CPU_TP = 0.0004;
Total_CPB_TP = 0.0571;

```

```

Total_Ca_SNHx = 0.95;
Total_Mg_SNHx = 0.23;
Total_Na_SNHx = 1.73;
Total_Cl_SNHx = 3.6;
Total_TIC_SNHx = 4.2;

```

```

% Parameters for urine

```

```

XU_CODpart_Urine = 0.1071;
XOHO_CODpart_Urine = 1E-50;
XOtherBiomass_CODpart_Urine = 1E-50;
XE_CODpart_Urine = 1E-50;
SVFA_CODsol_Urine = 0.57;
CB_CODpart_Urine = 0.214;
CU_CODpart_Urine = 0.036;
SMEOL_CODsol_Urine = 1E-50;
TCODinert_TCOD_Urine = 0.09;

```

```

TKNinert_TKN_Urine = 0.01;

```

```

Organic_TKN_Urine = 1 - (SNH_gperPEperd_Urine/TKN_gperPEperd_Urine);
XNU_TKN_Urine = 1E-50;
XNB_TKN_Urine = 0.015;
CNU_TKN_Urine = 1E-50;
CNB_TKN_Urine = 0.005;
SNO3_NOx_Urine = 0.5;

```

```

TPinert_TP_Urine = 0.001;

```

```

Organic_TP_Urine = 1 - (PO4_gperPEperd_Urine/TP_gperPEperd_Urine);
XPU_TP_Urine = 1E-50;
XPB_TP_Urine = 0.0075;
CPU_TP_Urine = 1E-50;
CPB_TP_Urine = 0.0025;

```

```

Ca_SNHx_Urine = 0.026;
Mg_SNHx_Urine = 0.022;

```

Na\_SNHx\_Urine = 0.392;  
 Cl\_SNHx\_Urine = 0.565;  
 TIC\_SNHx\_Urine = 1.57;

% Calculating new parameters for HH without urine source separated

XU\_CODpart =  

$$\frac{((\text{Total\_XU\_CODpart} * (\text{CODpart\_gperPEperd} + \text{CODpart\_gperPEperd\_Ind})) - (\text{XU\_CODpart\_Urine} * \text{CODpart\_gperPEperd\_SepUrine}))}{(\text{CODpart\_gperPEperd\_woUrine} + \text{CODpart\_gperPEperd\_Ind})}$$
 XOHO\_CODpart =  

$$\frac{((\text{Total\_XOHO\_CODpart} * (\text{CODpart\_gperPEperd} + \text{CODpart\_gperPEperd\_Ind})) - (\text{XOHO\_CODpart\_Urine} * \text{CODpart\_gperPEperd\_SepUrine}))}{(\text{CODpart\_gperPEperd\_woUrine} + \text{CODpart\_gperPEperd\_Ind})}$$
 XOtherBiomass\_CODpart =  

$$\frac{((\text{Total\_XOtherBiomass\_CODpart} * (\text{CODpart\_gperPEperd} + \text{CODpart\_gperPEperd\_Ind})) - (\text{XOtherBiomass\_CODpart\_Urine} * \text{CODpart\_gperPEperd\_SepUrine}))}{(\text{CODpart\_gperPEperd\_woUrine} + \text{CODpart\_gperPEperd\_Ind})}$$
 XE\_CODpart =  

$$\frac{((\text{Total\_XE\_CODpart} * (\text{CODpart\_gperPEperd} + \text{CODpart\_gperPEperd\_Ind})) - (\text{XE\_CODpart\_Urine} * \text{CODpart\_gperPEperd\_SepUrine}))}{(\text{CODpart\_gperPEperd\_woUrine} + \text{CODpart\_gperPEperd\_Ind})}$$
 SVFA\_CODsol =  

$$\frac{((\text{Total\_SVFA\_CODsol} * (\text{CODsol\_gperPEperd} + \text{CODsol\_gperPEperd\_Ind})) - (\text{SVFA\_CODsol\_Urine} * \text{CODsol\_gperPEperd\_SepUrine}))}{(\text{CODsol\_gperPEperd\_woUrine} + \text{CODsol\_gperPEperd\_Ind})}$$
 CB\_CODpart =  

$$\frac{((\text{Total\_CB\_CODpart} * (\text{CODpart\_gperPEperd} + \text{CODpart\_gperPEperd\_Ind})) - (\text{CB\_CODpart\_Urine} * \text{CODpart\_gperPEperd\_SepUrine}))}{(\text{CODpart\_gperPEperd\_woUrine} + \text{CODpart\_gperPEperd\_Ind})}$$
 CU\_CODpart =  

$$\frac{((\text{Total\_CU\_CODpart} * (\text{CODpart\_gperPEperd} + \text{CODpart\_gperPEperd\_Ind})) - (\text{CU\_CODpart\_Urine} * \text{CODpart\_gperPEperd\_SepUrine}))}{(\text{CODpart\_gperPEperd\_woUrine} + \text{CODpart\_gperPEperd\_Ind})}$$
 SMEOL\_CODsol =  

$$\frac{((\text{Total\_SMEOL\_CODsol} * (\text{CODsol\_gperPEperd} + \text{CODsol\_gperPEperd\_Ind})) - (\text{SMEOL\_CODsol\_Urine} * \text{CODsol\_gperPEperd\_SepUrine}))}{(\text{CODsol\_gperPEperd\_woUrine} + \text{CODsol\_gperPEperd\_Ind})}$$

TCODinert\_TCOD =  

$$\frac{((\text{Total\_TCODinert\_TCOD} * (\text{TotalCOD\_HH} + \text{TotalCOD\_Ind})) - (\text{TCODinert\_TCOD\_Urine} * \text{Total\_COD\_SepUrine}))}{(\text{Total\_COD\_woUrine} + \text{TotalCOD\_Ind})}$$

TKNinert\_TKN =  

$$\frac{((\text{Total\_TKNinert\_TKN} * (\text{TKN\_gperPEperd} + \text{TKN\_gperPEperd\_Ind})) - (\text{TKNinert\_TKN\_Urine} * \text{TKN\_gperPEperd\_SepUrine}))}{(\text{TKN\_gperPEperd\_woUrine} + \text{TKN\_gperPEperd\_Ind})}$$

Organic\_TKN =  

$$\frac{((\text{Total\_Organic\_TKN} * (\text{TKN\_gperPEperd} + \text{TKN\_gperPEperd\_Ind})) - (\text{Organic\_TKN\_Urine} * \text{TKN\_gperPEperd\_SepUrine}))}{(\text{TKN\_gperPEperd\_woUrine} + \text{TKN\_gperPEperd\_Ind})}$$

XNU\_TKN =  

$$\frac{((\text{Total\_XNU\_TKN} * (\text{TKN\_gperPEperd} + \text{TKN\_gperPEperd\_Ind})) - (\text{XNU\_TKN\_Urine} * \text{TKN\_gperPEperd\_SepUrine}))}{(\text{TKN\_gperPEperd\_woUrine} + \text{TKN\_gperPEperd\_Ind})}$$

XNB\_TKN =  

$$\frac{((\text{Total\_XNB\_TKN} * (\text{TKN\_gperPEperd} + \text{TKN\_gperPEperd\_Ind})) - (\text{XNB\_TKN\_Urine} * \text{TKN\_gperPEperd\_SepUrine}))}{(\text{TKN\_gperPEperd\_woUrine} + \text{TKN\_gperPEperd\_Ind})}$$

CNU\_TKN =  

$$\frac{((\text{Total\_CNU\_TKN} * (\text{TKN\_gperPEperd} + \text{TKN\_gperPEperd\_Ind})) - (\text{CNU\_TKN\_Urine} * \text{TKN\_gperPEperd\_SepUrine}))}{(\text{TKN\_gperPEperd\_woUrine} + \text{TKN\_gperPEperd\_Ind})}$$

CNB\_TKN =  

$$\frac{((\text{Total\_CNB\_TKN} * (\text{TKN\_gperPEperd} + \text{TKN\_gperPEperd\_Ind})) - (\text{CNB\_TKN\_Urine} * \text{TKN\_gperPEperd\_SepUrine}))}{(\text{TKN\_gperPEperd\_woUrine} + \text{TKN\_gperPEperd\_Ind})}$$

SNO3\_NOx =  

$$\frac{((\text{Total\_SNO3\_NOx} * (\text{NOx\_gperPEperd} + \text{NOx\_gperPEperd\_Ind})) - (\text{SNO3\_NOx\_Urine} * \text{NOx\_gperPEperd\_SepUrine}))}{(\text{NOx\_gperPEperd\_woUrine} + \text{NOx\_gperPEperd\_Ind})}$$

TPinert\_TP =  

$$\frac{((\text{Total\_TPinert\_TP} * (\text{TP\_gperPEperd} + \text{TP\_gperPEperd\_Ind})) - (\text{TPinert\_TP\_Urine} * \text{TP\_gperPEperd\_SepUrine}))}{(\text{TP\_gperPEperd\_woUrine} + \text{TP\_gperPEperd\_Ind})}$$

Organic\_TP =  

$$\frac{((\text{Total\_Organic\_TP} * (\text{TP\_gperPEperd} + \text{TP\_gperPEperd\_Ind})) - (\text{Organic\_TP\_Urine} * \text{TP\_gperPEperd\_SepUrine}))}{(\text{TP\_gperPEperd\_woUrine} + \text{TP\_gperPEperd\_Ind})}$$

XPU\_TP =  

$$\frac{((\text{Total\_XPU\_TP} * (\text{TP\_gperPEperd} + \text{TP\_gperPEperd\_Ind})) - (\text{XPU\_TP\_Urine} * \text{TP\_gperPEperd\_SepUrine}))}{(\text{TP\_gperPEperd\_woUrine} + \text{TP\_gperPEperd\_Ind})}$$

Supplementary Information

## Supplementary Information

```

XPB_TP = ((Total_XPB_TP*(TP_gperPEperd+TP_gperPEperd_Ind)) -
(XPB_TP_Urine*TP_gperPEperd_SepUrine))/(TP_gperPEperd_woUrine+TP_gpe
rPEperd_Ind);
CPU_TP = ((Total_CPU_TP*(TP_gperPEperd+TP_gperPEperd_Ind)) -
(CPU_TP_Urine*TP_gperPEperd_SepUrine))/(TP_gperPEperd_woUrine+TP_gpe
rPEperd_Ind);
CPB_TP = ((Total_CPB_TP*(TP_gperPEperd+TP_gperPEperd_Ind)) -
(CPB_TP_Urine*TP_gperPEperd_SepUrine))/(TP_gperPEperd_woUrine+TP_gpe
rPEperd_Ind);

Ca_SNHx = ((Total_Ca_SNHx*(SNH_gperPEperd+SNH_gperPEperd_Ind)) -
(Ca_SNHx_Urine*SNH_gperPEperd_SepUrine))/(SNH_gperPEperd_woUrine+S
NH_gperPEperd_Ind);
Mg_SNHx = ((Total_Mg_SNHx*(SNH_gperPEperd+SNH_gperPEperd_Ind)) -
(Mg_SNHx_Urine*SNH_gperPEperd_SepUrine))/(SNH_gperPEperd_woUrine+S
NH_gperPEperd_Ind);
Na_SNHx = ((Total_Na_SNHx*(SNH_gperPEperd+SNH_gperPEperd_Ind)) -
(Na_SNHx_Urine*SNH_gperPEperd_SepUrine))/(SNH_gperPEperd_woUrine+S
NH_gperPEperd_Ind);
Cl_SNHx = ((Total_Cl_SNHx*(SNH_gperPEperd+SNH_gperPEperd_Ind)) -
(Cl_SNHx_Urine*SNH_gperPEperd_SepUrine))/(SNH_gperPEperd_woUrine+S
NH_gperPEperd_Ind);
TIC_SNHx = ((Total_TIC_SNHx*(SNH_gperPEperd+SNH_gperPEperd_Ind)) -
(TIC_SNHx_Urine*SNH_gperPEperd_SepUrine))/(SNH_gperPEperd_woUrine+S
NH_gperPEperd_Ind);

% Initial values
% Urine
SVFA_in_Urine =
SVFA_CODsol_Urine*CODsol_gperPEperd_SepUrine/QperPE_SeparatedUrine*
1000;
SMEOL_in_Urine =
SMEOL_CODsol_Urine*CODsol_gperPEperd_SepUrine/QperPE_SeparatedUrin
e*1000;
CB_in_Urine =
CB_CODpart_Urine*CODpart_gperPEperd_SepUrine/QperPE_SeparatedUrine*1
000;

```

```

CU_in_Urine =
CU_CODpart_Urine*CODpart_gperPEperd_SepUrine/QperPE_SeparatedUrine*1
000;
XU_in_Urine =
XU_CODpart_Urine*CODpart_gperPEperd_SepUrine/QperPE_SeparatedUrine*1
000;
XE_in_Urine =
XE_CODpart_Urine*CODpart_gperPEperd_SepUrine/QperPE_SeparatedUrine*1
000;
XOHO_in_Urine =
XOHO_CODpart_Urine*CODpart_gperPEperd_SepUrine/QperPE_SeparatedUrin
e*1000;
XPAO_in_Urine =
XOtherBiomass_CODpart_Urine*CODpart_gperPEperd_SepUrine/QperPE_Sepa
ratedUrine*1000;
XMEOLO_in_Urine =
XOtherBiomass_CODpart_Urine*CODpart_gperPEperd_SepUrine/QperPE_Sepa
ratedUrine*1000;
XAOB_in_Urine =
XOtherBiomass_CODpart_Urine*CODpart_gperPEperd_SepUrine/QperPE_Sepa
ratedUrine*1000;
XNOB_in_Urine =
XOtherBiomass_CODpart_Urine*CODpart_gperPEperd_SepUrine/QperPE_Sepa
ratedUrine*1000;
XAMX_in_Urine =
XOtherBiomass_CODpart_Urine*CODpart_gperPEperd_SepUrine/QperPE_Sepa
ratedUrine*1000;
XAMETO_in_Urine =
XOtherBiomass_CODpart_Urine*CODpart_gperPEperd_SepUrine/QperPE_Sepa
ratedUrine*1000;
XHMETO_in_Urine =
XOtherBiomass_CODpart_Urine*CODpart_gperPEperd_SepUrine/QperPE_Sepa
ratedUrine*1000;
XB_in_Urine = (CODpart_gperPEperd_SepUrine/QperPE_SeparatedUrine*1000)
- CB_in_Urine - CU_in_Urine - XU_in_Urine - XE_in_Urine - XOHO_in_Urine -
XPAO_in_Urine - XMEOLO_in_Urine - XAOB_in_Urine - XNOB_in_Urine -
XAMX_in_Urine - XAMETO_in_Urine - XHMETO_in_Urine;

```

$SU_{in\_Urine} = (Total\_COD\_SepUrine * TCOD_{inert\_TCOD\_Urine} / Q_{perPE\_SeparatedUrine} * 1000) - XU_{in\_Urine} - CU_{in\_Urine};$   
 $SB_{in\_Urine} = (COD_{sol\_gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000) - SVFA_{in\_Urine} - SMEOL_{in\_Urine} - SU_{in\_Urine};$

$SNHx_{in\_Urine} = SNH_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000;$   
 $SNO3_{in\_Urine} = SNO3\_NOx_{Urine} * NOx_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000;$   
 $SNO2_{in\_Urine} = (NOx_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000) - SNO3_{in\_Urine};$   
 $CNB_{in\_Urine} = CNB\_TKN_{Urine} * TKN_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000;$   
 $XNB_{in\_Urine} = XNB\_TKN_{Urine} * TKN_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000;$   
 $CNU_{in\_Urine} = CNU\_TKN_{Urine} * TKN_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000;$   
 $XNU_{in\_Urine} = XNU\_TKN_{Urine} * TKN_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000;$   
 $SNU_{in\_Urine} = (TKN_{gperPEperd\_SepUrine} * TKN_{inert\_TKN_{Urine}} / Q_{perPE\_SeparatedUrine} * 1000) - XNU_{in\_Urine} - CNU_{in\_Urine};$   
 $SNB_{in\_Urine} = (TKN_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000) - SNHx_{in\_Urine} - SNO2_{in\_Urine} - SNO3_{in\_Urine} - CNB_{in\_Urine} - CNU_{in\_Urine} - XNB_{in\_Urine} - XNU_{in\_Urine} - SNU_{in\_Urine};$

$SPO4_{in\_Urine} = PO4_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000;$   
 $CPB_{in\_Urine} = CPB\_TP_{Urine} * TP_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000;$   
 $XPB_{in\_Urine} = XPB\_TP_{Urine} * TP_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000;$   
 $CPU_{in\_Urine} = CPU\_TP_{Urine} * TP_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000;$   
 $XPU_{in\_Urine} = XPU\_TP_{Urine} * TP_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000;$   
 $SPU_{in\_Urine} = (TP_{gperPEperd\_SepUrine} * TP_{inert\_TP_{Urine}} / Q_{perPE\_SeparatedUrine} * 1000) - XPU_{in\_Urine} - CPU_{in\_Urine};$

$SPB_{in\_Urine} = (TP_{gperPEperd\_SepUrine} / Q_{perPE\_SeparatedUrine} * 1000) - SPO4_{in\_Urine} - CPB_{in\_Urine} - CPU_{in\_Urine} - XPB_{in\_Urine} - XPU_{in\_Urine} - SPU_{in\_Urine};$

$TIC_{in\_Urine} = TIC\_SNHx_{Urine} * SNHx_{in\_Urine};$   
 $Ca_{in\_Urine} = Ca\_SNHx_{Urine} * SNHx_{in\_Urine};$   
 $Mg_{in\_Urine} = Mg\_SNHx_{Urine} * SNHx_{in\_Urine};$   
 $Na_{in\_Urine} = Na\_SNHx_{Urine} * SNHx_{in\_Urine};$   
 $Cl_{in\_Urine} = Cl\_SNHx_{Urine} * SNHx_{in\_Urine};$

%Others

$Contrib\_Other\_Q = 0.25;$   
 $Q_{perPE\_av} = (Q_{perPE\_WoUrine} + ((Q_{Ind\_weekday} * 1000) / PE)) + (Contrib\_Other\_Q * Q_{perPE\_Household} / (1 - Contrib\_Other\_Q));$

$SVFA_{in} = SVFA\_COD_{sol} * (COD_{sol\_gperPEperd\_woUrine} + COD_{sol\_gperPEperd\_Ind}) / (Q_{perPE\_av} * 1000);$   
 $SMEOL_{in} = SMEOL\_COD_{sol} * (COD_{sol\_gperPEperd\_woUrine} + COD_{sol\_gperPEperd\_Ind}) / (Q_{perPE\_av} * 1000);$   
 $CB_{in} = CB\_COD_{part} * (COD_{part\_gperPEperd\_woUrine} + COD_{part\_gperPEperd\_Ind}) / (Q_{perPE\_av} * 1000);$   
 $CU_{in} = CU\_COD_{part} * (COD_{part\_gperPEperd\_woUrine} + COD_{part\_gperPEperd\_Ind}) / (Q_{perPE\_av} * 1000);$   
 $XU_{in} = XU\_COD_{part} * (COD_{part\_gperPEperd\_woUrine} + COD_{part\_gperPEperd\_Ind}) / (Q_{perPE\_av} * 1000);$   
 $XE_{in} = XE\_COD_{part} * (COD_{part\_gperPEperd\_woUrine} + COD_{part\_gperPEperd\_Ind}) / (Q_{perPE\_av} * 1000);$   
 $XOHO_{in} = XOHO\_COD_{part} * (COD_{part\_gperPEperd\_woUrine} + COD_{part\_gperPEperd\_Ind}) / (Q_{perPE\_av} * 1000);$   
 $XPAO_{in} = XOtherBiomass\_COD_{part} * (COD_{part\_gperPEperd\_woUrine} + COD_{part\_gperPEperd\_Ind}) / (Q_{perPE\_av} * 1000);$

Supplementary Information

## Supplementary Information

$XMEOLO\_in =$   
 $XOtherBiomass\_CODpart * (CODpart\_gperPEperd\_woUrine + CODpart\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $XAOB\_in =$   
 $XOtherBiomass\_CODpart * (CODpart\_gperPEperd\_woUrine + CODpart\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $XNOB\_in =$   
 $XOtherBiomass\_CODpart * (CODpart\_gperPEperd\_woUrine + CODpart\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $XAMX\_in =$   
 $XOtherBiomass\_CODpart * (CODpart\_gperPEperd\_woUrine + CODpart\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $XAMETO\_in =$   
 $XOtherBiomass\_CODpart * (CODpart\_gperPEperd\_woUrine + CODpart\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $XHMETO\_in =$   
 $XOtherBiomass\_CODpart * (CODpart\_gperPEperd\_woUrine + CODpart\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $XB\_in =$   
 $((CODpart\_gperPEperd\_woUrine + CODpart\_gperPEperd\_Ind) / (QperPE\_av) * 1000)$   
 $- CB\_in - CU\_in - XU\_in - XE\_in - XOHO\_in - XPAO\_in - XMEOLO\_in -$   
 $XAOB\_in - XNOB\_in - XAMX\_in - XAMETO\_in - XHMETO\_in;$   
 $SU\_in = ((Total\_COD\_woUrine + TotalCOD\_Ind) *$   
 $TCODinert\_TCOD / (QperPE\_av) * 1000) - XU\_in - CU\_in;$   
 $SB\_in =$   
 $((CODsol\_gperPEperd\_woUrine + CODsol\_gperPEperd\_Ind) / (QperPE\_av) * 1000)$   
 $- SVFA\_in - SMEOL\_in - SU\_in;$   
  
 $SNHx\_in =$   
 $(SNH\_gperPEperd\_woUrine + SNH\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $SNO3\_in =$   
 $SNO3\_NOx * (NOx\_gperPEperd\_woUrine + NOx\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $SNO2\_in =$   
 $((NOx\_gperPEperd\_woUrine + NOx\_gperPEperd\_Ind) / (QperPE\_av) * 1000) -$   
 $SNO3\_in;$   
 $CNB\_in =$   
 $CNB\_TKN * (TKN\_gperPEperd\_woUrine + TKN\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$

$XNB\_in =$   
 $XNB\_TKN * (TKN\_gperPEperd\_woUrine + TKN\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $CNU\_in =$   
 $CNU\_TKN * (TKN\_gperPEperd\_woUrine + TKN\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $XNU\_in =$   
 $XNU\_TKN * (TKN\_gperPEperd\_woUrine + TKN\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $SNU\_in = ((TKN\_gperPEperd\_woUrine + TKN\_gperPEperd\_Ind) * TKNinert\_TKN / (QperPE\_av) * 1000) - XNU\_in - CNU\_in;$   
 $SNB\_in =$   
 $((TKN\_gperPEperd\_woUrine + TKN\_gperPEperd\_Ind) / (QperPE\_av) * 1000) -$   
 $SNHx\_in - SNO2\_in - SNO3\_in - CNB\_in - CNU\_in - XNB\_in - XNU\_in -$   
 $SNU\_in;$   
  
 $SPO4\_in =$   
 $(PO4\_gperPEperd\_woUrine + PO4\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $CPB\_in =$   
 $CPB\_TP * (TP\_gperPEperd\_woUrine + TP\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $XPB\_in =$   
 $XPB\_TP * (TP\_gperPEperd\_woUrine + TP\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $CPU\_in =$   
 $CPU\_TP * (TP\_gperPEperd\_woUrine + TP\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $XPU\_in =$   
 $XPU\_TP * (TP\_gperPEperd\_woUrine + TP\_gperPEperd\_Ind) / (QperPE\_av) * 1000;$   
 $SPU\_in = ((TP\_gperPEperd\_woUrine + TP\_gperPEperd\_Ind) * TPinert\_TP / (QperPE\_av) * 1000) - XPU\_in - CPU\_in;$   
 $SPB\_in = ((TP\_gperPEperd\_woUrine + TP\_gperPEperd\_Ind) / (QperPE\_av) * 1000) -$   
 $SPO4\_in - CPB\_in - CPU\_in - XPB\_in - XPU\_in - SPU\_in;$   
  
 $TIC\_in = TIC\_SNHx * SNHx\_in;$   
 $Ca\_in = Ca\_SNHx * SNHx\_in;$   
 $Mg\_in = Mg\_SNHx * SNHx\_in;$   
 $Na\_in = Na\_SNHx * SNHx\_in;$   
 $Cl\_in = Cl\_SNHx * SNHx\_in;$   
  
 $TSS\_in = COD\_TSS * (XB\_in + XU\_in + XOHO\_in + XPAO\_in + XMEOLO\_in + XAOB\_in + XNOB\_in + XAMX\_in + XAMETO\_in + XHMETO\_in + XE\_in);$

```

% Noise Others
factorVariables = 0.1;

SVFA_ns = 13122;
SVFA_nv = (factorVariables*(SVFA_in))^2;
SVFA_st = 1/sampling;
SVFA_max = 100*SVFA_in;
SVFA_min = 1E-50;

SB_ns = 13123;
SB_nv = (factorVariables*(SB_in))^2;
SB_st = 1/sampling;
SB_max = 100*SB_in;
SB_min = 1E-50;

SMEOL_ns = 13124;
SMEOL_nv = (factorVariables*(SMEOL_in))^2;
SMEOL_st = 1/sampling;
SMEOL_max = 100*SMEOL_in;
SMEOL_min = 1E-50;

CB_ns = 13125;
CB_nv = (factorVariables*(CB_in))^2;
CB_st = 1/sampling;
CB_max = 100*CB_in;
CB_min = 1E-50;

XB_ns = 13126;
XB_nv = (factorVariables*(XB_in))^2;
XB_st = 1/sampling;
XB_max = 100*XB_in;
XB_min = 1E-50;

SU_ns = 13127;
SU_nv = (factorVariables*(SU_in))^2;
SU_st = 1/sampling;
SU_max = 100*SU_in;
SU_min = 1E-50;

```

```

CU_ns = 13128;
CU_nv = (factorVariables*(CU_in))^2;
CU_st = 1/sampling;
CU_max = 100*CU_in;
CU_min = 1E-50;

XU_ns = 13129;
XU_nv = (factorVariables*(XU_in))^2;
XU_st = 1/sampling;
XU_max = 100*XU_in;
XU_min = 1E-50;

XE_ns = 13130;
XE_nv = (factorVariables*(XE_in))^2;
XE_st = 1/sampling;
XE_max = 100*XE_in;
XE_min = 1E-50;

XOHO_ns = 13131;
XOHO_nv = (factorVariables*(XOHO_in))^2;
XOHO_st = 1/sampling;
XOHO_max = 100*XOHO_in;
XOHO_min = 1E-50;

XPAO_ns = 13132;
XPAO_nv = (factorVariables*(XPAO_in))^2;
XPAO_st = 1/sampling;
XPAO_max = 100*XPAO_in;
XPAO_min = 1E-50;

XMEOLO_ns = 13133;
XMEOLO_nv = (factorVariables*(XMEOLO_in))^2;
XMEOLO_st = 1/sampling;
XMEOLO_max = 100*XMEOLO_in;
XMEOLO_min = 1E-50;

XAOB_ns = 13134;
XAOB_nv = (factorVariables*(XAOB_in))^2;

```

Supplementary Information

## Supplementary Information

```

XAOB_st = 1/sampling;
XAOB_max = 100*XAOB_in;
XAOB_min = 1E-50;

XNOB_ns = 13135;
XNOB_nv = (factorVariables*(XNOB_in))^2;
XNOB_st = 1/sampling;
XNOB_max = 100*XNOB_in;
XNOB_min = 1E-50;

XAMX_ns = 13136;
XAMX_nv = (factorVariables*(XAMX_in))^2;
XAMX_st = 1/sampling;
XAMX_max = 100*XAMX_in;
XAMX_min = 1E-50;

XAMETO_ns = 13137;
XAMETO_nv = (factorVariables*(XAMETO_in))^2;
XAMETO_st = 1/sampling;
XAMETO_max = 100*XAMETO_in;
XAMETO_min = 1E-50;

XHMETO_ns = 13138;
XHMETO_nv = (factorVariables*(XHMETO_in))^2;
XHMETO_st = 1/sampling;
XHMETO_max = 100*XHMETO_in;
XHMETO_min = 1E-50;

SNHx_ns = 13139;
SNHx_nv = (factorVariables*(SNHx_in))^2;
SNHx_st = 1/sampling;
SNHx_max = 100*SNHx_in;
SNHx_min = 1E-50;

SNO2_ns = 13140;
SNO2_nv = (factorVariables*(SNO2_in))^2;
SNO2_st = 1/sampling;
SNO2_max = 100*SNO2_in;
SNO2_min = 1E-50;

```

```

SNO3_ns = 13141;
SNO3_nv = (factorVariables*(SNO3_in))^2;
SNO3_st = 1/sampling;
SNO3_max = 100*SNO3_in;
SNO3_min = 1E-50;

SNB_ns = 13142;
SNB_nv = (factorVariables*(SNB_in))^2;
SNB_st = 1/sampling;
SNB_max = 100*SNB_in;
SNB_min = 1E-50;

CNB_ns = 13143;
CNB_nv = (factorVariables*(CNB_in))^2;
CNB_st = 1/sampling;
CNB_max = 100*CNB_in;
CNB_min = 1E-50;

XNB_ns = 13144;
XNB_nv = (factorVariables*(XNB_in))^2;
XNB_st = 1/sampling;
XNB_max = 100*XNB_in;
XNB_min = 1E-50;

SNU_ns = 13145;
SNU_nv = (factorVariables*(SNU_in))^2;
SNU_st = 1/sampling;
SNU_max = 100*SNU_in;
SNU_min = 1E-50;

CNU_ns = 13146;
CNU_nv = (factorVariables*(CNU_in))^2;
CNU_st = 1/sampling;
CNU_max = 100*CNU_in;
CNU_min = 1E-50;

XNU_ns = 13147;
XNU_nv = (factorVariables*(XNU_in))^2;

```

```

XNU_st = 1/sampling;
XNU_max = 100*XNU_in;
XNU_min = 1E-50;

SPO4_ns = 13148;
SPO4_nv = (factorVariables*(SPO4_in))^2;
SPO4_st = 1/sampling;
SPO4_max = 100*SPO4_in;
SPO4_min = 1E-50;

SPB_ns = 13149;
SPB_nv = (factorVariables*(SPB_in))^2;
SPB_st = 1/sampling;
SPB_max = 100*SPB_in;
SPB_min = 1E-50;

CPB_ns = 13150;
CPB_nv = (factorVariables*(CPB_in))^2;
CPB_st = 1/sampling;
CPB_max = 100*CPB_in;
CPB_min = 1E-50;

XPB_ns = 13151;
XPB_nv = (factorVariables*(XPB_in))^2;
XPB_st = 1/sampling;
XPB_max = 100*XPB_in;
XPB_min = 1E-50;

SPU_ns = 13152;
SPU_nv = (factorVariables*(SPU_in))^2;
SPU_st = 1/sampling;
SPU_max = 100*SPU_in;
SPU_min = 1E-50;

CPU_ns = 13153;
CPU_nv = (factorVariables*(CPU_in))^2;
CPU_st = 1/sampling;
CPU_max = 100*CPU_in;
CPU_min = 1E-50;

```

```

XPU_ns = 13154;
XPU_nv = (factorVariables*(XPU_in))^2;
XPU_st = 1/sampling;
XPU_max = 100*XPU_in;
XPU_min = 1E-50;

TIC_ns = 13155;
TIC_nv = (factorVariables*(TIC_in))^2;
TIC_st = 1/sampling;
TIC_max = 100*TIC_in;
TIC_min = 1E-50;

Ca_ns = 13156;
Ca_nv = (factorVariables*(Ca_in))^2;
Ca_st = 1/sampling;
Ca_max = 100*Ca_in;
Ca_min = 1E-50;

Mg_ns = 13157;
Mg_nv = (factorVariables*(Mg_in))^2;
Mg_st = 1/sampling;
Mg_max = 100*Mg_in;
Mg_min = 1E-50;

Na_ns = 13158;
Na_nv = (factorVariables*(Na_in))^2;
Na_st = 1/sampling;
Na_max = 100*Na_in;
Na_min = 1E-50;

Cl_ns = 13159;
Cl_nv = (factorVariables*(Cl_in))^2;
Cl_st = 1/sampling;
Cl_max = 100*Cl_in;
Cl_min = 1E-50;

polnoisewitch = all_noises;

```

Supplementary Information

## Supplementary Information

```
% Noise Urine
factorVariables_Urine = 0.01;
```

```
SVFA_ns_Urine = 13222;
SVFA_nv_Urine = (factorVariables_Urine*(SVFA_in_Urine))^2;
SVFA_st_Urine = 1/sampling;
SVFA_max_Urine = 100*SVFA_in_Urine;
SVFA_min_Urine = 1E-50;
```

```
SB_ns_Urine = 13223;
SB_nv_Urine = (factorVariables_Urine*(SB_in_Urine))^2;
SB_st_Urine = 1/sampling;
SB_max_Urine = 100*SB_in_Urine;
SB_min_Urine = 1E-50;
```

```
SMEOL_ns_Urine = 13224;
SMEOL_nv_Urine = (factorVariables_Urine*(SMEOL_in_Urine))^2;
SMEOL_st_Urine = 1/sampling;
SMEOL_max_Urine = 100*SMEOL_in_Urine;
SMEOL_min_Urine = 1E-50;
```

```
CB_ns_Urine = 13225;
CB_nv_Urine = (factorVariables_Urine*(CB_in_Urine))^2;
CB_st_Urine = 1/sampling;
CB_max_Urine = 100*CB_in_Urine;
CB_min_Urine = 1E-50;
```

```
XB_ns_Urine = 13226;
XB_nv_Urine = (factorVariables_Urine*(XB_in_Urine))^2;
XB_st_Urine = 1/sampling;
XB_max_Urine = 100*XB_in_Urine;
XB_min_Urine = 1E-50;
```

```
SU_ns_Urine = 13227;
SU_nv_Urine = (factorVariables_Urine*(SU_in_Urine))^2;
SU_st_Urine = 1/sampling;
SU_max_Urine = 100*SU_in_Urine;
SU_min_Urine = 1E-50;
```

```
CU_ns_Urine = 13228;
CU_nv_Urine = (factorVariables_Urine*(CU_in_Urine))^2;
CU_st_Urine = 1/sampling;
CU_max_Urine = 100*CU_in_Urine;
CU_min_Urine = 1E-50;
```

```
XU_ns_Urine = 13229;
XU_nv_Urine = (factorVariables_Urine*(XU_in_Urine))^2;
XU_st_Urine = 1/sampling;
XU_max_Urine = 100*XU_in_Urine;
XU_min_Urine = 1E-50;
```

```
XE_ns_Urine = 13230;
XE_nv_Urine = (factorVariables_Urine*(XE_in_Urine))^2;
XE_st_Urine = 1/sampling;
XE_max_Urine = 100*XE_in_Urine;
XE_min_Urine = 1E-50;
```

```
XOHO_ns_Urine = 13231;
XOHO_nv_Urine = (factorVariables_Urine*(XOHO_in_Urine))^2;
XOHO_st_Urine = 1/sampling;
XOHO_max_Urine = 100*XOHO_in_Urine;
XOHO_min_Urine = 1E-50;
```

```
XPAO_ns_Urine = 13232;
XPAO_nv_Urine = (factorVariables_Urine*(XPAO_in_Urine))^2;
XPAO_st_Urine = 1/sampling;
XPAO_max_Urine = 100*XPAO_in_Urine;
XPAO_min_Urine = 1E-50;
```

```
XMEOLO_ns_Urine = 13233;
XMEOLO_nv_Urine = (factorVariables_Urine*(XMEOLO_in_Urine))^2;
XMEOLO_st_Urine = 1/sampling;
XMEOLO_max_Urine = 100*XMEOLO_in_Urine;
XMEOLO_min_Urine = 1E-50;
```

```
XAOB_ns_Urine = 13234;
XAOB_nv_Urine = (factorVariables_Urine*(XAOB_in_Urine))^2;
XAOB_st_Urine = 1/sampling;
```

XAOB\_max\_Urine = 100\*XAOB\_in\_Urine;  
 XAOB\_min\_Urine = 1E-50;  
  
 XNOB\_ns\_Urine = 13235;  
 XNOB\_nv\_Urine = (factorVariables\_Urine\*(XNOB\_in\_Urine))^2;  
 XNOB\_st\_Urine = 1/sampling;  
 XNOB\_max\_Urine = 100\*XNOB\_in\_Urine;  
 XNOB\_min\_Urine = 1E-50;  
  
 XAMX\_ns\_Urine = 13236;  
 XAMX\_nv\_Urine = (factorVariables\_Urine\*(XAMX\_in\_Urine))^2;  
 XAMX\_st\_Urine = 1/sampling;  
 XAMX\_max\_Urine = 100\*XAMX\_in\_Urine;  
 XAMX\_min\_Urine = 1E-50;  
  
 XAMETO\_ns\_Urine = 13237;  
 XAMETO\_nv\_Urine = (factorVariables\_Urine\*(XAMETO\_in\_Urine))^2;  
 XAMETO\_st\_Urine = 1/sampling;  
 XAMETO\_max\_Urine = 100\*XAMETO\_in\_Urine;  
 XAMETO\_min\_Urine = 1E-50;  
  
 XHMETO\_ns\_Urine = 13238;  
 XHMETO\_nv\_Urine = (factorVariables\_Urine\*(XHMETO\_in\_Urine))^2;  
 XHMETO\_st\_Urine = 1/sampling;  
 XHMETO\_max\_Urine = 100\*XHMETO\_in\_Urine;  
 XHMETO\_min\_Urine = 1E-50;  
  
 SNHx\_ns\_Urine = 13239;  
 SNHx\_nv\_Urine = (factorVariables\_Urine\*(SNHx\_in\_Urine))^2;  
 SNHx\_st\_Urine = 1/sampling;  
 SNHx\_max\_Urine = 100\*SNHx\_in\_Urine;  
 SNHx\_min\_Urine = 1E-50;  
  
 SNO2\_ns\_Urine = 13240;  
 SNO2\_nv\_Urine = (factorVariables\_Urine\*(SNO2\_in\_Urine))^2;  
 SNO2\_st\_Urine = 1/sampling;  
 SNO2\_max\_Urine = 100\*SNO2\_in\_Urine;  
 SNO2\_min\_Urine = 1E-50;

SNO3\_ns\_Urine = 13241;  
 SNO3\_nv\_Urine = (factorVariables\_Urine\*(SNO3\_in\_Urine))^2;  
 SNO3\_st\_Urine = 1/sampling;  
 SNO3\_max\_Urine = 100\*SNO3\_in\_Urine;  
 SNO3\_min\_Urine = 1E-50;  
  
 SNB\_ns\_Urine = 13242;  
 SNB\_nv\_Urine = (factorVariables\_Urine\*(SNB\_in\_Urine))^2;  
 SNB\_st\_Urine = 1/sampling;  
 SNB\_max\_Urine = 100\*SNB\_in\_Urine;  
 SNB\_min\_Urine = 1E-50;  
  
 CNB\_ns\_Urine = 13243;  
 CNB\_nv\_Urine = (factorVariables\_Urine\*(CNB\_in\_Urine))^2;  
 CNB\_st\_Urine = 1/sampling;  
 CNB\_max\_Urine = 100\*CNB\_in\_Urine;  
 CNB\_min\_Urine = 1E-50;  
  
 XNB\_ns\_Urine = 13244;  
 XNB\_nv\_Urine = (factorVariables\_Urine\*(XNB\_in\_Urine))^2;  
 XNB\_st\_Urine = 1/sampling;  
 XNB\_max\_Urine = 100\*XNB\_in\_Urine;  
 XNB\_min\_Urine = 1E-50;  
  
 SNU\_ns\_Urine = 13245;  
 SNU\_nv\_Urine = (factorVariables\_Urine\*(SNU\_in\_Urine))^2;  
 SNU\_st\_Urine = 1/sampling;  
 SNU\_max\_Urine = 100\*SNU\_in\_Urine;  
 SNU\_min\_Urine = 1E-50;  
  
 CNU\_ns\_Urine = 13246;  
 CNU\_nv\_Urine = (factorVariables\_Urine\*(CNU\_in\_Urine))^2;  
 CNU\_st\_Urine = 1/sampling;  
 CNU\_max\_Urine = 100\*CNU\_in\_Urine;  
 CNU\_min\_Urine = 1E-50;  
  
 XNU\_ns\_Urine = 13247;  
 XNU\_nv\_Urine = (factorVariables\_Urine\*(XNU\_in\_Urine))^2;  
 XNU\_st\_Urine = 1/sampling;

Supplementary Information

## Supplementary Information

```
XNU_max_Urine = 100*XNU_in_Urine;
XNU_min_Urine = 1E-50;
```

```
SPO4_ns_Urine = 13248;
SPO4_nv_Urine = (factorVariables_Urine*(SPO4_in_Urine))^2;
SPO4_st_Urine = 1/sampling;
SPO4_max_Urine = 100*SPO4_in_Urine;
SPO4_min_Urine = 1E-50;
```

```
SPB_ns_Urine = 13249;
SPB_nv_Urine = (factorVariables_Urine*(SPB_in_Urine))^2;
SPB_st_Urine = 1/sampling;
SPB_max_Urine = 100*SPB_in_Urine;
SPB_min_Urine = 1E-50;
```

```
CPB_ns_Urine = 13250;
CPB_nv_Urine = (factorVariables_Urine*(CPB_in_Urine))^2;
CPB_st_Urine = 1/sampling;
CPB_max_Urine = 100*CPB_in_Urine;
CPB_min_Urine = 1E-50;
```

```
XPB_ns_Urine = 13251;
XPB_nv_Urine = (factorVariables_Urine*(XPB_in_Urine))^2;
XPB_st_Urine = 1/sampling;
XPB_max_Urine = 100*XPB_in_Urine;
XPB_min_Urine = 1E-50;
```

```
SPU_ns_Urine = 13252;
SPU_nv_Urine = (factorVariables_Urine*(SPU_in_Urine))^2;
SPU_st_Urine = 1/sampling;
SPU_max_Urine = 100*SPU_in_Urine;
SPU_min_Urine = 1E-50;
```

```
CPU_ns_Urine = 13253;
CPU_nv_Urine = (factorVariables_Urine*(CPU_in_Urine))^2;
CPU_st_Urine = 1/sampling;
CPU_max_Urine = 100*CPU_in_Urine;
CPU_min_Urine = 1E-50;
```

```
XPU_ns_Urine = 13254;
XPU_nv_Urine = (factorVariables_Urine*(XPU_in_Urine))^2;
XPU_st_Urine = 1/sampling;
XPU_max_Urine = 100*XPU_in_Urine;
XPU_min_Urine = 1E-50;
```

```
TIC_ns_Urine = 13255;
TIC_nv_Urine = (factorVariables_Urine*(TIC_in_Urine))^2;
TIC_st_Urine = 1/sampling;
TIC_max_Urine = 100*TIC_in_Urine;
TIC_min_Urine = 1E-50;
```

```
Ca_ns_Urine = 13256;
Ca_nv_Urine = (factorVariables_Urine*(Ca_in_Urine))^2;
Ca_st_Urine = 1/sampling;
Ca_max_Urine = 100*Ca_in_Urine;
Ca_min_Urine = 1E-50;
```

```
Mg_ns_Urine = 13257;
Mg_nv_Urine = (factorVariables_Urine*(Mg_in_Urine))^2;
Mg_st_Urine = 1/sampling;
Mg_max_Urine = 100*Mg_in_Urine;
Mg_min_Urine = 1E-50;
```

```
Na_ns_Urine = 13258;
Na_nv_Urine = (factorVariables_Urine*(Na_in_Urine))^2;
Na_st_Urine = 1/sampling;
Na_max_Urine = 100*Na_in_Urine;
Na_min_Urine = 1E-50;
```

```
Cl_ns_Urine = 13259;
Cl_nv_Urine = (factorVariables_Urine*(Cl_in_Urine))^2;
Cl_st_Urine = 1/sampling;
Cl_max_Urine = 100*Cl_in_Urine;
Cl_min_Urine = 1E-50;
```

```
polnoiseswitch_Urine = all_noises;
%% 9. First flush effect
```

```

FFfraction = 0.25;           % Fraction of the TSS that is able to settle
in the sewers

% State values
FF_XINIT=[TSS_in XB_in XU_in XE_in XOHO_in XPAO_in XMEOLO_in
XAOB_in XNOB_in XAMX_in XAMETO_in XHMETO_in XNB_in XNU_in
XPB_in XPU_in]; % Initial conditions (7 states) XINIT= [TSS XI XS
XBH XBA XP XND]

% Parameters
M_Max = 1000;               % kg SS
Q_lim = 70000;             % m3/d
n = 15;                    % Dimensionless
Ff = 500;                  % Dimensionless, gain
SSPARS=[M_Max Q_lim n Ff];

%% 10. Sewer model

subarea = 4;

% Initialisation of the individual sewer model blocks
VARS_SEWERINIT =[zeros(1,39) 0.001];

% Parameters for individual sewer model block S-functions
A=1100;                    % Area (m2)
C=150000;                 % Tuning constant
Hmin=0.00;                % Minimum water level in tank
SPAR = [A C Hmin];

%% 11 Parameters temperature model block
TAmp = 5;                 % Sine wave amplitude (deg. C)
TBias = 15;               % Sine wave bias (m3/d) (= average
infiltration flow rate)
TFreq = 2*pi/364;         % Sine wave frequency (rad/d)
TPhase = pi*8.5/24;      % Sine wave phase shift

TdAmp = 0.5;              % Sine wave amplitude (deg. C)
TdBias = 0;               % Sine wave bias (m3/d) (= average
infiltration flow rate)

```

```

TdFreq = 2*pi;           % Sine wave frequency (rad/d)
TdPhase = pi*0.8;        % Sine wave phase shift

%% 12 Profiles
QdayHS_SeparatedUrine = struct('signals'
,struct('values',(SNH_day_HS.signals.values - 1) * 0.4 + 1), 'time', []);
QdayHS_woUrine = struct('signals',struct('values',Q_day_HS.signals.values),
'time', []);

CODsoldayHS_SeparatedUrine = struct('signals'
,struct('values',(CODsol_day_HS.signals.values - 1) * 0.4 + 1), 'time', []);
CODsoldayHS_woUrine = struct('signals'
,struct('values',CODsol_day_HS.signals.values), 'time', []);

CODpartdayHS_SeparatedUrine = struct('signals'
,struct('values',(CODpart_day_HS.signals.values - 1) * 0.4 + 1), 'time', []);
CODpartdayHS_woUrine = struct('signals'
,struct('values',CODpart_day_HS.signals.values), 'time', []);

TKNdayHS_SeparatedUrine = struct('signals'
,struct('values',(TKN_day_HS.signals.values - 1) * 0.4 + 1), 'time', []);
TKNdayHS_woUrine = struct('signals'
,struct('values',TKN_day_HS.signals.values), 'time', []);

SNHdayHS_SeparatedUrine = struct('signals'
,struct('values',(SNH_day_HS.signals.values - 1) * 0.4 + 1), 'time', []);
SNHdayHS_woUrine = struct('signals'
,struct('values',SNH_day_HS.signals.values), 'time', []);

TPdayHS_SeparatedUrine = struct('signals'
,struct('values',(TP_day_HS.signals.values - 1) * 0.4 + 1), 'time', []);
TPdayHS_woUrine = struct('signals',struct('values',TP_day_HS.signals.values),
'time', []);

PO4dayHS_SeparatedUrine = struct('signals'
,struct('values',(PO4_day_HS.signals.values - 1) * 0.4 + 1), 'time', []);
PO4dayHS_woUrine = struct('signals'
,struct('values',PO4_day_HS.signals.values), 'time', []);

```

## C. Supplementary Information for chapters IV and V

### C.1. Adapted Sumo2 Gujer matrix

The original Sumo2 Gujer matrix was developed by Dynamita. For more details, please refer to [www.dynamita.com/the-sumo/](http://www.dynamita.com/the-sumo/)

	Name	Unit
$S_{VFA}$	VFAs	g COD.m <sup>-3</sup>
$S_B$	Readily biodegradable substrate (non-VFA)	g COD.m <sup>-3</sup>
$S_{MEOL}$	Methanol	g COD.m <sup>-3</sup>
$C_B$	Colloidal biodegradable substrate	g COD.m <sup>-3</sup>
$X_B$	Slowly biodegradable substrate	g COD.m <sup>-3</sup>
$S_U$	Soluble unbiodegradable organics	g COD.m <sup>-3</sup>
$C_U$	Colloidal unbiodegradable organics	g COD.m <sup>-3</sup>
$X_U$	Particulate unbiodegradable organics	g COD.m <sup>-3</sup>
$X_{PHA}$	Stored PHA	g COD.m <sup>-3</sup>
$X_E$	Endogenous decay products	g COD.m <sup>-3</sup>
$X_{OHO}$	Ordinary heterotrophs	g COD.m <sup>-3</sup>
$X_{PAO}$	Phosphorus accumulating organisms	g COD.m <sup>-3</sup>
$X_{MEOLO}$	Anoxic methanol utilizers	g COD.m <sup>-3</sup>
$X_{AOB}$	Aerobic ammonia oxidizers	g COD.m <sup>-3</sup>
$X_{NOB}$	Nitrite oxidizers	g COD.m <sup>-3</sup>
$X_{AMX}$	Anammox organisms	g COD.m <sup>-3</sup>
$X_{AMETO}$	Acidoclastic methanogens (VFA)	g COD.m <sup>-3</sup>

$X_{HMETO}$	Hydrogenotrophic methanogens	g COD.m <sup>-3</sup>
$S_{NHx}$	Total ammonia	g N.m <sup>-3</sup>
$S_{NO2}$	Nitrite	g N.m <sup>-3</sup>
$S_{NO3}$	Nitrate	g N.m <sup>-3</sup>
$S_{N2}$	Dissolved Nitrogen	g N.m <sup>-3</sup>
$S_{N,B}$	Soluble biodegradable organic N (from $S_B$ )	g N.m <sup>-3</sup>
$C_{N,B}$	Colloidal biodegradable organic N	g N.m <sup>-3</sup>
$X_{N,B}$	Particulate biodegradable organic N	g N.m <sup>-3</sup>
$S_{N,U}$	Soluble unbiodegradable organic N	g N.m <sup>-3</sup>
$C_{N,U}$	Colloidal unbiodegradable organic N	g N.m <sup>-3</sup>
$X_{N,U}$	Particulate unbiodegradable organic N	g N.m <sup>-3</sup>
$S_{PO4}$	Orthophosphate	g P.m <sup>-3</sup>
$X_{PP,LO}$	Releasable stored polyphosphate	g P.m <sup>-3</sup>
$X_{PP,HI}$	Non-releasable stored polyphosphate	g P.m <sup>-3</sup>
$S_{P,B}$	Soluble biodegradable organic P (from $S_B$ )	g P.m <sup>-3</sup>
$C_{P,B}$	Colloidal biodegradable organic P	g P.m <sup>-3</sup>
$X_{P,B}$	Particulate biodegradable organic P	g P.m <sup>-3</sup>
$S_{P,U}$	Soluble unbiodegradable organic P content	g P.m <sup>-3</sup>

<b>C<sub>P,U</sub></b>	Colloidal unbiodegradable organic P content	g P.m <sup>-3</sup>
<b>X<sub>P,U</sub></b>	Particulate unbiodegradable organic P content	g P.m <sup>-3</sup>
<b>S<sub>O2</sub></b>	Dissolved oxygen	g O <sub>2</sub> .m <sup>-3</sup>
<b>S<sub>CH4</sub></b>	Dissolved methane	g COD.m <sup>-3</sup>
<b>S<sub>H2</sub></b>	Dissolved hydrogen	g COD.m <sup>-3</sup>
<b>S<sub>CO2</sub></b>	Total inorganic carbon	g CO <sub>2</sub> .m <sup>-3</sup>
<b>X<sub>INORG</sub></b>	Inorganic suspended solids	g TSS.m <sup>-3</sup>
<b>S<sub>Mg</sub></b>	Magnesium	g Mg.m <sup>-3</sup>
<b>S<sub>Ca</sub></b>	Calcium	g Ca.m <sup>-3</sup>
<b>S<sub>CAT</sub></b>	Sodium (strong cation)	g.m <sup>-3</sup>
<b>S<sub>AN</sub></b>	Chloride (strong anion)	g.m <sup>-3</sup>
<b>S<sub>Fe</sub></b>	Soluble Fe	g Fe.m <sup>-3</sup>
<b>X<sub>HFO,L</sub></b>	Active, unused hydrous ferric oxide with low surface area	g Fe.m <sup>-3</sup>
<b>X<sub>HFO,H</sub></b>	Active, unused hydrous ferric oxide with high surface area	g Fe.m <sup>-3</sup>
<b>X<sub>HFO,L,P</sub></b>	Inactive, used hydrous ferric oxide with low surface area	g Fe.m <sup>-3</sup>
<b>X<sub>HFO,H,P</sub></b>	Inactive, used hydrous ferric oxide with high surface area	g Fe.m <sup>-3</sup>
<b>X<sub>HFO,H,P,old</sub></b>	Inert used HFO with high surface area	g Fe.m <sup>-3</sup>
<b>X<sub>HFO,L,P,old</sub></b>	Inert used HFO with low surface area	g Fe.m <sup>-3</sup>
<b>X<sub>HFO,old</sub></b>	Aged HFO from other four hydrous ferric oxide states	g Fe.m <sup>-3</sup>
<b>X<sub>STR</sub></b>	Struvite	g TSS.m <sup>-3</sup>
<b>G<sub>CO2</sub></b>	Carbon dioxide gas	ppm
<b>G<sub>CH4</sub></b>	Methane gas	ppm
<b>G<sub>H2</sub></b>	Hydrogen gas	ppm
<b>G<sub>O2</sub></b>	Oxygen gas	ppm
<b>G<sub>N2</sub></b>	Nitrogen gas	ppm

Supplementary Information



Ordinary heterotrophs organisms

	Name	S <sub>VFA</sub>	S <sub>B</sub>	S <sub>MEOL</sub>	X <sub>B</sub>	X <sub>E</sub>	X <sub>OHO</sub>	X <sub>MEOLO</sub>	S <sub>NHx</sub>	S <sub>NO2</sub>	S <sub>NO3</sub>	S <sub>N2</sub>	X <sub>N,B</sub>	S <sub>P04</sub>	X <sub>P,B</sub>	S <sub>O2</sub>	S <sub>H2</sub>	S <sub>CO2</sub>	X <sub>INORG</sub>	S <sub>CAT</sub>	S <sub>AN</sub>
r1	OHO growth on VFAs, O <sub>2</sub>	-1/Y <sub>OHO,VFA,O2</sub>					1		-i <sub>N,BIO</sub>					-ip <sub>BIO</sub>		-(1-Y <sub>OHO,VFA,O2</sub> )/Y <sub>OHO,VFA,O2</sub>		1.375*(1-Y <sub>OHO,VFA,O2</sub> )/Y <sub>OHO,VFA,O2</sub>	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )
r2	OHO growth on VFAs, NO <sub>2</sub>	-1/Y <sub>OHO,VFA,NOx</sub>					1		-i <sub>N,BIO</sub>	-(1-Y <sub>OHO,VFA,NOx</sub> )/(EEQ <sub>N2,NO2</sub> *Y <sub>OHO,VFA,NOx</sub> )		(1-Y <sub>OHO,VFA,NOx</sub> )/(EEQ <sub>N2,NO2</sub> *Y <sub>OHO,VFA,NOx</sub> )		-ip <sub>BIO</sub>				1.375*(1-Y <sub>OHO,VFA,NOx</sub> )/Y <sub>OHO,VFA,NOx</sub>	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )
r3	OHO growth on VFAs, NO <sub>3</sub>	-1/Y <sub>OHO,VFA,NOx</sub>					1		-i <sub>N,BIO</sub>	(1-Y <sub>OHO,VFA,NOx</sub> )/(EEQ <sub>NO2,NO3</sub> *Y <sub>OHO,VFA,NOx</sub> )	-(1-Y <sub>OHO,VFA,NOx</sub> )/(EEQ <sub>NO2,NO3</sub> *Y <sub>OHO,VFA,NOx</sub> )			-ip <sub>BIO</sub>				1.375*(1-Y <sub>OHO,VFA,NOx</sub> )/Y <sub>OHO,VFA,NOx</sub>	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )
r4	OHO growth on S <sub>B</sub> , O <sub>2</sub>		-1/Y <sub>OHO,SB,O2</sub>				1		-i <sub>N,BIO</sub>					-ip <sub>BIO</sub>		-(1-Y <sub>OHO,SB,O2</sub> )/Y <sub>OHO,SB,O2</sub>		1.375*(1-Y <sub>OHO,SB,O2</sub> )/Y <sub>OHO,SB,O2</sub>	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )
r5	OHO growth on S <sub>B</sub> , NO <sub>2</sub>		-1/Y <sub>OHO,SB,NOx</sub>				1		-i <sub>N,BIO</sub>	-(1-Y <sub>OHO,SB,NOx</sub> )/(EEQ <sub>N2,NO2</sub> *Y <sub>OHO,SB,NOx</sub> )		(1-Y <sub>OHO,SB,NOx</sub> )/(EEQ <sub>N2,NO2</sub> *Y <sub>OHO,SB,NOx</sub> )		-ip <sub>BIO</sub>				1.375*(1-Y <sub>OHO,SB,NOx</sub> )/Y <sub>OHO,SB,NOx</sub>	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )
r6	OHO growth on S <sub>B</sub> , NO <sub>3</sub>		-1/Y <sub>OHO,SB,NOx</sub>				1		-i <sub>N,BIO</sub>	(1-Y <sub>OHO,SB,NOx</sub> )/(EEQ <sub>NO2,NO3</sub> *Y <sub>OHO,SB,NOx</sub> )	-(1-Y <sub>OHO,SB,NOx</sub> )/(EEQ <sub>NO2,NO3</sub> *Y <sub>OHO,SB,NOx</sub> )			-ip <sub>BIO</sub>				1.375*(1-Y <sub>OHO,SB,NOx</sub> )/Y <sub>OHO,SB,NOx</sub>	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )
r7	S <sub>B</sub> fermentation (OHO growth, anaerobic)	(1-Y <sub>OHO,SB,ANA</sub> -Y <sub>OHO,H2,ANA</sub> )/Y <sub>OHO,SB,ANA</sub>	-1/Y <sub>OHO,SB,ANA</sub>				1		-i <sub>N,BIO</sub>					-ip <sub>BIO</sub>			Y <sub>OHO,H2,ANA</sub> /Y <sub>OHO,SB,ANA</sub>	f <sub>CHL,SB</sub> *1.375*Y <sub>OHO,CO2,ANA</sub> *(1-Y <sub>OHO,SB,ANA</sub> -Y <sub>OHO,H2,ANA</sub> )/Y <sub>OHO,SB,ANA</sub>	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )
r8	OHO growth on S <sub>MEOL</sub> , O <sub>2</sub>			-1/Y <sub>OHO,SMEOL,O2</sub>			1		-i <sub>N,BIO</sub>					-ip <sub>BIO</sub>		-(1-Y <sub>OHO,SMEOL,O2</sub> )/Y <sub>OHO,SMEOL,O2</sub>		1.375*(1-Y <sub>OHO,SMEOL,O2</sub> )/Y <sub>OHO,SMEOL,O2</sub>	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )
r9	OHO decay				1-f <sub>E</sub>	f <sub>E</sub>	-1						(1-f <sub>E</sub> )*i <sub>N,BIO</sub>		(1-f <sub>E</sub> )*ip <sub>BIO</sub>				-i <sub>IG</sub>	i <sub>IG</sub> *f <sub>Na</sub>	i <sub>IG</sub> *(1-f <sub>Na</sub> )
r10	MEOLO growth, NO <sub>2</sub>			-1/Y <sub>MEOLO</sub>				1	-i <sub>N,BIO</sub>	-(1-Y <sub>MEOLO</sub> )/(EEQ <sub>N2,NO2</sub> *Y <sub>MEOLO</sub> )		(1-Y <sub>MEOLO</sub> )/(EEQ <sub>N2,NO2</sub> *Y <sub>MEOLO</sub> )		-ip <sub>BIO</sub>				1.375*(1-Y <sub>MEOLO</sub> )/Y <sub>MEOLO</sub>	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )
r11	MEOLO growth, NO <sub>3</sub>			-1/Y <sub>MEOLO</sub>				1	-i <sub>N,BIO</sub>	(1-Y <sub>MEOLO</sub> )/(EEQ <sub>NO2,NO3</sub> *Y <sub>MEOLO</sub> )	-(1-Y <sub>MEOLO</sub> )/(EEQ <sub>NO2,NO3</sub> *Y <sub>MEOLO</sub> )			-ip <sub>BIO</sub>				1.375*(1-Y <sub>MEOLO</sub> )/Y <sub>MEOLO</sub>	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )
r12	MEOLO decay				1-f <sub>E</sub>	f <sub>E</sub>	-1						(1-f <sub>E</sub> )*i <sub>N,BIO</sub>		(1-f <sub>E</sub> )*ip <sub>BIO</sub>				-i <sub>IG</sub>	i <sub>IG</sub> *f <sub>Na</sub>	i <sub>IG</sub> *(1-f <sub>Na</sub> )

Rate expression (r <sub>j</sub> )
$\mu_{OHO,T} * Msat_{SVFA,KVFA} * X_{OHO} * Msat_{SO2,KO2,OHO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,BIO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{HOHO}$
$\mu_{OHO,T} * \eta_{biox,OHO} * Msat_{SVFA,KVFA} * X_{OHO} * Msat_{NO2,KNO2,OHO} * Minh_{SO2,KO2,OHO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,BIO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{HOHO}$
$\mu_{OHO,T} * \eta_{biox,OHO} * Msat_{SVFA,KVFA} * X_{OHO} * Msat_{NO3,KNO3,OHO} * Minh_{SO2,KO2,OHO} * Minh_{SNO2,KNO2,OHO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,BIO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{HOHO}$
$\mu_{OHO,T} * Msat_{SB,KSb} * X_{OHO} * Minh_{SVFA,KVFA} * Msat_{SO2,KO2,OHO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,BIO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{HOHO}$
$\mu_{OHO,T} * \eta_{biox,OHO} * Msat_{SB,KSb} * X_{OHO} * Minh_{SVFA,KVFA} * Msat_{NO2,KNO2,OHO} * Minh_{SO2,KO2,OHO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,BIO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{HOHO}$
$\mu_{OHO,T} * \eta_{biox,OHO} * Msat_{SB,KSb} * X_{OHO} * Minh_{SVFA,KVFA} * Msat_{NO3,KNO3,OHO} * Minh_{SO2,KO2,OHO} * Minh_{SNO2,KNO2,OHO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,BIO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{HOHO}$
$\mu_{FERM,OHO,T} * Msat_{SB,KSb,ANA} * X_{OHO} * Minh_{SO2,KO2,OHO} * Minh_{SNOx,kin,KNOx,OHO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,BIO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{HOHO}$
$\mu_{OHO,T} * Msat_{SMEOL,KMEOL,OHO} * X_{OHO} * Msat_{SO2,KO2,OHO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,BIO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{HOHO}$
$b_{OHO,T} * X_{OHO} * (Msat_{SO2,KO2,OHO} + \eta_{biox,b} * Msat_{SNOx,kin,KNOx,OHO} * Minh_{SO2,KO2,OHO} + \eta_{ana,b} * Minh_{SNOx,KNOx,OHO} * Minh_{SO2,KO2,OHO})$
$\mu_{MEOLO,T} * Msat_{SMEOL,KMEOL} * X_{MEOLO} * Msat_{NO2,KNO2,MEOLO} * Minh_{SO2,KO2,MEOLO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,BIO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{HMEOLO}$
$\mu_{MEOLO,T} * Msat_{SMEOL,KMEOL} * X_{MEOLO} * Msat_{NO3,KNO3,MEOLO} * Minh_{SO2,KO2,MEOLO} * Minh_{SNO2,KNO2,MEOLO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,BIO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{HMEOLO}$
$b_{MEOLO,T} * X_{MEOLO} * (Msat_{SO2,KO2,MEOLO} + \eta_{biox,b} * Msat_{SNOx,kin,KNOx,MEOLO} * Minh_{SO2,KO2,MEOLO} + \eta_{ana,b} * Minh_{SNOx,KNOx,MEOLO} * Minh_{SO2,KO2,MEOLO})$



Phosphorus accumulating organisms

	Name	S <sub>VFA</sub>	X <sub>B</sub>	X <sub>PHA</sub>	X <sub>E</sub>	X <sub>PAO</sub>	S <sub>NHx</sub>	S <sub>NO2</sub>	S <sub>NO3</sub>	S <sub>N2</sub>	X <sub>N,B</sub>	S <sub>PO4</sub>	X <sub>PP,LO</sub>	X <sub>PP,HI</sub>	X <sub>P,B</sub>	S <sub>O2</sub>	S <sub>CO2</sub>	X <sub>INORG</sub>	S <sub>CAT</sub>	S <sub>AN</sub>	
r13	PAO growth on PHA, O <sub>2</sub>			-1/Y <sub>PAO,PHA,O2</sub>		1	-i <sub>N,BIO</sub>					$\frac{f_{PHA,PP,O2}/Y_{PAO,PHA,O2}}{f_{PHA,PP,O2}/Y_{PAO,PHA,O2}}$	$\frac{Y_{PPL0}^*}{(f_{PHA,PP,O2}/Y_{PAO,PHA,O2})}$	$\frac{(1-Y_{PPL0})^*}{(f_{PHA,PP,O2}/Y_{PAO,PHA,O2})}$		$\frac{-(1-Y_{PAO,PHA,O2})}{Y_{PAO,PHA,O2}}$	$\frac{1.375^*(1-Y_{PAO,PHA,O2})}{Y_{PAO,PHA,O2}}$	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )	
r14	PAO growth on PHA, NO <sub>2</sub>			-1/Y <sub>PAO,PHA,NOx</sub>		1	-i <sub>N,BIO</sub>	$\frac{-(1-Y_{PAO,PHA,NOx})}{(EEQ_{N2,NO2}^* Y_{PAO,PHA,NOx})}$				$\frac{-(1-Y_{PAO,PHA,NOx})}{(EEQ_{N2,NO2}^* Y_{PAO,PHA,NOx})}$	$\frac{Y_{PPL0}^*}{(f_{PHA,PP,NOx}/Y_{PAO,PHA,NOx})}$	$\frac{(1-Y_{PPL0})^*}{(f_{PHA,PP,NOx}/Y_{PAO,PHA,NOx})}$			$\frac{1.375^*(1-Y_{PAO,PHA,NOx})}{Y_{PAO,PHA,NOx}}$	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )	
r15	PAO growth on PHA, NO <sub>3</sub>			-1/Y <sub>PAO,PHA,NOx</sub>		1	-i <sub>N,BIO</sub>	$\frac{-(1-Y_{PAO,PHA,NOx})}{(EEQ_{NO2,NO3}^* Y_{PAO,PHA,NOx})}$	$\frac{-(1-Y_{PAO,PHA,NOx})}{(EEQ_{NO2,NO3}^* Y_{PAO,PHA,NOx})}$			$\frac{-(f_{PHA,PP,NOx}/Y_{PAO,PHA,NOx})}{i_{P,BIO}}$	$\frac{Y_{PPL0}^*}{(f_{PHA,PP,NOx}/Y_{PAO,PHA,NOx})}$	$\frac{(1-Y_{PPL0})^*}{(f_{PHA,PP,NOx}/Y_{PAO,PHA,NOx})}$			$\frac{1.375^*(1-Y_{PAO,PHA,NOx})}{Y_{PAO,PHA,NOx}}$	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )	
r16	PAO growth on PHA, O <sub>2</sub> ; PO <sub>4</sub> limited			-1/Y <sub>PAO,PHA,O2</sub>		1	-i <sub>N,BIO</sub>						-i <sub>P,BIO</sub>			$\frac{-(1-Y_{PAO,PHA,O2})}{Y_{PAO,PHA,O2}}$	$\frac{1.375^*(1-Y_{PAO,PHA,O2})}{Y_{PAO,PHA,O2}}$	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )	
r17	PAO growth on PHA, NO <sub>2</sub> ; PO <sub>4</sub> limited			-1/Y <sub>PAO,PHA,NOx</sub>		1	-i <sub>N,BIO</sub>	$\frac{-(1-Y_{PAO,PHA,NOx})}{(EEQ_{N2,NO2}^* Y_{PAO,PHA,NOx})}$					-i <sub>P,BIO</sub>				$\frac{1.375^*(1-Y_{PAO,PHA,NOx})}{Y_{PAO,PHA,NOx}}$	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )	
r18	PAO growth on PHA, NO <sub>3</sub> ; PO <sub>4</sub> limited			-1/Y <sub>PAO,PHA,NOx</sub>		1	-i <sub>N,BIO</sub>	$\frac{-(1-Y_{PAO,PHA,NOx})}{(EEQ_{NO2,NO3}^* Y_{PAO,PHA,NOx})}$	$\frac{-(1-Y_{PAO,PHA,NOx})}{(EEQ_{NO2,NO3}^* Y_{PAO,PHA,NOx})}$				-i <sub>P,BIO</sub>				$\frac{1.375^*(1-Y_{PAO,PHA,NOx})}{Y_{PAO,PHA,NOx}}$	i <sub>IG</sub>	-i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1-f <sub>Na</sub> )	
r19	PHA storage from VFAs	-1		1								f <sub>P,VFA</sub>	-f <sub>P,VFA</sub>								
r20	PAO decay		1-f <sub>E,PAO</sub>		f <sub>E,PAO</sub>	-1					$\frac{(1-f_{E,PAO})}{i_{N,BIO}}$							$\frac{(1-f_{E,PAO})}{i_{P,BIO}}$	-i <sub>IG</sub>	i <sub>IG</sub> *f <sub>Na</sub>	i <sub>IG</sub> *(1-f <sub>Na</sub> )
r21	PHA release on PAO decay	1		-1																	
r22	PPlow release on PAO decay											1	-1								
r23	PPhigh release on PAO decay											1		-1							
r24	PPlow cleavage for anaerobic maintenance											1	-1								

Rate expression (r <sub>j</sub> )
$\mu_{PAO,T} * MR_{satX_{PHA},X_{PAO},K_{PHA}} * X_{PAO} * Msat_{SO2,KO2,PAO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,PAO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{H_{PAO}}$
$\mu_{PAO,T} * \eta_{limox,PAO} * MR_{satX_{PHA},X_{PAO},K_{PHA}} * X_{PAO} * Msat_{NO2,KNO2,PAO} * Minh_{SO2,KO2,PAO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,PAO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{H_{PAO}}$
$\mu_{PAO,T} * \eta_{limox,PAO} * MR_{satX_{PHA},X_{PAO},K_{PHA}} * X_{PAO} * Msat_{NO3,KNO3,PAO} * Minh_{SO2,KO2,PAO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,PAO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{H_{PAO}}$
$\mu_{PAO,LIMIT} * MR_{satX_{PHA},X_{PAO},K_{PHA}} * X_{PAO} * Msat_{SO2,KO2,PAO} * Msat_{SNHx,KNHx,BIO} * Minh_{SPO4,KPO4,lim} * Msat_{XPP,LO,KPP,lim} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{H_{PAO}}$
$\mu_{PAO,LIMIT} * \eta_{limox,PAO} * MR_{satX_{PHA},X_{PAO},K_{PHA}} * X_{PAO} * Msat_{NO2,KNO2,PAO} * Msat_{SNHx,KNHx,BIO} * Minh_{SPO4,KPO4,lim} * Msat_{XPP,LO,KPP,lim} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{H_{PAO}}$
$\mu_{PAO,LIMIT} * \eta_{limox,PAO} * MR_{satX_{PHA},X_{PAO},K_{PHA}} * X_{PAO} * Msat_{NO3,KNO3,PAO} * Minh_{NO2,KNO2,PAO} * Msat_{SNHx,KNHx,BIO} * Minh_{SPO4,KPO4,lim} * Msat_{XPP,LO,KPP,lim} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * Bellinhp_{H_{PAO}}$
$Q_{PAO,PHA,T} * X_{PAO} * Msat_{SVFA,KSTORE,VFA} * MR_{satX_{PP,LO},X_{PAO},K_{PP,LO}}$
$b_{PAO,T} * X_{PAO} * (Msat_{SO2,KO2,PAO} + \eta_{limox,b} * Msat_{SNOx,kin,KNOx,PAO} * Minh_{SO2,KO2,PAO} + \eta_{limox,b} * Minh_{SNOx,kin,KNOx,PAO} * Minh_{SO2,KO2,PAO})$
$r_{20} * X_{PHA} / X_{PAO}$
$r_{20} * X_{PP,LO} / X_{PAO}$
$r_{20} * X_{PP,HI} / X_{PAO}$
$b_{PPL0,ANA,T} * X_{PAO} * Minh_{SO2,KO2,PAO} * Minh_{SNOx,kin,KNO3,PAO} * Msat_{XPP,LO,KPO4,PAO}$







*Acidoclastic methanogens (VFA) and Hydrogenotrophic methanogens*

	Name	S <sub>VFA</sub>	X <sub>B</sub>	X <sub>E</sub>	X <sub>AMETO</sub>	X <sub>HMETO</sub>	S <sub>NHx</sub>	X <sub>N,B</sub>	S <sub>PO4</sub>	X <sub>P,B</sub>	S <sub>CH4</sub>	S <sub>H2</sub>	S <sub>CO2</sub>	X <sub>INORG</sub>	S <sub>CAT</sub>	S <sub>AN</sub>
r31	AMETO growth	- 1/Y <sub>AMETO</sub>			1		- i <sub>N,BIO</sub>		- i <sub>P,BIO</sub>		(1- Y <sub>AMETO</sub> )/Y <sub>AMETO</sub>		MM <sub>CO2</sub> /MM <sub>EQ,GCH4</sub> *(1- Y <sub>AMETO</sub> )/Y <sub>AMETO</sub>	i <sub>IG</sub>	- i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1- f <sub>Na</sub> )
r32	AMETO decay		1- f <sub>E</sub>	f <sub>E</sub>	-1		(1- f <sub>E</sub> )*i <sub>N,BIO</sub>		(1- f <sub>E</sub> )*i <sub>P,BIO</sub>					-i <sub>IG</sub>	i <sub>IG</sub> *f <sub>Na</sub>	i <sub>IG</sub> *(1-f <sub>Na</sub> )
r33	HMETO growth					1	- i <sub>N,BIO</sub>		- i <sub>P,BIO</sub>		(1- Y <sub>HMETO</sub> )/Y <sub>HMETO</sub>	- 1/Y <sub>HMETO</sub>	-MM <sub>CO2</sub> /(MM <sub>EQ,GH2</sub> *4)*1/Y <sub>HMETO</sub>	i <sub>IG</sub>	- i <sub>IG</sub> *f <sub>Na</sub>	-i <sub>IG</sub> *(1- f <sub>Na</sub> )
r34	HMETO decay		1- f <sub>E</sub>	f <sub>E</sub>		-1	(1- f <sub>E</sub> )*i <sub>N,BIO</sub>		(1- f <sub>E</sub> )*i <sub>P,BIO</sub>					-i <sub>IG</sub>	i <sub>IG</sub> *f <sub>Na</sub>	i <sub>IG</sub> *(1-f <sub>Na</sub> )

Rate expression (r <sub>j</sub> )	
$\mu_{AMETO,T}$	$*Msat_{SVFA,KVFA,AMETO} * X_{AMETO} * Minh_{SO2,KO2,AMETO} * Minh_{SNOx,kin,KNOx,AMETO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,BIO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * BellinhpH_{AMETO}$
$b_{AMETO,T}$	$* X_{AMETO} * (Msat_{SO2,KO2,AMETO} + \eta_{anox,b} * Msat_{SNOx,kin,KNOx,AMETO} * Minh_{SO2,KO2,AMETO} + \eta_{ana,b} * Minh_{SNOx,kin,KNOx,AMETO} * Minh_{SO2,KO2,AMETO})$
$\mu_{HMETO,T}$	$* Msat_{CO2,KCO2,HMETO} * Msat_{SH2,KH2,HMETO} * X_{HMETO} * Minh_{SO2,KO2,HMETO} * Minh_{SNOx,kin,KNOx,HMETO} * Msat_{SNHx,KNHx,BIO} * Msat_{SPO4,KPO4,BIO} * Msat_{SCAT,KCAT} * Msat_{SAN,KAN} * BellinhpH_{HMETO}$
$b_{HMETO,T}$	$* X_{HMETO} * (Msat_{SO2,KO2,HMETO} + \eta_{anox,b} * Msat_{SNOx,kin,KNOx,HMETO} * Minh_{SO2,KO2,HMETO} + \eta_{ana,b} * Minh_{SNOx,kin,KNOx,HMETO} * Minh_{SO2,KO2,HMETO})$

## Supplementary Information

*Flocculation, hydrolysis and other conversion reactions*

	Name	S <sub>VFA</sub>	S <sub>B</sub>	S <sub>MEOl</sub>	C <sub>B</sub>	X <sub>B</sub>	C <sub>U</sub>	X <sub>U</sub>	X <sub>E</sub>	X <sub>OHO</sub>	S <sub>NHx</sub>	S <sub>NO<sub>2</sub></sub>	S <sub>NO<sub>3</sub></sub>	S <sub>N<sub>B</sub></sub>	C <sub>N,B</sub>	X <sub>N,B</sub>	C <sub>N,U</sub>	X <sub>N,U</sub>	S <sub>PO4</sub>	S <sub>P,B</sub>	C <sub>P,B</sub>	X <sub>P,B</sub>	C <sub>P,U</sub>	X <sub>P,U</sub>	S <sub>CO2</sub>	S <sub>CAT</sub>	
r35	C <sub>B</sub> flocculation				-1	1																					
r36	C <sub>U</sub> flocculation						-1	1																			
r37	C <sub>N,B</sub> flocculation														-1	1											
r38	C <sub>N,U</sub> flocculation																-1	1									
r39	C <sub>P,B</sub> flocculation																				-1	1					
r40	C <sub>P,U</sub> flocculation																						-1	1			
r41	X <sub>B</sub> hydrolysis		1			-1																					
r42	X <sub>N,B</sub> hydrolysis													1		-1											
r43	X <sub>P,B</sub> hydrolysis																			1		-1					
r44	S <sub>N,B</sub> ammonification										1			-1													
r45	S <sub>P,B</sub> conversion to PO <sub>4</sub>																		1	-1							i <sub>CAT,P</sub>
r46	X <sub>E</sub> conversion					1			-1							i <sub>N,BIO</sub>							i <sub>P,BIO</sub>				
r47	Anaerobic methanol conversion	1		-1																							
r48	NO <sub>2</sub> assimilative reduction									-EEQ <sub>NO2</sub>	1+EEQ <sub>NO2</sub> *i <sub>N,BIO</sub>	-1							EEQ <sub>NO2</sub> *i <sub>P,BIO</sub>							1.375*EEQ <sub>NO2</sub>	
r49	NO <sub>3</sub> assimilative reduction									-EEQ <sub>NO3</sub>	1+EEQ <sub>NO3</sub> *i <sub>N,BIO</sub>		-1						EEQ <sub>NO3</sub> *i <sub>P,BIO</sub>							1.375*EEQ <sub>NO3</sub>	

Rate expression (r <sub>j</sub> )
$q_{FLOC,T} * X_{BIO} * MR_{sat_{CB,XBIO,kin,KFLOC}}$
$q_{FLOC,T} * X_{BIO} * MR_{sat_{CU,XBIO,kin,KFLOC}}$
$C_{N,B}/C_B * r_{35}$
$C_{N,U}/C_U * r_{36}$
$C_{P,B}/C_B * r_{35}$
$C_{P,U}/C_U * r_{36}$
$q_{HYD,T} * X_{BIO,kin} * MR_{sat_{XB,XBIO,kin,KHYD}} * (Msat_{SO2,KO2,OHO} + \eta_{anox,hyd} * Msat_{SNOx,kin,KNOx,OHO} * Min_{h_{SO2,KO2,OHO}} + \eta_{ana,hyd} * Min_{h_{SNOx,kin,KNOx,OHO}} * Min_{h_{SO2,KO2,OHO}})$
$X_{N,B}/X_B * r_{41}$
$X_{P,B}/X_B * r_{41}$
$q_{AMMON,T} * S_{N,B} * X_{BIO,kin}$
$q_{PO4conv,T} * S_{P,B} * X_{BIO,kin}$
$q_{EtOB,T} * X_E$
$0 * S_{MEOL}$
$q_{ASSIM,T} * Msat_{SNO2,KNO2,ASSIM} * Min_{h_{SNHx,KNHx,ASSIM}} * Msat_{XOHO,KOHO,ASSIM} * X_{BIO,kin}$
$q_{ASSIM,T} * Msat_{SNO3,KNO3,ASSIM} * Min_{h_{SNO2,KNO2,ASSIM}} * Min_{h_{SNHx,KNHx,ASSIM}} * Msat_{XOHO,KOHO,ASSIM} * X_{BIO,kin}$



Rate expression (r <sub>j</sub> )
$Q_{aging,H} * X_{HFO,H}$
$Q_{aging,L} * X_{HFO,L}$
$Q_{Pcoprecip} * S_{PO4} / (K_P + S_{PO4}) * X_{HFO,H}$
$Q_{Pbinding} * S_{PO4} / (K_P + S_{PO4}) * X_{HFO,L}$
$Q_{aging,H} * X_{HFO,H,P}$
$Q_{aging,L} * X_{HFO,L,P}$
$Q_{diss,H} * K_{p,diss} / (K_{p,diss} + S_{PO4}) * X_{HFO,H,P}$
$Q_{diss,L} * K_{p,diss} / (K_{p,diss} + S_{PO4}) * X_{HFO,L,P}$
$Q_{prec} * Minh_{SO2,KO2,prec} * Minh_{NO3,KNO3,prec} * Minh_{NO2,KNO2,prec} * Msat_{SPO4,KSPO4,prec} * BellinhpH_{prec} * Msat_{XHFO,old,KXHFO,old,prec}$
$Q_{STR} * DrivingForce_{STR} * MM_{STR} * 1000 * X_{STR} / (K_{P,STR} + X_{STR})$

## Supplementary Information

## Gas transfer

	Name	S <sub>N2</sub>	S <sub>O2</sub>	S <sub>CH4</sub>	S <sub>H2</sub>	S <sub>CO2</sub>	G <sub>CO2</sub>	G <sub>CH4</sub>	G <sub>H2</sub>	G <sub>O2</sub>	G <sub>N2</sub>
r61	Carbon dioxide gas transfer					1	$-1 * C_{ppm,Vconc} / MM_{EQ,GCO2} * R * T_{null} / P_{St} * f_{volume,L,G}$				
r62	Methane gas transfer			1				$-1 * C_{ppm,Vconc} / MM_{EQ,GCH4} * R * T_{null} / P_{St} * f_{volume,L,G}$			
r63	Hydrogen gas transfer				1				$1 * C_{ppm,Vconc} / MM_{EQ,GH2} * R * T_{null} / P_{St} * f_{volume,L,G}$		
r64	Oxygen gas transfer		1							$-1 * C_{ppm,Vconc} / MM_{EQ,GO2} * R * T_{null} / P_{St} * f_{volume,L,G}$	
r65	Nitrogen gas transfer	1									$1 * C_{ppm,Vconc} / MM_{EQ,GN2} * R * T_{null} / P_{St} * f_{volume,L,G}$

Rate expression (r <sub>j</sub> )
k <sub>transfer,GCO2</sub>
k <sub>transfer,GCH4</sub>
k <sub>transfer,GH2</sub>
k <sub>transfer,GO2</sub>
k <sub>transfer,GN2</sub>

*Functions*

<b>Symbol</b>	<b>Name</b>	<b>Expression</b>
Msat(var; k)	Monod saturation	$\text{var} / (\text{k} + \text{var})$
MsatpH(var;k;varpH;kpH)	Monod saturation with check for pH availability	$\text{If}(\text{Sumo\_pHEffects}; \text{varpH}/(\text{kpH}+\text{varpH}); \text{var}/(\text{k}+\text{var}))$
Minh(var; k)	Monod inhibition	$\text{k} / (\text{k} + \text{var})$
MinhpH(var;k;varpH;kpH)	Monod inhibition with check for pH availability	$\text{If}(\text{Sumo\_pHEffects}; \text{kpH}/(\text{kpH}+\text{varpH}); \text{k}/(\text{k}+\text{var}))$
MRSat(s;x;k)	Monod ratio saturation	$(\text{s}/\text{x})/(\text{s}/\text{x}+\text{k})$
MRinh(s;x;k)	Monod ratio inhibition	$(\text{k})/(\text{s}/\text{x}+\text{k})$
Bellinh(var; K <sub>lo</sub> ; K <sub>hi</sub> )	Bell-shaped inhibition	$(1 + 2 * 10^{(0.5 * (\text{Klo} - \text{Khi}))}) / (1 + 10^{(\text{var} - \text{Khi})} + 10^{(\text{Klo} - \text{var})})$
BellinhpH(var; K <sub>lo</sub> ; K <sub>hi</sub> )	Bell-shaped inhibition with check for pH availability	$\text{If}(\text{Sumo\_pHEffects}; (1 + 2 * 10^{(0.5 * (\text{Klo} - \text{Khi}))}) / (1 + 10^{(\text{var} - \text{Khi})} + 10^{(\text{Klo} - \text{var})}); 1)$
Logsat(var; slope; halfval)	Logistic saturation	$1 / (1 + \text{Exp}((\text{halfval} - \text{var}) * \text{slope}))$
LogsatpH(var; halfval; slope; varpH; halfvalpH; slopepH)	Logistic saturation with check for pH availability	$\text{If}(\text{Sumo\_pHEffects}; 1 / (1 + \text{Exp}((\text{halfvalpH} - \text{varpH}) * \text{slopepH}))); 1/((1 + \text{Exp}((\text{halfval} - \text{var}) * \text{slope}))))$
Loginh(var; slope; halfval)	Logistic inhibition	$1 / (1 + \text{Exp}((\text{var} - \text{halfval}) * \text{slope}))$
LoginhpH(var; halfval; slope; varpH; halfvalpH; slopepH)	Logistic inhibition with check for pH availability	$\text{If}(\text{Sumo\_pHEffects}; 1 / (1 + \text{Exp}((\text{varpH} - \text{halfvalpH}) * \text{slopepH}))); 1/((1 + \text{Exp}((\text{var} - \text{halfval}) * \text{slope}))))$

## Supplementary Information

*Parameters***Heterotrophic kinetics**

<b>Symbol</b>	<b>Name</b>	<b>Default</b>	<b>Unit</b>
$\mu_{\text{OHO}}$	Maximum specific growth rate of OHOs	4.0	$\text{d}^{-1}$
$K_{\text{SB}}$	Substrate half saturation for OHOs	5.0	$\text{g COD.m}^{-3}$
$K_{\text{VFA}}$	VFA half saturation for OHOs	1.0	$\text{g COD.m}^{-3}$
$K_{\text{MEOL,OHO}}$	Methanol half saturation for OHOs (aerobic)	0.5	$\text{g COD.m}^{-3}$
$K_{\text{O}_2,\text{OHO}}$	O <sub>2</sub> half saturation for OHOs	0.05	$\text{g O}_2.\text{m}^{-3}$
$K_{\text{NO}_3,\text{OHO}}$	NO <sub>3</sub> half saturation for OHOs	0.10	$\text{g N.m}^{-3}$
$K_{\text{NO}_2,\text{OHO}}$	NO <sub>2</sub> half saturation for OHOs	0.05	$\text{g N.m}^{-3}$
$\eta_{\text{anox,OHO}}$	Anoxic growth reduction for OHOs	0.60	-
$b_{\text{OHO}}$	Aerobic decay rate coefficient for OHOs	0.62	$\text{d}^{-1}$
$\mu_{\text{FERM,OHO}}$	Fermentation rate coefficient	0.4	$\text{d}^{-1}$
$K_{\text{SB,ANA}}$	Substrate half saturation during fermentation	5.0	$\text{g COD.m}^{-3}$
$\text{pHl}_{\text{OHO}}$	pH inhibition - low value	3.5	pH unit
$\text{pHhi}_{\text{OHO}}$	pH inhibition - high value	10.0	pH unit

**AOB kinetics**

<b>Symbol</b>	<b>Name</b>	<b>Default</b>	<b>Unit</b>
$\mu_{\text{AOB}}$	Maximum specific growth rate of AOBs	0.85	$\text{d}^{-1}$
$K_{\text{NH}_x,\text{AOB}}$	Ammonia half saturation for AOBs	0.7	$\text{g N.m}^{-3}$
$K_{\text{CO}_2,\text{AOB}}$	CO <sub>2</sub> half saturation for AOBs	10.000	$\text{g CO}_2.\text{m}^{-3}$
$K_{\text{CO}_2,\text{AOB,pH}}$	HCO <sub>3</sub> <sup>-</sup> half saturation for AOBs	0.0001	$\text{mol}[\text{HCO}_3^-]/\text{L}$

$K_{O_2,AOB}$	Oxygen half saturation for AOBs	0.25	$g\ O_2.m^{-3}$
$K_{NOx,AOB}$	Half saturation for anoxic conditions for AOBs	0.03	$g\ N.m^{-3}$
$b_{AOB}$	Aerobic decay rate coefficient for AOBs	0.17	$d^{-1}$
$K_{SNO_2,AOB}$	SNO2 half saturation for AOBs	9999.00	$g\ N.m^{-3}$
$K_{HNO_2,AOB,pH}$	HNO2 half saturation for AOBs	0.00	mol/L
$pH_{lo,AOB}$	pH inhibition - low value	5.50	pH unit
$pH_{hi,AOB}$	pH inhibition - high value	9.50	pH unit

#### NOB kinetics

Symbol	Name	Default	Unit
$\mu_{NOB}$	Maximum specific growth rate of NOBs	0.65	$d^{-1}$
$K_{NO_2,NOB}$	Nitrite half saturation for NOBs	0.10	$g\ N.m^{-3}$
$K_{CO_2,NOB}$	CO2 half saturation for NOBs	1.00	$g\ CO_2.m^{-3}$
$K_{CO_2,NOB,pH}$	$HCO_3^-$ half saturation for NOBs	1.00E-10	mol[ $HCO_3^-$ ]/L
$K_{O_2,NOB}$	Oxygen half saturation for NOBs	0.25	$g\ O_2.m^{-3}$
$K_{NOx,NOB}$	Half saturation for anoxic conditions for NOBs	0.03	$g\ N.m^{-3}$
$b_{NOB}$	Aerobic decay rate coefficient for NOBs	0.15	$d^{-1}$
$K_{NH_3,NOB}$	SNHx half saturation for NOBs	9999.00000	$g\ N.m^{-3}$
$K_{NH_3,NOB,pH}$	[ $NH_3$ ] half saturation for NOBs	0.00008	mol/L
$pH_{lo,NOB}$	pH inhibition - low value	5.50	pH unit
$pH_{hi,NOB}$	pH inhibition - high value	9.50	pH unit

#### Anammox kinetics

Symbol	Name	Default	Unit
$\mu_{AMX}$	Maximum specific growth rate of Anammox	0.1	$d^{-1}$

Supplementary Information

## Supplementary Information

$K_{NHx,AMX}$	Ammonia half saturation for Anammox	2	$g\ N.m^{-3}$
$K_{NO2,AMX}$	Nitrite half saturation for Anammox	1	$g\ N.m^{-3}$
$K_{CO2,AMX}$	CO2 half saturation for Anammox	10	$g\ CO_2.m^{-3}$
$K_{CO2,AMX,pH}$	$HCO_3^-$ half saturation for Anammox	0.0001	$mol[HCO_3^-]/L$
$K_{O2,AMX}$	Oxygen half saturation for Anammox	0.4	$g\ O_2.m^{-3}$
$K_{NOx,AMX}$	Half saturation for anoxic conditions for Anammox	0.1	$g\ N.m^{-3}$
$b_{AMX}$	Aerobic decay rate coefficient for Anammox	0.019	$d^{-1}$
$K_{SNO2,AMX}$	$SNO_2$ half saturation for Anammox	1	$mol/L$
$K_{HNO2,AMX,pH}$	$HNO_2$ half saturation for Anammox	1	$mol/L$
$pH_{lo,AMX}$	pH inhibition - low value	5.5	pH unit
$pH_{hi,AMX}$	pH inhibition - high value	9.5	pH unit

**Methylotroph kinetics**

<b>Symbol</b>	<b>Name</b>	<b>Default</b>	<b>Unit</b>
$\mu_{MEOLO}$	Methylotroph maximum specific growth rate	1.30	$d^{-1}$
$K_{MEOL}$	Methanol half saturation coefficient	0.50	$g\ COD.m^{-3}$
$K_{O2,MEOLO}$	$O_2$ half saturation for MEOLOs	0.05	$g\ O_2.m^{-3}$
$K_{NO2,MEOLO}$	$NO_2$ half saturation for MEOLOs	0.02	$g\ N.m^{-3}$
$K_{NO3,MEOLO}$	$NO_3$ half saturation for MEOLOs	0.05	$g\ N.m^{-3}$
$b_{MEOLO}$	Aerobic decay rate coefficient for methylotrophs	0.05	$d^{-1}$
$pH_{lo,MEOLO}$	pH inhibition - low value	4	pH unit
$pH_{hi,MEOLO}$	pH inhibition - high value	9.5	pH unit

**PAO kinetics**

Symbol	Name	Default	Unit
$\mu_{PAO}$	Maximum specific growth rate of PAOs	0.95	d <sup>-1</sup>
$\mu_{PAO,LIM}$	Maximum specific growth rate of PAOs, P limited	0.42	d <sup>-1</sup>
$K_{PHA}$	PHA half saturation coefficient	0.05	-
$K_{O_2,PAO}$	Oxygen half saturation for PAOs	0.05	g O <sub>2</sub> .m <sup>-3</sup>
$K_{NO_2,PAO}$	NO <sub>2</sub> half saturation for PAOs	0.05	g N.m <sup>-3</sup>
$K_{NO_3,PAO}$	NO <sub>3</sub> half saturation for PAOs	0.1	g N.m <sup>-3</sup>
$\eta_{anox,PAO}$	PAO anoxic growth factor	0.33	-
$b_{PAO}$	Aerobic decay rate coefficient for PAOs	0.20	d <sup>-1</sup>
$b_{PPLO,ANA}$	Anaerobic maintenance PP cleavage	0.03	d <sup>-1</sup>
$q_{PAO,PHA}$	PHA storage rate	6.0	d <sup>-1</sup>
$K_{STORE,VFA}$	VFA half saturation for storage	5.0	g COD.m <sup>-3</sup>
$K_{PP,LO}$	PP-low half saturation for storage	0.01	g P.m <sup>-3</sup>
$K_{PO_4,PAO}$	PO <sub>4</sub> half saturation for PAOs	0.10	g P.m <sup>-3</sup>
$K_{PP,lim}$	PP limitation as nutrient	0.001	g P.m <sup>-3</sup>
$K_{PO_4,lim}$	PO <sub>4</sub> limitation as nutrient	0.001	g P.m <sup>-3</sup>
$pH_{lo,PAO}$	pH inhibition - low value	4	pH unit
$pH_{hi,PAO}$	pH inhibition - high value	9.5	pH unit

#### VFA (Acido)clastic methanogen kinetics

Symbol	Name	Default	Unit
$\mu_{AMETO}$	Maximum specific growth rate of AMETO	0.50	d <sup>-1</sup>
$K_{VFA,AMETO}$	VFA half saturation for AMETO	100	g COD.m <sup>-3</sup>
$K_{O_2,AMETO}$	Oxygen half saturation for AMETO	0.05	g O <sub>2</sub> .m <sup>-3</sup>

Supplementary Information

## Supplementary Information

$K_{NOx,AMETO}$	NOx half saturation for AMETO	0.05	$g\ N.m^{-3}$
$b_{AMETO}$	Decay rate for AMETO (aerobic)	0.52	$d^{-1}$
$pH_{lo,AMETO}$	pH inhibition - low value	5.5	pH unit
$pH_{hi,AMETO}$	pH inhibition - high value	9.5	pH unit

**Hydrogenotrophic methanogen kinetics**

<b>Symbol</b>	<b>Name</b>	<b>Default</b>	<b>Unit</b>
$\mu_{HMETO}$	Maximum specific growth rate of HMETO	1.50	$d^{-1}$
$K_{CO2,HMETO}$	CO2 half saturation for HMETO	1.0	$g.m^{-3}$
$K_{H2,HMETO}$	H2 half saturation for HMETO	0.1	$g\ COD.m^{-3}$
$K_{O2,HMETO}$	Oxygen half saturation for HMETO	0.05	$g\ O_2.m^{-3}$
$K_{NOx,HMETO}$	NOx half saturation for HMETO	0.05	$g\ N.m^{-3}$
$b_{HMETO}$	Decay rate for HMETO (aerobic)	0.52	$d^{-1}$
$pH_{lo,HMETO}$	pH inhibition - low value	5.5	pH unit
$pH_{hi,HMETO}$	pH inhibition - high value	9.5	pH unit

**Common switches**

<b>Symbol</b>	<b>Name</b>	<b>Default</b>	<b>Unit</b>
$K_{NHx,BIO}$	NHx half saturation for biomasses	0.005	$g\ N.m^{-3}$
$K_{PO4,BIO}$	PO4 half saturation for biomasses	0.002	$g\ P.m^{-3}$
$\eta_{anox,b}$	Anoxic reduction of decay	0.50	-
$\eta_{ana,b}$	Anaerobic reduction of decay	0.25	-
$\eta_{anox,hyd}$	Anoxic reduction of hydrolysis	0.50	-
$\eta_{ana,hyd}$	Anaerobic reduction of hydrolysis	0.50	-

$K_{b,CH4}$	Methane switch (to indicate anaerobic conditions)	10.00	$g.m^{-3}$
$K_{CAT}$	Sodium half saturation for synthesis inorganics	0.1	$g.m^{-3}$
$K_{AN}$	Choride half saturation for synthesis inorganics	0.1	$g.m^{-3}$

#### Conversion kinetics

Symbol	Name	Default	Unit
$q_{FLOC}$	Flocculation rate coefficient	50.0	$d^{-1}$
$K_{FLOC}$	Flocculation half saturation coefficient	0.001	$g\ COD.m^{-3}$
$q_{HYD}$	Hydrolysis rate coefficient	2.0	$d^{-1}$
$K_{HYD}$	Hydrolysis half saturation coefficient	0.05	-
$q_{AMMON}$	Ammonification rate coefficient	0.05	$d^{-1}$
$q_{PO4conv}$	Phosphate release rate coefficient	0.05	$d^{-1}$
$q_{EtOB}$	Endogenous residue conversion rate coefficient	0.007	$d^{-1}$
$q_{ASSIM}$	Assimilative $NH_x$ production rate coefficient	1.0	$d^{-1}$
$K_{NHx,ASSIM}$	Assimilative $NH_x$ half saturation	0.0005	$g\ N.m^{-3}$
$K_{NO2,ASSIM}$	Assimilative $NO_2$ half saturation	0.001	$g\ N.m^{-3}$
$K_{NO3,ASSIM}$	Assimilative $NO_3$ half saturation	0.001	$g\ N.m^{-3}$
$K_{OHO,ASSIM}$	Assimilative OHO half saturation	0.001	$g\ COD.m^{-3}$

#### Operational inputs

Symbol	Name	Default	Unit
T	Temperature	15.0	$C^{\circ}$
Tbase	Arrhenius base temperature	20.0	$C^{\circ}$

#### Temperature dependency

Supplementary Information

## Supplementary Information

<b>Symbol</b>	<b>Name</b>	<b>Default</b>	<b>Unit</b>
$\theta_{\mu, \text{OHO}}$	Arrhenius coefficient	1.04	-
$\theta_{\text{FERM}, \text{OHO}}$	Arrhenius coefficient	1.04	-
$\theta_{\text{b}, \text{OHO}}$	Arrhenius coefficient	1.03	-
$\theta_{\mu, \text{MEOLO}}$	Arrhenius coefficient	1.06	-
$\theta_{\text{b}, \text{MEOLO}}$	Arrhenius coefficient	1.03	-
$\theta_{\mu, \text{PAO}}$	Arrhenius coefficient	1.04	-
$\theta_{\mu, \text{PAO}, \text{LIM}}$	Arrhenius coefficient	1.04	-
$\theta_{\text{q}, \text{PAO}, \text{PHA}}$	Arrhenius coefficient	1.04	-
$\theta_{\text{b}, \text{PAO}}$	Arrhenius coefficient	1.03	-
$\theta_{\text{b}, \text{PPLO}, \text{ANA}}$	Arrhenius coefficient	1.03	-
$\theta_{\mu, \text{AOB}}$	Arrhenius coefficient	1.072	-
$\theta_{\text{b}, \text{AOB}}$	Arrhenius coefficient	1.03	-
$\theta_{\mu, \text{NOB}}$	Arrhenius coefficient	1.06	-
$\theta_{\text{b}, \text{NOB}}$	Arrhenius coefficient	1.03	-
$\theta_{\mu, \text{AMX}}$	Arrhenius coefficient	1.01	-
$\theta_{\text{b}, \text{AMX}}$	Arrhenius coefficient	1.03	-
$\theta_{\mu, \text{AMETO}}$	Arrhenius coefficient	1.03	-
$\theta_{\text{b}, \text{AMETO}}$	Arrhenius coefficient	1.03	-
$\theta_{\mu, \text{HMETO}}$	Arrhenius coefficient	1.03	-
$\theta_{\text{b}, \text{HMETO}}$	Arrhenius coefficient	1.03	-
$\theta_{\text{q}, \text{FLOC}}$	Arrhenius coefficient	1.0	-
$\theta_{\text{q}, \text{HYD}}$	Arrhenius coefficient	1.029	-

$\theta_{q,AMMON}$	Arrhenius coefficient	1	-
$\theta_{q,PO4conv}$	Arrhenius coefficient	1	-
$\theta_{q,EtoB}$	Arrhenius coefficient	1	-
$\theta_{q,ASSIM}$	Arrhenius coefficient	1	-

#### Heterotrophic stoichiometry

Symbol	Name	Default	Unit
$Y_{OHO,VFA,O2}$	Aerobic yield of OHOs on VFA	0.60	
$Y_{OHO,VFA,NOx}$	Anoxic yield of OHOs on VFA	0.45	
$Y_{OHO,SB,O2}$	Aerobic yield of OHOs on substrate	0.67	
$Y_{OHO,SB,NOx}$	Anoxic yield of OHOs on substrate	0.54	
$Y_{OHO,SB,ANA}$	Anaerobic yield of OHOs on substrate	0.1	
$Y_{OHO,H2,ANA}$	Anaerobic yield of H <sub>2</sub> production in fermentation	0.35	
$Y_{OHO,CO2,ANA}$	Anaerobic yield of CO <sub>2</sub> production in fermentation	0.35	
$fr_{CH,SB}$	Carbohydrate fraction in S <sub>B</sub>	1	
$Y_{OHO,SMEOL,O2}$	Aerobic yield of OHOs on methanol	0.4	

#### Methylotroph stoichiometry

Symbol	Name	Default	Unit
$Y_{MEOLO}$	MEOLO yield	0.4	

#### Ammonia oxidizer stoichiometry

Symbol	Name	Default	Unit
$Y_{AOB}$	AOB yield	0.15	

Supplementary Information

## Supplementary Information

**Nitrite oxidizer stoichiometry**

<b>Symbol</b>	<b>Name</b>	<b>Default</b>	<b>Unit</b>
$Y_{\text{NOB}}$	NOB yield	0.09	

**Phosphorus accumulating stoichiometry**

<b>Symbol</b>	<b>Name</b>	<b>Default</b>	<b>Unit</b>
$Y_{\text{PAO,PHA,O}_2}$	Aerobic yield of PAOs on PHA	0.639	
$Y_{\text{PAO,PHA,NO}_x}$	Anoxic yield of PAOs on PHA	0.52	
$Y_{\text{PPLO}}$	PPlow yield on PP storage (rest goes to PPhigh)	0.94	
$f_{\text{PHA,PP,O}_2}$	PHA to PP ratio, aerobic	0.95	
$f_{\text{PHA,PP,NO}_x}$	PHA to PP ratio, anoxic	0.35	
$f_{\text{P,VFA}}$	P release to VFA ratio	0.49	
$i_{\text{TSS,PP}}$	TSS content of PP	3.5	

**Methanogenic stoichiometry**

<b>Symbol</b>	<b>Name</b>	<b>Default</b>	<b>Unit</b>
$Y_{\text{HMETO}}$	HMETO yield	0.1	
$Y_{\text{AMETO}}$	AMETO yield	0.1	

**General stoichiometry**

<b>Symbol</b>	<b>Name</b>	<b>Default</b>	<b>Unit</b>
$f_{\text{E}}$	Endogenous fraction (death-regeneration)	0.08	
$f_{\text{E,PAO}}$	Endogenous fraction (death-regeneration) for PAO	0.25	
$i_{\text{N,BIO}}$	N content of biomasses	0.070	

$i_{P,BIO}$	P content of biomasses	0.020	
$i_{CV,BIO}$	Biomass XCOD/VSS ratio	1.42	g COD / g VSS
$i_{CV,B}$	X <sub>b</sub> XCOD/VSS ratio	1.80	g COD / g VSS
$i_{CV,U}$	X <sub>u</sub> XCOD/VSS ratio	1.30	g COD / g VSS
$Y_{BOD,U}$	Yield on ultimate BOD	0.95	-
$f_{BOD5,BODu}$	BOD5 to ultimate BOD ratio	0.66	-
$i_{CV,PHA}$	PHA XCOD/VSS ratio	1.67	g COD / g VSS
$i_{CV,E}$	X <sub>e</sub> XCOD/VSS ratio	1.42	g COD / g VSS
$i_{IG}$	Synthesis inorganics in active biomass	0.11	g TSS / g COD
$i_{P,XSTR}$	Phosphorus content of struvite	0.13	gP / gTSS
$i_{CAT,P}$	Cation content of S <sub>P,B</sub>	0.00	mg CAT/mg P
$f_{Na}$	Sodium mass fraction in NaCl	0.393	mg CAT/mg

<b>Anammox stoichiometry</b>			
<b>Symbol</b>	<b>Name</b>	<b>Default</b>	<b>Unit</b>
$Y_{NO2,AMX}$	$Y_{NO2,AMX}$	1.32	
$Y_{NO3,AMX}$	$Y_{NO3,AMX}$	0.26	

<b>P precipitation kinetics</b>			
<b>Symbol</b>	<b>Name</b>	<b>Default</b>	<b>Unit</b>
$q_{aging,H}$	Aging coefficient for X <sub>HFO,H</sub>	200	
$q_{aging,L}$	Aging coefficient for X <sub>HFO,L</sub>	30	
$q_{Pcoprecip}$	Maximum precipitation rate of X <sub>HFO,H</sub>	238	
$q_{STR,precip}$	Struvite precipitation rate	30000000000	d-1
$q_{STR,dissolve}$	Struvite dissolution rate	3E+11	d-1

Supplementary Information

## Supplementary Information

$K_{P,STR}$	Struvite half saturation	1	g TSS.m-3
$q_{Pbinding}$	Maximum binding rate of $X_{HFO,L}$	8.8	
$q_{diss,H}$	Redissolution rate coefficient - $X_{HFO,H,P}$	36	
$q_{diss,L}$	Redissolution rate coefficient - $X_{HFO,L,P}$	36	
$K_{p,diss}$	Inhibition coefficient for $S_{PO4}$ for redissolution	0.03	
$K_P$	Half saturation coefficient for $S_{PO4}$	0.5	
$q_{prec}$	Precipitation rate under anaerobic conditions (in digester)	40	
$K_{O_2,prec}$	$O_2$ half saturation for P precipitation in digester	0.01	
$K_{NO_3,prec}$	$S_{NO_3}$ half saturation for P precipitation in digester	0.01	
$K_{NO_2,prec}$	$S_{NO_2}$ half saturation for P precipitation in digester	0.01	
$K_{SPO_4,prec}$	$S_{PO_4}$ half saturation for P precipitation in digester	60	
$pH_{lo,prec}$	pH inhibition - low value	4	
$pH_{hi,prec}$	pH inhibition - high value	8	
$K_{XHFO,old,prec}$	Half saturation coefficient for HFO old	80	

**Stoichiometric parameters of P precipitation**

Symbol	Name	Default	Unit
$ASF_H$	Active site factor for $HFO_H$	1.2	molP/molFe
$ASF_L$	Active site factor for $HFO_L$	0.2	molP/molFe



Wastewater treatment plants are moving towards energy and nutrients recovery facilities. Simultaneously, they are submitted to stricter regulation with respect to environment and human health. Facing the great challenge of reducing operational costs along with the reduction of environmental impacts and the guaranty of plants robustness, tools might be developed in order to provide an integrated assessment. The goal of this work is to develop a reliable and predictive framework containing rigorous dynamic wide-plant modelling, extended boundaries life cycle assessment for scenarios evaluation and an efficient multi-objective optimization tool. The developed framework for environmental evaluation coupled to dynamic modelling was initially applied to several case studies including urine source separation, enhanced primary clarification and urine treatment by nitrification/ anaerobic ammonium oxidation, offering both performance results and environmental hotspots. Given the important benefits of the urine source separation provided by the previous results, a flexible and dynamic phenomenological influent generator was adapted in order to provide realistic dynamic data concerning urine and wastewater streams in different urine retention scenarios. Finally, as the complex combination of biological, chemical and physical processes leads to a computational expensive problem, a feasibility study (computational time and reliability) on the multi-objective optimization was conducted. Obtaining a set of solutions that avoids any prior discrimination among costs, environment and performance allowed thus the discussion of the involved trade-offs. Finally, the complete framework was applied to several case studies lightening on operational aspects of more sustainable options on wastewater management and treatment.

*Keywords: Wastewater; Modelling; Life Cycle Assessment; Multi-Objective Optimization; Urine Source Separation*

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Les stations d'épuration se tournent actuellement vers des installations de récupération d'énergie et des nutriments. Dans le même temps, elles sont soumises à une réglementation de plus en plus stricte en ce qui concerne l'environnement et la santé humaine. Face au défi ambitieux de réduire les coûts d'exploitation et les impacts environnementaux tout en garantissant la robustesse du procédé, il est nécessaire de développer des outils capables de fournir une évaluation intégrée du procédé. L'objectif de ce travail est de développer une plateforme réaliste et prédictive contenant trois aspects: la modélisation rigoureuse et dynamique de l'ensemble de la station d'épuration; l'analyse de cycle de vie aux frontières étendues pour l'évaluation des scénarios et enfin un outil d'optimisation multi-objectif efficace. La plateforme développée pour l'évaluation environnementale couplée à la modélisation dynamique a d'abord été appliquée à plusieurs cas d'étude. Ainsi des résultats de performance et d'impacts environnementaux ont été obtenus pour la séparation de l'urine à la source, la décantation primaire avancée et le traitement de l'urine par nitrification/ oxydation anaérobie de l'ammonium, et d'autres filières. Compte tenu des importants avantages de la séparation de l'urine établis par les résultats précédents, un générateur d'influents phénoménologique, flexible et dynamique a été adapté afin de fournir des données dynamiques réalistes concernant les flux d'urine et des eaux usées dans les différents scénarios de rétention d'urine. Enfin, comme la combinaison complexe de processus biologiques, chimiques et physiques conduit à un problème lourd en calcul, une étude de faisabilité (temps de calcul et fiabilité) a été réalisée sur l'optimisation multi-objectif. L'obtention d'un ensemble de solutions qui évite toute discrimination préalable entre les coûts, l'environnement et les performances ont permis la discussion des enjeux impliqués. Finalement, la plateforme complète a été appliquée à plusieurs cas d'étude et clarifie les aspects opérationnels des options plus durables en matière de gestion et de traitement des eaux usées.

*Mots-clés: Eaux usées; Modélisation; Analyse de Cycle de Vie; Optimisation Multi-Objectif; Séparation de l'Urine à la Source*