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Ph.D. dissertation

Development of an integrated tool for Process Modelling and Life Cycle Assessment

Ecodesign of process plants and application to drinking water treatment

Développement d'un outil intégré pour la Modélisation de Procédés et l'Analyse de Cycle de Vie - Ecoconception d'usines de procédés et application à la production d'eau potable

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Abstract

Adapted tools for tackling environmental issues are necessary but they are still missing in industry. Indeed, the introduction of ecodesign practices in the process industry is hindered by the lack of realism and flexibility of related tools.

The main objectives of this research work were the development of a fully integrated tool for Process Modelling & Life Cycle Assessment (PM-LCA), and the formulation of an affiliated methodological approach for process ecodesign. The software tool and the methodological approach are meant to be applied to water treatment technologies.

The literature review leads to a better comprehension of the required research efforts. The main guidelines for the development of the software tool are stated accordingly.

The developed tool, named EVALEAU, consists in a library of unit process models allowing life cycle inventory calculation in function of process parameters. The tool is embedded in Umberto® LCA software and is complementary to Ecoinvent database. A sensitivity analysis toolbox, based on the Morris method, was included for the identification of the process parameters mainly affecting the life cycle impact assessment results.

EVALEAU tool was tested through two case studies - two existing drinking water plants. The reliability of the modelling approach was demonstrated through water quality simulation, energy and materials inventory simulation, compared with site real data. An ecodesign procedure was experienced on a complex water treatment chain, demonstrating the relevance of simulation results and the usefulness of sensitivity analysis for an optimal choice of operation parameters.

This first developed PM-LCA tool is dedicated to foster the introduction of ecodesign practices in the water industry.

Keywords

Process modelling - Life Cycle Assessment (LCA) - Ecodesign tool - Sensitivity analysis - Decision-making support - Drinking water treatment

Résumé

Des outils adaptés pour s'attaquer aux problématiques environnementales sont nécessaires mais malheureusement absents de l'industrie. En effet, l'introduction de nouvelles pratiques d'écoconception dans l'industrie des procédés est entravée par le manque de réalisme et de flexibilité des outils associés.

Les objectifs principaux de ce travail de recherche étaient le développement d'un outil intégré pour la modélisation de procédés et l'analyse de cycle de vie (PM-LCA), ainsi que la formulation d'une approche méthodologique affiliée pour l'écoconception de procédés. L'outil logiciel et l'approche méthodologique sont appliqués à la production d'eau potable.

La revue de la littérature scientifique a permis d'appréhender les efforts de recherche nécessaires. Les principales lignes directrices sont établies en conséquence.

L'outil développé, nommé EVALEAU, consiste en une bibliothèque logicielle de modèles de procédés unitaires permettant le calcul d'inventaire de données en fonction de paramètres de procédés. L'outil est embarqué dans le logiciel ACV Umberto® en complément de la base de données Ecoinvent. Une boîte à outils pour l'analyse de sensibilité, basée sur la méthode de Morris, est implémentée pour l'identification des paramètres de procédés ayant une influence majeure sur les résultats d'impacts environnementaux.

L'outil EVALEAU est testé sur deux études de cas - deux usines de production d'eau potable existantes. La fiabilité de l'approche est démontrée à travers la comparaison des calculs de qualité de l'eau, de consommations d'énergie et de matériaux avec les données réelles recueillies sur site. Une procédure d'écoconception est expérimentée sur une chaîne de traitement complexe démontrant ainsi la pertinence des résultats de simulations et l'utilité de l'analyse de sensibilité pour un choix optimal des paramètres opératoires.

En conséquence, ce premier outil PM-LCA est censé promouvoir l'introduction de pratiques d'écoconception dans l'industrie de l'eau.

Mots clés

Modélisation de procédés - Analyse de Cycle de Vie (ACV) - Outil d'écoconception - Analyse de sensibilité - Aide à la décision - Production d'eau potable

Scientific production

Scientific papers published in international and peer reviewed journals

Méry Y., Tiruta-Barna L., Benetto E., Baudin I. *An integrated « Process Modelling-Life Cycle Assessment » approach for process evaluation and eco-design* (2012) International Journal of Life Cycle Assessment.

Igos E., Benetto E., Baudin I., Tiruta-Barna L., Méry Y., Arbault D. *Cost-performance indicator for comparative assessment of water treatment plants* (2012) Science of the Total Environment.

Igos E., Benetto E., Dalle A., Tiruta-Barna L., Baudin I., Méry Y. *Life cycle assessment of water treatment : the role of infrastructure vs operation at unit process level*. Submitted to the journal Cleaner Production in 2012.

In progress

Méry Y., Tiruta-Barna L., Benetto E., Baudin I. *Ecodesign and environmental assessment of a drinking water treatment plant - a case study* To be submitted to the journal Water Research in January, 2013.

Scientific papers published in international journals (not peer reviewed)

Méry Y., Tiruta-Barna L., Baudin I., Roustan M. *Evaluation of environmental impacts of ozone plants - a case study.* Ozone News, 2012.

Conferences with full text and proceedings

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Igos E., Benetto E., Tiruta-Barna L., Ambec S., Bobtcheff C., Rasgelener C., Reynauld A., Baudin I., Méry Y. *Comparative LCA of potable water production plants using economic valuation*. Oral presentation, 6th world congress of the Society of Environmental Toxicology And Chemistry, SETAC, Berlin, 2012.

Tiruta-Barna L., Baudin I., Méry Y., Benetto E. *Eco-conception des procédés de traitement de l'eau: outil intégré « modélisation de procédés - évaluation environnementale ». Application à plusieurs usines d'eau potable*. Oral presentation, Journée Techniques Eaux et Déchets, Toulouse, 2012.

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Summary

CHAPTER 3. MATHEMATICAL MODELLING OF UNIT PROCESSES.................. 63

CHAPTER 4. AN INTEGRATED « PROCESS MODELLING-LIFE CYCLE ASSESSMENT » TOOL FOR THE ASSESSMENT AND DESIGN OF WATER TREATMENT PROCESSES - A PILOT STUDY 87

CHAPTER 5. DETAILED CASE STUDY OF A DRINKING WATER TREATMENT PLANT 109

List of abbreviations

BCAA	Bromochloroacetic acid
BOD	Biological Oxygen Demand
BOD5	Biological Oxygen Demand over a five-day period
CBA	Cost-Benefit Analysis
COD	Chemical Oxygen Demand
CSTR	Continuously Stirred Tank Reactors
DBAA	Dibromoacetic acid
DBCAA	Dibromochloroacetic acid
DBP	Disinfection By-Products
DCAA	Dichloroacetic acid
DCBAA	Dichlorobromoacetic acid
DfE	Design for Environment
DOC	Dissolved Organic Carbon
EE	Elementary effect
EIA	Environmental Impact Assessment
ERA	Environmental Risk Assessment
FAST	Fourier Amplitude Sensitivity Test
GAC	Granular Activated Carbon
HAA	Haloacetic acids
ISO	International Standard Organisation
IT	Information Technology
LCA (ACV)	Life Cycle Assessment (Analyse de Cycle de Vie)
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LHS	Latin Hypercube Sampling
MBAA	Monobromoacetic acid
MCAA	Monochloroacetic acid
MEC	Mean Elimination Capacity
MED	Multi-Effect Distillation

MFA	Material Flow Analysis
moMINLP	Multi-objective Mixed Integer Non Linear Problem
MSF	Multi-Stage Flash
OECD	Organisation for Economic Cooperation and Development
OOP	Object-Oriented Programming
PAC	Powdered Activated Carbon
PM-LCA	Process Modelling - Life Cycle Assessment
POC	Particulate Organic Carbon
PSE	Process Systems Engineering
RO	Reverse Osmosis
SM	Suspended Matter
TAC or CAT	Complete Alkalinity Titration
TBAA	Tribromoacetic acid
TCAA	Trichloroacetic acid
TH	Total Hardness
THM1	Tribromomethane (CHBr3)
THM2	Dibromochloromethane (CHClBr2)
THM3	Bromodichloromethane (CHCl2Br)
THM4	Trichloromethane (CHCl3)
TOC	Total Organic Carbon
Total 5 HAA	Sum of MCAA, DCAA, TCAA, MBAA and DBAA.
Total 9 HAA	Sum of the nine haloacetic acids
Total THM	Total Trihalomethanes
UNEP	United Nations Environment Programme
UNESCO	United Nations Educational, Scientific & Cultural Organisation
UP	Unit Process
USEPA	United States Environmental Protection Agency
USGS	United States Geographical Survey
UVA	UV Absorbance at 254 nm
WHO	World Health Organization

Introduction

Introduction [FR]

De nos jours, le contexte mondial change rapidement, et ce à divers égards. Les sociétés humaines n'ont jamais été confrontées par le passé à des changements aussi importants et elles en portent la plus grande responsabilité. Les révolutions industrielles ont amené des innovations technologiques décisives, qui à leur tour ont façonné notre culture. L'environnement, lui aussi, a été affecté par ces activités industrielles de grande intensité et de progression rapide. A la fin du vingtième siècle, plusieurs indicateurs cruciaux ont atteint des niveaux alarmants, tels que l'utilisation de ressources non-renouvelables et la production de déchets (OECD 2008). En réaction, la prise de conscience collective de ces problèmes a progressé dans les sociétés modernes.

Dans un rapport des Nations Unies datant de 1987 (le dénommé rapport Brundtland), le développement durable s'est vu défini comme le fait de « satisfaire les besoins actuels sans compromettre la possibilité pour les générations futures de satisfaire leurs propres besoins » (Nations Unies 1987). Ce concept a été érigé en principe directeur pour les instances publiques et privées des Nations Unies, et cette définition générale a été reformulée et élargie en fonction du contexte.

La classe politique et les industriels sont maintenant censés prendre des mesures en faveur du développement durable. Le rôle de l'industrie est crucial vis-à-vis de ce problème, car c'est elle qui fournit l'énergie et les matières premières assurant le niveau de vie dans les pays développés ou émergents.

L'industrie des procédés a une place centrale dans l'économie mondiale. Derrière chaque produit (ou du moins ses composants), il y a au moins un procédé permettant d'extraire et/ou transformer les matières premières. Par conséquent, ce secteur industriel se retrouve dans toutes les chaines d’approvisionnement, et joue un rôle primordial dans l'économie moderne.

Plusieurs initiatives dans le monde (par exemple SusChem, la plateforme technologique européenne pour la chimie durable, http://www.suschem.fr) visent à promouvoir une industrie des procédés plus verte, par le biais du recyclage des déchets, de l'efficacité énergétique et d'une gestion raisonnée des ressources. De fait, le but de développement durable tel que le formule le rapport Brundtland ne saurait être atteint sans considérer très attentivement le cas de l'industrie des procédés.

Le secteur de l'eau est confronté à des défis supplémentaires, tels que la rareté grandissante des ressources en eau et l'adaptation aux changements climatiques, la dégradation de la qualité de l'eau, et les exigences du public contre les risques en matière de santé. Un rapport de l'UNESCO attire l'attention sur ces problèmes et met en garde contre l'instabilité politique et les conflits qui peuvent en découler (UNESCO 2009). Lors de son discours au Forum Economique Mondial de Davos en 2008, le secrétaire général des Nations Unies Ban Ki-Moon fit une remarque acerbe à propos des pénuries en eau : « Elles créent des tensions dans des régions sujettes aux conflits. Trop souvent, là où manque l'eau, on trouve des armes. » (Ban Ki-moon 2008). De fait, les problèmes relatifs à l'eau ont des effets de grande ampleur dans nos sociétés et peuvent affecter des aspects essentiels de la vie. Il faut les prévenir grâce à une planification stratégique et une politique environnementale à long terme.

La pénurie en eau est un problème bien connu dans certaines parties du monde, mais il s'étend actuellement à des régions qui ne connaissaient pas la sècheresse par le passé. Elle a de fortes répercussions sur les ressources locales, en ce sens que leur accès et leur traitement sont rendus plus difficiles. La dégradation de la qualité de l'eau s'observe pour certaines ressources en eau, par exemple les eaux souterraines contaminées par des pesticides, et cela rend plus complexe et plus énergivore la chaine de procédés permettant leur traitement.
En parallèle, les problèmes de santé publique liés à l'eau sont cruciaux et les critères afférents se font de plus en plus contraignants dans la plupart des pays.

On demande donc à l'industrie de l'eau de produire de l'eau potable de meilleure qualité, alors que les ressources se font plus rares et plus polluées. Etant donné que l'écart de qualité entre l'eau brute et l'eau potable s'accroit, la réalisation du traitement nécessite naturellement plus d'énergie et/ou de produits chimiques. Ces considérations techniques sont en contradiction avec le principe de développement durable. En d'autres termes, les usines de traitement de l'eau doivent améliorer simultanément leurs performances techniques et environnementales et il peut s'avérer difficile, dans la plupart des cas, de trouver un compromis satisfaisant.

Il y a une impérieuse nécessité de changement de paradigme dans l'industrie et plus largement dans la société. Les ressources naturelles doivent être utilisées avec parcimonie et les déchets doivent être perçus comme des ressources potentielles. Les modes de consommation dans les pays industrialisés doivent changer à brève échéance (UNEP 2002). De tels défis entrainent de nombreuses difficultés, mais ce changement de contexte à l'échelle planétaire est également favorable à l'innovation.

Le travail de recherche présenté dans cette thèse fait partie d'un projet de recherche dénommé EVALEAU (2009-2012). Ce projet a été financé par l'Agence Nationale pour la Recherche (ANR) et le Centre de Recherche Publique Henri Tudor (Luxembourg). Le but principal était d'élaborer une nouvelle approche méthodologique et les outils connexes, afin d'évaluer les performances d'usines de production d'eau potable sur les plans environnemental, économique, technique et sanitaire, afin d'apporter une aide objective au processus de prise de décision dans le domaine de l'eau potable. Améliorer la pertinence des critères thermodynamiques (c'est-à-dire l'exergie et l'émergie) et économiques pour l'évaluation environnementale était aussi un des objectifs originaux de ce projet.

Un partenariat fondé sur la diversité et la complémentarité des compétences ont permis d'atteindre les objectifs de recherche. Les partenaires impliqués dans le projet apparaissent dans la liste suivante :

- Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés LISBP (Université de Toulouse, INSA Toulouse, CNRS, INRA)
- Centre des Ressources pour les Technologies et l'Environnement CRTE (Centre de Recherche Public Henri Tudor, Luxembourg)
- Centre International de Recherche Sur l'Eau et l'Environnement CIRSEE (Suez Environnement, Paris)
- Laboratoire d'Economie des Ressources NAturelles LERNA (Université de Toulouse, INRA)

Les objectifs principaux de ce travail de recherche sont le développement d'un outil intégré pour la modélisation de procédés et l'analyse de cycle de vie, ainsi que la formulation d'une approche méthodologique affiliée pour l'écoconception de procédés. L'outil logiciel et l'approche méthodologique sont appliqués à la production d'eau potable.

Cette thèse est structurée autour de cinq chapitres qui sont brièvement décrits ci-dessous.

Le chapitre 1 passe en revue la littérature existante sur la méthodologie ACV (Analyse de Cycle de Vie), les outils et les applications connexes dans les industries des procédés et de l'eau. Les objectifs du projet de recherche sont formulés en conséquence.

Le chapitre 2 décrit en détail le cadre méthodologique, l'architecture de l'outil logiciel, les approches de modélisation proposées, et les pratiques d'éco-conception adéquates qui en découlent. Les concepts présentés dans ce chapitre sont censés être transposables à d'autres industries des procédés.

Le chapitre 3 introduit la modélisation des procédés unitaires du point de vue de l'ingénierie logicielle. En outre, les procédés unitaires pour la production d'eau potable apparaissant dans la bibliothèque logicielle sont listés, et leur modélisation mathématique est passée au crible dans une annexe technique dédiée, garantissant ainsi la transparence de ce travail.

Le chapitre 4 présente succinctement l'outil EVALEAU et ses principales caractéristiques, avant d'illustrer les concepts mis en avant à l'aide d'une étude pilote. Ce chapitre se veut une introduction au cadre méthodologique de l'outil. Ce chapitre est en fait un article scientifique publié dans un journal référencé à comité de lecture.

Le chapitre 5 est une étude de cas détaillée d'une usine de production d'eau potable située dans la région parisienne. Suite à la validation de la modélisation de la qualité de l'eau, un modèle prédictif de l'usine est établi en tant que scénario de base. Une analyse approfondie est menée permettant ainsi une meilleure compréhension du fonctionnement de l'usine. Des solutions alternatives de traitement sont ensuite étudiées des points de vue environnemental et économique. Cette étude de cas détaillée vise à montrer comment l'écoconception peut être mise en œuvre dans l'industrie de l'eau.

Introduction [EN]

Nowadays, the worldwide context is rapidly changing in various aspects. Human societies have never faced such important changes in the past and they are mostly responsible for these. Industrial revolutions lead to some major technological innovations which shape human culture in return. The environment has also been affected by these intense and fast-growing industrial activities. At the end of the twentieth century, several key indicators have reached alarming levels such as use of non-renewable resources or waste generation (OECD 2008). Public awareness of these concerns has increased in modern societies as a reaction.

In a report of the United Nations dated of 1987 (the so-called Brundtland report), sustainable development was defined as the fact of « meeting the needs of the present without compromising the ability of future generations to meet their own needs » (United Nations 1987). This concept has been given as a guiding principle for public and private entities of the United Nations and this general definition has been reformulated and extended depending on the context.

Policy makers and industry managers are now expected to take action towards sustainability. The role of industry is critical regarding this issue as it is the provider for energy and raw materials supporting the standard of living in developed and emerging countries.

The process industry is central in the worldwide economy. Behind every product (or its components), there is at least one process to extract and/or transform the required raw materials. Therefore, this industrial sector is present in every value chain and plays a major role in the modern economy.

Several initiatives around the world (e.g. SusChem, the European technology platform for sustainable chemistry; http://www.suschem.fr) promote a greener process industry through waste recycling, energy and resource efficiency. Indeed, the goal of sustainable development as formulated in the definition of the Brundtland report cannot be achieved without considering carefully the case of the process industry.

The water sector is confronted to additional challenges like water scarcity and adaptation to climate change, deterioration of water quality, public heath demands against sanitary risks. A UNESCO report points at these issues and warns about political instability and conflicts that they may cause (UNESCO 2009). During his speech at the Davos World Economic Forum in 2008, United Nations Secretary-General Ban Ki-moon made a sharp remark about water shortages : « They create tensions in conflict-prone regions. Too often, where we need water we find guns. » (Ban Ki-moon 2008). Indeed, water related problems have effects on a large scale in our society and essential aspects of life can be affected. They must be prevented thanks to strategic planning and long-term environmental policy.

Water scarcity is a well-known problem in some places of the world but it is spreading over regions where no drought occurred in the past. It strongly affects the local water resources, i.e. the access to these sources and the water treatment based on them become more difficult. Deterioration of water quality is recorded for some water resources (e.g. ground waters contaminated by pesticides). It makes the process chain treating these water sources more complex and more energy-consuming.
In the mean time, public health issues related to water are crucial and the relative standards are becoming more and more restrictive in most countries.

The water industry is therefore asked to produce better drinking water quality while resources are becoming scarcer and more polluted. As the quality gap between raw water and drinking water is increasing, it logically requires more energy and/or chemicals to achieve the treatment. This technical consideration is in contradiction to the precepts of sustainable development. In other words, water treatment plants must improve their technical and environmental performances at the same time and it may be difficult to find a suitable trade-off in most cases.

There is an imperative for a paradigm shift in industry and more generally in society. Natural resources must be used sparingly and waste must be seen as potential resources. The consumption patterns of citizens in industrialised countries must change in the near future (UNEP 2002). Numerous difficulties come with these challenges but this changing context is also favourable for innovation.

The research work presented in this Ph.D. dissertation is part of the research project named EVALEAU (2009-2012). This project was funded by the French National Research Agency (ANR) and the Public Research Centre Henri Tudor (Luxemburg). The main purpose was to develop a methodological approach and the related tools in order to assess the environmental, economic, technical and sanitary performances of drinking water treatment plants and to support the decision-making process in the field of drinking water. Improving the consistency of thermodynamic (i.e. exergy and emergy) and economic criteria for environmental assessment was also an original objective of this project.

A complementary and multi-skills partnership ensured the achievement of the research objectives. The partners involved in the project are listed below :

- Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés LISBP (Université de Toulouse, INSA Toulouse, CNRS, INRA)
- Centre des Ressources pour les Technologies et l'Environnement CRTE (Centre de Recherche Public Henri Tudor, Luxembourg)
- Centre International de Recherche Sur l'Eau et l'Environnement CIRSEE (Suez Environnement, Paris)
- Laboratoire d'Economie des Ressources NAturelles LERNA (Université de Toulouse, INRA)

The objectives of the research work presented in this Ph.D. dissertation are the development of a software tool for the full integration of Process Modelling and Life Cycle Assessment (PM-LCA), and the formulation of a methodological framework for process ecodesign, applied to the water treatment industry.

This Ph.D. dissertation is structured around five chapters which are briefly presented below.
Chapter 1 is a literature review on LCA methodology, related tools and applications in the process and water industries. The objectives of the research project are consequently stated in the light of the state-of-the-art.
Chapter 2 describes in detail the methodological framework, the IT tool architecture, the proposed modelling approaches and the resulting proper ecodesign practices. The concepts presented in this chapter are meant to be transposable to other process industries.
Chapter 3 introduces the modelling of unit processes from a software engineering point of view. Besides, the unit processes for drinking water production that appear in the

computational library are listed and their mathematical modelling is scrutinized in a dedicated technical appendix as a guarantee of transparency.

Chapter 4 briefly presents the EVALEAU tool and its main features, and then illustrates the concepts put forward with a short case study. This chapter aims at introducing the methodological framework of the tool. This chapter is in fact a scientific paper published in a peer reviewed journal.

Chapter 5 is a detailed case study of a drinking water treatment plant located in the Paris area. After validating water quality modelling, a predictive plant model is established as a ground modelling scenario and an in-depth analysis is carried out which provides a better understanding of the current functioning of the plant. Alternative treatment solutions are then studied from environmental and economic points of view. This detailed case study intends to demonstrate how ecodesign can be put into practice in the water industry.

Chapter 1.

Literature review and research objectives

Résumé du chapitre 1. Revue de la littérature scientifique et objectifs de recherche.

Ce chapitre débute par une revue complète de la littérature scientifique ayant trait aux différentes méthodes d'évaluation environnementale. Parmi les principales méthodes, on peut citer l'évaluation des risques pour l'environnement, l'évaluation des impacts sur l'environnement ou encore l'analyse coûts-bénéfices, et bien sûr l'analyse de cycle de vie (ACV). Ces méthodes d'évaluation environnementale diffèrent sur certains points (par exemple, certaines peuvent avoir une valeur locale tandis que d'autres ont une portée plus large) mais chacune a son intérêt.

L'ACV est une méthode qui a été dûment normée, ce qui a aidé à sa reconnaissance dans les milieux scientifique et industriel. Une de ses caractéristiques est de s'intéresser à l'ensemble du cycle de vie d'un produit/procédé. Le fait de considérer les différentes étapes de la vie d'un produit/procédé permet d'éviter le transfert d'impact, et cela est assurément un gage d'objectivité.

Pour mener à bien une ACV, il faut passer par quatre étapes indispensables à l'application de cette méthodologie telle que définie dans la norme ISO 14040-2006 :

1. Définition des objectifs et du champ de l'étude.
2. Recueil de l'inventaire de données et analyse de celui-ci.
3. Evaluation des impacts environnementaux.
4. Interprétation des résultats

Les premières applications de l'ACV concernaient des produits, mais de plus en plus d'études adoptent une approche procédé. De nombreux auteurs ont ainsi argumenté que l'ACV pouvait être un bon complément au dimensionnement et à l'analyse de procédés dans une optique d'écoconception (Azapagic and Clift 1999; Bakshi and Fiksel 2003; Grossman and Westerberg 2000; Grossman et al. 2004; Jacquemin et al. 2012; Kniel et al. 1996).

Mais les applications concrètes manquent encore cruellement. Des outils de modélisation flexibles sont nécessaires pour mettre l'ACV au service de l'écoconception de procédés et à l'heure actuelle, aucun n'est vraiment adapté pour intégrer parfaitement l'ACV au stade du dimensionnement d'une usine de procédés.

Dans une revue récente sur l'ACV dans l'industrie des procédés (Jacquemin et al. 2012), il est recommandé par les auteurs d'étudier l'influence du dimensionnement et des conditions opératoires sur les résultats d'impacts environnementaux. A notre connaissance, seulement deux études relèvent en partie ce défi. Guillén-Gosálbez et al. ont intégré des calculs d'ACV dans un programme de simulation de procédés, ce qui leur a permis d'optimiser la configuration des procédés dans l'usine simulée (Guillén-Gosálbez et al. 2008). Gerber et al. ont étudié quant à eux l'influence des conditions opératoires d'un procédé de production énergétique à partir de biomasse lignocellulosique (Gerber et al. 2011).

Dans le domaine du traitement de l'eau, un outil ACV appliqué à la production d'eau potable a été développé par Vince et al. (Vince et al. 2008a). Les auteurs ont ensuite étudié l'influence du dimensionnement et des conditions opératoires d'une usine d'osmose inverse sur les impacts environnementaux générés (Vince et al. 2008b). Cependant, il ne s'agissait pas réellement des impacts calculés par la méthode ACV, mais seulement d'un paramètre censé être représentatif des impacts générés par une usine, à savoir la consommation électrique. Par conséquent, l'étude manque d'objectivité et peut être mise en doute puisqu'il peut y avoir eu transfert d'impact. Ceci est dû au fait que l'outil développé n'intègre pas en une seule structure tous les aspects (environnementaux, techniques et économiques) et les calculs ACV ne sont que superposés à la simulation de procédés.

Concernant les outils de modélisation des procédés de production d'eau potable, une revue très complète a été rédigée par Dudley et al. 2008 (Dudley et al. 2008). La principale conclusion est que l'approche de modélisation adoptée dans le domaine du traitement de l'eau est trop souvent empirique. Les modèles ainsi développés ont par conséquent besoin de beaucoup de données pour être calibrés, et sont spécifiques à un site de production ou à un contexte très particulier, le meilleur exemple étant celui du procédé de coagulation. C'est pourquoi l'industrie de l'eau manque d'outils de modélisation fiables et pratiques.

Partant de ces différents constats, les objectifs de recherche du projet et les lignes directrices pour le développement de l'outil ont été établis.

Chapter 1. Literature review and research objectives.

1. Literature review

This section presents the state-of-the-art regarding fundamental issues for this research work. Firstly, the LCA methodology and general principles are introduced. Applications of LCA in the process and water industries are then presented to show the potential outcomes of this methodology and the required research efforts. Coupling of process modelling and LCA is further investigated and limitations in the context of drinking water production are explained.

The point of view adopted for this literature review is the one of the process industry (the water industry being part of it). Specific water issues are not considered intentionally (e.g. water footprint and water use in LCA methodology).

1.1 LCA methodology and general principles

In the second part of the twentieth century, depletion of natural resources and environmental damages on ecosystems provoked by human activities encouraged governments to establish new environmental regulations. They were not coordinated at the international level but they compelled the industry to initiate actions on these environmental issues (Harold and Ogunnaike 2000). At first, mitigation measures were the response proposed by the industry to deal with generated environmental impacts. They progressively become anticipatory measures meant to avoid irreversible environmental impacts (Young et al. 1997).

Several techniques and methodologies for environmental assessment have been developed to better understand the issues at stake and to make appropriate decisions. Among all these techniques, some are more often used and they are briefly introduced below :

- Environmental Risk Assessment (ERA) evaluates the risks due to an industrial activity for the surrounding ecosystems and human populations (Burgess and Brennan 2001). Risk management is put into practice based on this technique and industrial disasters are avoided thanks to prevention measures.

- Environmental Impact Assessment (EIA) provides qualitative and quantitative information in a predictive manner. Environmental impacts are well assessed but this technique has one important limitation. It is case specific in terms of location, time and industrial activity (Burgess and Brennan 2001).
- Cost-Benefit Analysis (CBA) intends to integrate environmental quality (improvement or deterioration) as an economic value in a conventional cost-benefit analysis of a project (Pearce 2006).
- Life Cycle Assessment (LCA) consists in assessing the environmental impacts of a product, process or service considering all the steps of its life cycle (raw material extraction, manufacturing, use and maintenance, end-of-life and disposal, etc.).

These environmental assessment techniques give different insights on the considered system and do not allow concluding about the same aspects. The technique used within a project must be selected depending on the study's objectives and the questions to be answered. They could also be used in combination as they are complementary.

The acceptance of the LCA methodology is increasing both in the scientific community and in industry. It provides a comprehensive understanding of the system under study and its environmental impacts which are classified in different impact categories and assessed quantitatively. Besides, the LCA methodological framework has been standardised (ISO Standard 14040 2006) and this makes the LCA methodology more widely trusted.

The regular sequence of an LCA study must always be constructed as defined in the ISO standard. There are 4 steps in the LCA methodology :

1. *Goal and scope definition*. LCA starts by defining the context and the purpose of the study, the objectives and the information sought for. The people to whom the results are intended to be communicated must be explicitly stated. Practical information must include the functional unit (the function delivered by the system which is often a reference material or service) and the system boundaries. Assumptions and/or limitations are also part of this exhaustive description of the study as they can bias the interpretation of the results.
2. *Inventory analysis*. The inventory is a list of all inputs and outputs of the system called the Life Cycle Inventory (LCI). Energy demand and raw materials typically represent inputs and pollutant emissions to air, soil or water are the outputs of the system as well

as the delivered functional unit. Elementary flows crossing the system boundaries are calculated/measured/estimated in relation with the functional unit. LCA databases provide LCI for conventional and widely used products or processes (e.g. electricity production).

3. *Environmental impact assessment*. This step is also called Life Cycle Impact Assessment (LCIA). Potential impacts due to input and output flows (i.e. LCI flows) are evaluated. An evaluation method (i.e. LCIA method) and impact categories must be selected to be consistent with the objectives and the scope of the study. An evaluation method calculates the contribution of each LCI flow to the different impact categories through characterization factors.
4. *Interpretation*. In this final step, the goal and scope of the study strongly influence the conclusions drawn from the LCI and LCIA results. Major contributions to environmental impacts can be identified and quantified. Recommendations can be stated and improvement levers may be detected. Assumptions and limitations of the study must be reminded when they change the interpretation of the results.

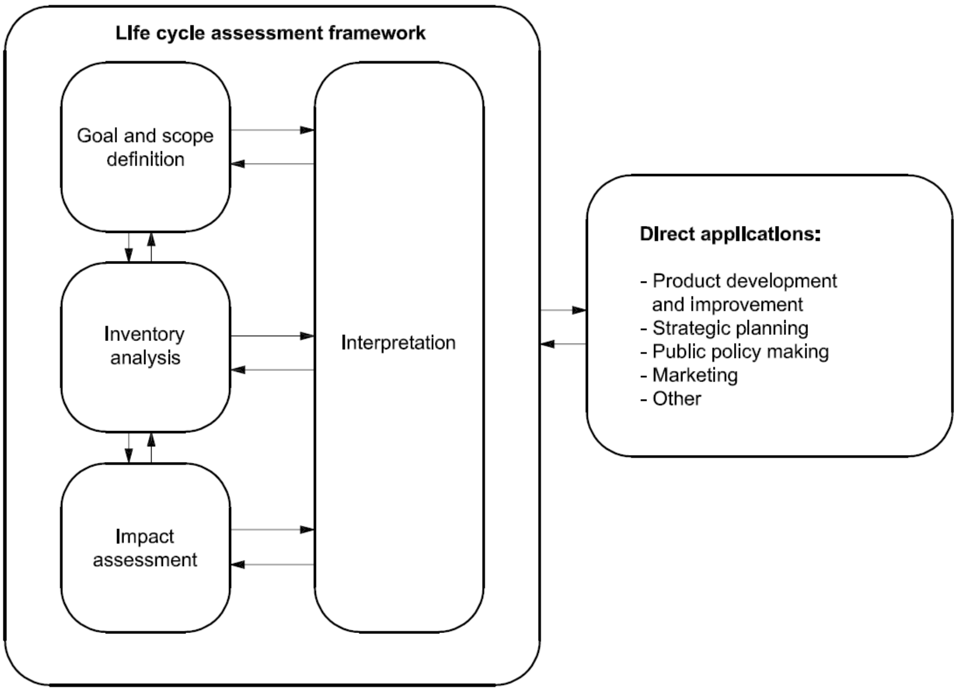


Figure 1-1. The 4 steps of an LCA (from ISO Standard 14040 2006).

Goal and scope definition must be explicitly and precisely defined to ensure the quality of the results' interpretation. Any ambiguity leads to distorted interpretation of the results and this is justifiably the criticism most often voiced against LCA studies.

A distinctive feature of this approach is that all life cycle steps (usually from cradle to grave) are part of the environmental assessment. Conclusions of an LCA study take into account the entire life cycle avoiding mistakes due for instance to pollution transfer between two life cycle steps. Therefore, it makes LCA a robust and objective aid for decision-making.

A plethora of publications on LCA methodology are henceforth available in the literature. Numerous LCA reviews (Pennington et al. 2004; Rebitzer et al. 2004; Bare 2010) give detailed information on LCA methodological framework, current practices and applications.
Another LCA review written by Finnveden et al. focuses more on recent methodological developments and emerging issues related to LCA applications (Finnveden et al. 2009). Important LCA challenges for future developments are discussed such as attributional and consequential LCA, allocation procedures, system boundaries (considering time and geographic limits), data uncertainty, LCA databases and tools. Among other things, the authors stress the need to develop LCA tools for subsystems or unit processes when they are not within the scope of common LCA databases. They mention examples of LCA modelling tools from waste management and chemical industries. They outline the utility of "detailed models with enhanced flexibility" encouraging the development of this sort of model.

The first applications of the LCA methodology were mostly on products. The aim was to identify key life cycle steps and major environmental impacts due to the use or consumption of a product. LCA studies on processes have only gained importance more recently (Burgess and Brennan 2001; Jacquemin et al. 2012).

1.2 LCA in the process industry

1.2.1 A new challenge for the process industry

In the last decade, several studies have argued that process analysis and design can be improved and complemented by including environmental considerations at early design stage. A major challenge arises from this opportunity and many authors acknowledge that LCA is a methodology suited for this task (Azapagic and Clift 1999; Bakshi and Fiksel 2003; Grossman and Westerberg 2000; Grossman et al. 2004; Jacquemin et al. 2012; Kniel et al. 1996). Coupling of process modelling and LCA tools is necessary to effectively perform ecodesign and this must be tackled for introducing ecodesign practices in the process industry. (Azapagic et al. 2006; Grossman et al. 2004).

The integration of environmental considerations into Process System Engineering (PSE) tools for process analysis has lead to the concept of Design for Environment (DfE) (Sroufe et al. 2001). It is a predictive approach put into practice at the design stage and it is standardised in the ISO standard 14062 EMS (ISO Standard 14062 2003). Typical DfE applications for the process industry are redesign and use of green chemicals for example (Bakshi and Fiksel 2003).

1.2.2 Need for detailed and flexible models

Despite the incentives to integrate sustainability criteria into process design, only a few attempts are found in the literature (Azapagic et al. 2006). The main scientific barrier is the inflexibility of models representing process plants in LCA. This is a legacy of the product approach of the very first LCA applications where these life cycle steps were modelled as black boxes. In this context, production processes were not optimised regarding environmental performances as they were conventionally and rigidly designed.

The first author to follow the LCA methodology on a process system model was Furuholt in 1995 (Furuholt 1995). The author modelled a refinery as a sequence of unit processes, each of them consuming energy and/or chemicals and releasing pollutants in the environment. The unit process models were black boxes (i.e. fixed process functioning) but still, the accuracy of the method was sufficiently improved and the analysis of the plant regarding environmental issues was made possible. The production and use of three fuel products were compared and unit processes heaving the most on LCA results were identified.

As the modelling of process systems became more advanced in LCA applications, it allowed environmental impacts to be part of the design criteria. The use of LCA as a design tool for processes was firstly affirmed by Kniel et al. in their research work on a nitric acid plant (Kniel et al. 1996). The authors attempt to optimise the plant from both environmental and economic points of view.

The international research community insisted on this area of investigations and numerous approaches were proposed. Khan et al. described a methodology for process ecodesign called “GreenPro” (Khan et al. 2001). Sugiyama et al. reported about a decision framework aimed at process design integrating technical, economic and environmental issues (Sugiyama et al.

2008). A major problem was yet unresolved in the sense that detailed process modelling was achieved prior to the LCA calculations as an upstream step. In other words, environmental impacts were calculated consecutively to a conventional process design obtained with a regular simulation tool (Baratto and Diwekar 2005; Bojarski et al. 2008; Iosif et al. 2010; Portha et al. 2010; Kikuchi et al. 2010; Kniel et al. 1996) and LCA was in fact studied on different black box models (corresponding to different process functioning). A genuine ecodesign activity must not consider technical, economic and environmental issues in successive steps but rather at the same time, in order to support decisions objectively from the start.

Guillén-Gosálbez et al. overcame this technical limitation of current IT tools by integrating LCA calculations within a flowsheeting program (Guillén-Gosálbez et al. 2008). They optimised the configuration of the studied plant (i.e. the sequence of unit processes) regarding LCA results within a multi-objective Mixed Integer Non Linear Problem (moMINLP). The optimisation was based on the process sequence and not on their operating conditions.
The influence of process design and operating conditions on LCA results was studied by Gerber et al. (Gerber et al. 2011). The case study was about energy production from lignocellulosic biomass. To our knowledge, it is the only LCA study that fully integrates process design and functioning aspects and their repercussions on the different result categories in an automated manner thanks to efficient programming.

Within the product approach, supply chain management is put into practice because it is not possible to act on the production processes. The main option to reduce environmental impacts of a product is to select the best supply chain (comprising fixed functioning processes). Within the process approach, it is normally possible to undertake actions on the operating conditions and design facts because these are parameters under control on the field so they should be in the modelling scenario as well. Moreover, ecodesigning one process plant often leads to an improvement of environmental performances of all the supply chains in which it is involved. It definitely makes this approach powerful because of its wide range of influence. Thus the process industry should be actively involved in LCA future developments and more particularly in the development of fully integrated PSE-LCA tools (Jacquemin et al. 2012).

Process scientists and engineers need to understand the system's behaviour in order to make it more efficient. They cannot meet ecodesign objectives with black box models. Unit process models must take into consideration operating conditions and design parameters in order to study their influence on the different result categories (technical, economic and environmental). The approach has been recently recommended by many authors since the prospects are promising and encouraging (Jacquemin et al. 2012).

1.2.3 Decision-support with mathematical techniques

In addition, as the LCI usually gives access to mass and energy balances, multi-optimization on environmental and economic issues is then feasible within an ecodesign perspective (Dietz et al. 2006; Ouattara et al. 2011). One prerequisite is the development of fully integrated tools to automatize this kind of mathematical analysis (Grossmann and Guillén-Gosálbez 2010; Chen et al. 2004). A large number of calculations may be ordered by multi-optimization techniques and they could not be handled manually. Other mathematical analysis techniques can be envisaged as well (e.g. sensitivity and uncertainty analysis).

1.2.4 Knowledge transfer into practice

Ernzer et al. carried out interviews of industrial actors and desk research about the use of DfE tools and ecodesign practices in industry. They observed that “most results end up in scientific publications rather than being transferred into practice” (Ernzer et al. 2003). Therefore, more efforts are required to make ecodesign tools more practical and easily understandable for non experts. Research scientists and process engineers must remedy this situation in order to act effectively towards sustainable development.

1.3 LCA in the water industry

1.3.1 Contribution of plant life cycle phases to LCA results

The life cycle of a water treatment plant can be divided into three phases : construction, operation and decommissioning. The relative contribution of each phase to the total environmental impacts has been evaluated only by a few authors.

Friedrich studied it on one conventional and one membrane-based water treatment plants (Friedrich 2001). Both case studies showed that the construction phase is responsible for approximately 15% of the total environmental impacts and the decommissioning phase for less than 1%. The environmental impacts of the construction phase were mainly due to steel production (about 80%). The operation phase was the main contributor to the total environmental impacts.

Raluy et al. published a study on three water treatment plants based on different types of desalination technology : Multi-Effect Distillation (MED), Multi-Stage Flash desalination (MSF) and Reverse Osmosis (RO) membrane separation (Raluy et al. 2005). The environmental impacts of the decommissioning phase were negligible (less than 1%) and those of the construction phase were less than 4% (except for the MED-based plant impacts evaluated with the Ecopoints 97 method). Desalination technologies (particularly thermal desalination technologies, MED and MSF) are intensive energy-consuming processes and consequently, the contribution of the operation phase is even more important than the one obtained by Friedrich (Friedrich 2001).

Special attention has been dedicated to this issue during the EVALEAU research project. An LCA study has been carried out to assess the respective contributions of the construction and operation phases to the global environmental impacts of two drinking water treatment plants (Igos et al. 2012). Environmental impacts of both life cycle phases were evaluated at unit process level. The LCIA evaluation method used were Recipe (Goedkoop et al. 2009) and Impact 2002+ (Jolliet et al. 2003).

The study confirmed the results published in the literature (Friedrich 2001; Raluy et al. 2005). The environmental impacts of the construction phase for the two studied plants were 11% and 6% with the Recipe method and 7% and 4% with the Impact 2002+ method. The main source of impacts was steel production. At unit process level, the contribution of the construction phase was approximately the same even though the infrastructure of some processes (e.g. disinfection) is responsible for proportionally higher environmental impacts.

The operation phase is thus considered the main life cycle phase contributing to the environmental impacts generated by a drinking water treatment plant and the other phases can be neglected for sake of simplicity. The scientific literature is not abundant on this topic and definitive conclusions should not be drawn from such limited results. For instance, investment costs for plant construction are often proportionally higher for small water treatment plants. This scale effect can influence the environmental impacts analogously and potentially leads to a higher contribution of the construction phase. This is only a hypothesis since there is no such study in the scientific literature but it is realistic and it has to be kept in mind.

1.3.2 Range of LCA applications in the water industry

Numerous LCA papers on water treatment technologies have been recently published in the scientific literature. The range of these case studies is large and can be summarised with the following areas of investigation :

1. drinking water treatment
2. industrial and urban wastewater treatment
3. strategic planning
4. environmental and economic assessment

LCA studies on drinking water mostly focused on membrane and desalination technologies. These technologies usually generate higher on-site energy consumptions than conventional ones. LCA methodology is used to assess whether their global life cycle is responsible for higher environmental impacts or not (Friedrich 2002; Raluy et al. 2005; Sombekke et al. 1997). Indeed, LCA is suited for fairly comparing water treatment technologies by taking into account off-site emissions due to chemical production for instance. Results from the literature show that desalination plants are not necessarily more polluting than conventional ones.

During the last decade, various alternatives for wastewater treatment have been investigated on the basis of LCA methodology. Lundin et al. compared urine separation (from the rest of the urban wastewater mix) with conventional wastewater treatment (Lundin et al. 2000). Better results were obtained by the authors for the urine separation scenario because of reduced emissions to water bodies and nutrient recovery and reuse in agriculture. Lundin et al. argued that the system's boundaries should be extended to take into account fertilizer production when studying such alternative treatment solutions. Benetto et al. studied a decentralised system for wastewater treatment and reported about its potential for reducing environmental impacts of small-scale unit (Benetto et al. 2009).

Renou et al. used five different LCIA evaluation methods on one wastewater treatment plant and compared the results (Renou et al. 2007). The authors observed that the impact assessment methods lead to similar results for some impact categories but significantly different ones for others, thus highlighting requirements for future research on LCIA evaluation methods.

Besides, even if scientific papers mostly deal with urban wastewater, environmental impacts of industrial wastewater treatment have also been studied in the literature (Vlasopoulos et al. 2006).

On a larger scale, Muñoz et al. compared two strategies concerning water supply for Mediterranean regions in Spain (Muñoz et al. 2010). The authors considered the previous strategy (based on transfer between watersheds) and the present one (based on use of alternative resources). They quantified the environmental impacts induced by both scenarios and highlighted how LCA can contribute efficiently to the decision-making process. Lundie et al. also applied LCA methodology for strategic planning in the Sydney area. (Lundie et al. 2004). The originality is that the authors considered both drinking water production and wastewater treatment.

An environmental and economic assessment has been carried out on drinking water production for the Amsterdam area by Barrios et al. and Tapia et al. (Barrios et al. 2008; Tapia et al. 2008). A ground scenario served as a basis for future alternative scenarios while considering both environmental and economic aspects of the project. The objective of reducing costs as well as environmental impacts was clearly displayed in this two-part study.

LCA methodology has found many applications in the water industry over the last few years. Nevertheless, the effects of design and operating conditions of unit processes are still often disregarded despite recommendations of the scientific community in this respect (Jacquemin et al. 2012). The main reason is a lack of generic and flexible models for unit processes involved in water treatment.

To our knowledge, Vince et al. are the only authors that managed to take into consideration design and operating conditions of drinking water production plants in LCA thanks to a dedicated tool (Vince et al. 2008a). Unfortunately, the decision variables are not explicitly detailed in this first paper. The authors focused on desalination technologies in a second paper. They studied the influence of design and operating conditions for RO desalination plants within a multi-objective optimisation framework (Vince et al. 2008b). The pre-treatment chain was not included in the simulation and only the membrane system was optimised. Environmental impacts were not calculated through LCA methodology, only electricity consumption was taken into account as an objective for optimization. Although this criterion is supposed to be representative of the environmental impacts of a desalination plant, it is not based on LCA methodology and it lacks objectivity for environmental impact assessment.

1.4 Process modelling for drinking water treatment

The history of water treatment goes back to ancient times. In the Egyptian civilisation, clarification of water was achieved by coagulation since approximately 2000 B.C. (Bratby 2006). The coagulant agents were crushed seeds (e.g. almonds) used during seasonal flood events due to the Nile River. In more recent times, use of aluminium-based coagulants for water treatment has been reported in England since 1757 (Faust and Aly 1998).

Despite the long history of water treatment processes, their mathematical analysis is not a mature scientific discipline as possibly expected. For instance, there is an agreement on the fact that coagulation modelling is still an issue for water engineers (Dudley et al. 2008). This unit process is designed with rules of thumb and basic experimentation (e.g. jar-tests). The corresponding models are data-driven and site-specific.

For instance, neural network models to predict coagulant doses were applied on water treatment plants in Canada and Australia (Gagnon et al. 1997; Maier et al. 2003). In the work of Gagnon et al., the aim was to develop a tool able to predict the required coagulant dose based on four input water quality parameters (pH, turbidity, conductivity and temperature). More than 500,000 measurements for each of the four input water quality parameters were necessary to develop a robust neural network. Despite all the efforts, the neural network was linking the input water quality to the coagulant dose determined by the plant operator with conventional jar-test experimentation. In fact, the neural network had learnt about the empirical knowledge of the plant operator and reproduced it.

A review on predictive models for Disinfection By-Products (DBP) formation in drinking water listed all the models on this topic available in the literature (Sadiq and Rodriguez 2003). The authors noted that they all contain empirical equations requiring extensive data for calibration.

Mathematical modelling of water treatment processes most often suggests site-specific and data-intensive approaches. This is not complying with basic recommendations for the use of process models in design tools. Therefore, the water industry consequently lacks efficient modelling tools in spite of the benefit of hindsight.

The balance between empirical approaches and formal mathematical modelling must be reconsidered in water treatment simulation. There is a need for more mechanistic models.

A literature review written by Dudley et al. (Dudley et al. 2008) leads to the same observation. Three reasons are given by the authors to explain the non use (or bad use) of mathematical modelling and flowsheeting programs in the water industry :

1. There are only a few available process models (i.e. the completeness of computational model libraries is not satisfactory).
2. Mathematical modelling is perceived as an academic exercise as opposed to field operations (i.e. it is remote from the issues faced by water engineers working on the field).
3. Expectations among water engineers about process modelling are often too high.

Development of an IT tool is an adaptive and iterative work which requires modelling and research efforts as well as collaboration of future users (Agile manifesto website). Time is also needed. Thus water engineers should not expect too much from a modelling tool at first and they should preferably be disposed to contribute to its development.

However, in the review on water treatment simulators (Dudley et al. 2008), the authors focused on the most relevant modelling tools applied to water treatment because of interesting features. The tested tools were Otter (WRc), Stimela (TU Delft), WTP (US EPA), Metrex (TU Duisberg), WatPro (Hydromantis). The main issues related to process flowsheeting are part of the review (e.g. recycle loops and handling of any discontinuities within dynamic simulations) but these mathematical considerations are not specific of the water sector and they will not be tackled in this research project.

The development of a modelling tool is strongly affected by its objectives and the questions to be answered with it. As the five studied modelling tools do not have the same goals, there are differences and the main ones are listed below :

1. dynamic or steady-state simulations
2. targeted end-users (practising engineers or researchers)
3. water quality parameters under consideration
4. unit processes under consideration
5. Empiricism of the process models and data requirements for calibration (empirical models versus mechanistic models)

Two special features are of great interest and must be an inspiration for the development of future modelling tools.

1. In the Stimela framework, unit process models are stored in a library freely accessible to the user. The source code is open, that is to say the user has access to the code lines defining the process models which can be modified and/or extended. Complementary unit process models can be stored in the library. This very flexible modelling environment enables the user to integrate additional knowledge in the model library and to use it as a collaborative platform for research and development.
2. In the software Metrex, two modelling approaches have been created : the operation mode and the design mode. Required data for calibration and study objectives are different depending on the situation (operation or design of the plant), so the models must be different as well. This is a very relevant modelling approach for water treatment processes and it certainly leads to more consistent modelling scenarios.

The authors conclude the review on water treatment simulators by presenting the main weak point of the studied modelling tools : extensive data requirements for calibration of empirical models, especially coagulation models. This issue must be tackled while developing the next-generation IT tools for water treatment modelling.

Numerous other tools for water treatment simulation exist. Private companies and public laboratories often develop their own modelling tools based on specific knowledge and objectives.

Tools from other scientific disciplines are sometimes appropriated for water treatment. For instance, the geochemical software PHREEQC® (PHREEQC website) has been used in research studies on water treatment (Telzhensky et al. 2011). This is an interesting approach since water treatment simulation could benefit from modelling efforts of previous research in other scientific areas.

2. Conclusion and objectives

Within a perspective of sustainable development, industrial systems must be designed on the basis of technical, economic and environmental criteria. LCA is a methodology recognised by the scientific community for considering environmental issues during the decision-making process. Moreover, it has been standardised by the International Organization for Standardization and that makes it more widely trusted.

Ecodesign practices must be introduced in the process industry but there is still one major requirement to make progress : the development of detailed and flexible models at unit process level. Operating conditions and design parameters must be part of this modelling approach and their influence on LCA results should be further investigated in order to find action levers on the field.

In addition, mathematical analysis techniques can effectively support the ecodesign activity by improving the understanding of the process system under study.

The main scientific obstacle to performing ecodesign on drinking water treatment plants is the lack of generic and flexible models in this area. Mechanistic models should be favoured over empirical and statistical ones for next-generation IT tools related to drinking water treatment.

Regarding the current state-of-the-art, the global objective of the EVALEAU research project was to develop an IT tool for multi-criteria decision support in the field of drinking water production. The underlying objectives were to provide the water industry with a genuine ecodesign tool and to foster related engineering practices.

The development of the EVALEAU tool was achieved in three main steps which are presented below :

1. Development of a model library for unit processes involved in drinking water treatment.
2. Integration in a computer framework enabling plant flowsheeting and providing access to common LCA databases.
3. Development of a toolbox for mathematical analysis in order to support the ecodesign activity.

The first step was fundamental and it was the core task of the research project. Recommendations from the literature were carefully taken into consideration and since then, some of the technical requirements for the development of the computational library have been established in view of the state-of-the-art. They are listed below with no particular order of importance :

- The library must comprise models for unit processes involved in conventional drinking water treatment in order to cover most cases encountered. Special attention must be dedicated to the coagulation process as it is the most problematic in terms of modelling.
- Two distinct modelling approaches must be available : the retrofit approach for when the plant is already in operation, and the predictive approach for when the plant is about to be designed.
- Mechanistic models must be favoured over empirical and statistical ones.
- The unit process models must be able to provide a reliable and predictive list of material consumptions (i.e. energy and chemicals) as it is a prerequisite for ecodesign.
- The three result categories (technical, economic and environmental) must be calculated in parallel and not in successive steps.
- Environmental impacts must be calculated using LCA methodology and any LCIA evaluation method must be available for selection.
- Engineering design facts and operating conditions of a unit process must be parameters of the corresponding model as they must be variables for decision making.

The development of the EVALEAU tool necessarily relies on a multidisciplinary approach, combining very different domains : process engineering and water treatment, environmental assessment, applied mathematics and software engineering. This no doubt increases considerably the difficulty of the work carried out, but also, just as clearly, the interest of the results achieved.

Chapter 2.

EVALEAU tool and related modelling approaches

Résumé du chapitre 2. L'outil EVALEAU et les approches de modélisation associées.

L'outil EVALEAU est ici décrit dans sa globalité et les approches de modélisation associées sont introduites. Les concepts présentés sont supposés pouvoir être repris et appliqués dans d'autres secteurs liés à l'industrie des procédés.

La structure de l'outil est tout d'abord détaillée. L'approche modulaire permet de créer de toutes pièces n'importe quelle configuration d'usine et de calculer la qualité de l'eau traitée ainsi que les consommations d'énergie et de réactifs (fonction *modélisation de procédés*). Les impacts environnementaux associés sont calculés sur la base de ce calcul de bilans matière et énergie, i.e. l'inventaire de données (fonction *diagnostic environnemental*). Les composants de l'outil sont listés ci-dessous :

- Le logiciel Umberto®, qui est en fait l'environnement de travail à proprement parler.
- La bibliothèque logicielle, dénommée EVALEAU, qui est composée de modules (i.e. des modèles de procédés unitaires) pour la simulation d'usines de production d'eau potable. Les modules EVALEAU peuvent être connectés à des logiciels externes, comme PHREEQC® par exemple.
- La base de données ACV.
- La base de données sur la qualité de l'eau.
- La boîte à outils pour l'analyse de sensibilité.

Les modules EVALEAU sont codés dans le langage Python^{TM} et chacun représente un procédé unitaire. Le fort paramétrage et la généricité de ces modèles leur confèrent une importante flexibilité, indispensable pour s'adapter aux spécificités et aux contraintes techniques d'un projet. Les calculs sont basés sur la qualité de l'eau en entrée et sur les paramètres du modèle qui représentent des données de dimensionnement, des conditions opératoires ainsi que des contraintes techniques/légales. Les résultats obtenus sont la qualité de l'eau après traitement, les consommations de matériaux ainsi que des données techniques utiles au stade du dimensionnement d'une usine et sauvegardées sous forme d'un rapport.

La base de données sur la qualité de l'eau est constituée de trois tableurs. Le premier concerne l'eau brute et contient notamment des données moyennes de qualité d'eau de différentes ressources exploitées par l'industriel partenaire de ce projet. Le deuxième tableur concerne l'eau traitée. Les résultats de modélisation peuvent y être sauvegardés et comparés avec différentes normes et recommandations. Le troisième tableur concerne les boues. L'ensemble des données de qualité d'eau compte 170 paramètres représentant une sorte de *vecteur eau*.

La base de données ACV actuellement utilisée est Ecoinvent. Son utilisation est double. Elle permet d'accéder aux inventaires de données des procédés d'arrière-plan et de mettre à disposition les méthodes d'évaluation des impacts.

La boîte à outils pour l'analyse de sensibilité est basée sur la méthode de Morris. Cette méthode est peu utilisée, quoique simple et efficace à la fois. L'utilisation qui en est faite dans le cadre de l'outil EVALEAU est originale. Le but est de fournir une méthode compréhensible pour évaluer l'influence des choix de dimensionnement et de conditions opératoires sur les résultats d'impacts environnementaux.

Les deux principales approches de modélisation pour les modules EVALEAU sont ensuite décrites, à savoir l'approche rétrospective et l'approche prédictive. Dans les deux approches les consommations d'électricité sont prédites car en effet, il est impossible de détailler ces consommations par procédé unitaire lors du recueil de données sur un site industriel. Par contre, les consommations de réactifs peuvent être détaillées par procédé. Dans l'approche rétrospective, les consommations de réactifs sont définies par l'utilisateur et les calculs de qualité d'eau et les performances de procédés associées en découlent. Dans l'approche prédictive, ces consommations sont calculées sur la base d'objectifs de traitements (i.e. performance de traitement attendue) définis par l'utilisateur. L'approche prédictive est évidemment plus instructive et plus appropriée pour la pratique de l'écoconception mais l'approche rétrospective n'est pas dénuée d'intérêt puisqu'elle permet de valider la modélisation de la qualité de l'eau indépendamment des autres calculs.

Finalement, une procédure technique pour l'écoconception de procédés est proposée sur la base de l'outil présenté. La formulation et la structuration de cette approche méthodologique a permis de formaliser l'écoconception dans le domaine du traitement de l'eau.

Chapter 2. EVALEAU tool and related modelling approaches.

This chapter describes in detail the tool developed during this research work. First, the working environment and its main components are presented as well as the original features of this LCA tool. Then, two modelling approaches that can be embraced by the user are introduced in order to better understand the different uses of the tool. Finally, a technical procedure is suggested for performing process ecodesign thanks to EVALEAU tool.

It must be underlined that the concepts and modelling approaches presented in this chapter are applied to drinking water treatment in the following chapters but they are intended to be transposed in different process industries.

1. Framework of the EVALEAU tool

The EVALEAU tool relies on the software Umberto® which is used as a working environment. It has been selected for this research project because it is the best suited LCA software regarding the project's requirements. It was originally developed for Material Flow Analysis (MFA) hence its ability to model process networks and complex industrial systems. It evolved as an LCA software subsequently. Besides, it gives the possibility to do integrated scripting with object-oriented programming languages, which is an interesting feature regarding the need for informatics development.

The framework of the EVALEAU tool is presented in figure 2-1. It illustrates the relations at work between the main components of the tool during the modelling of a drinking water treatment plant. These components are :

- The *software Umberto®.*
- The *EVALEAU library*, which is composed of modules (i.e. unit process models) for simulating drinking water treatment plants. The *EVALEAU modules* can be linked to external specialised software tools like *PHREEQC®* for instance.
- The *LCA Database.*
- The *Water Quality Database.*
- The *Sensitivity Analysis Toolbox.*

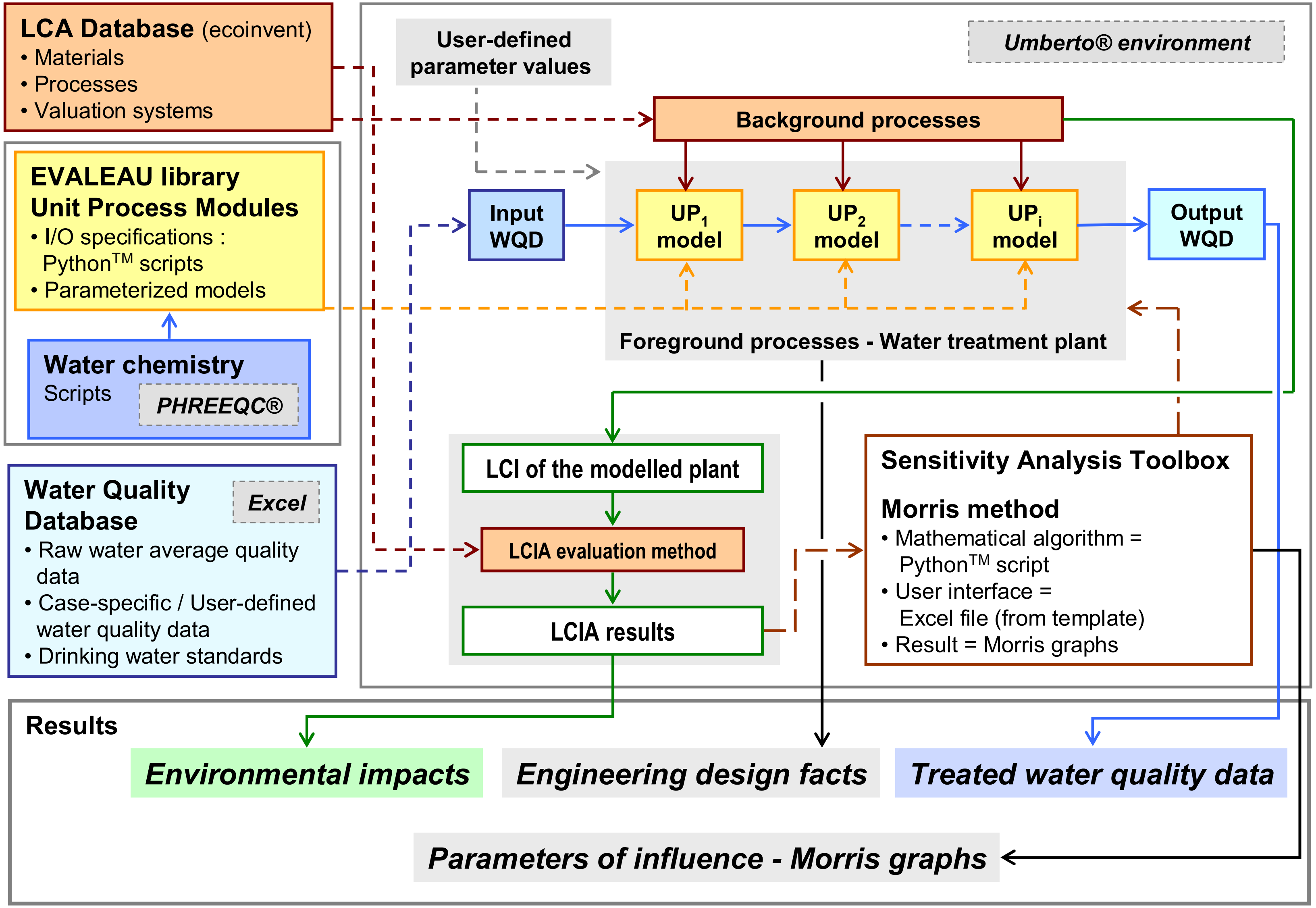


Figure 2-1. Framework of the EVALEAU tool.

The EVALEAU tool allows flowchart building for any water treatment plant and calculation of material and energy inputs/outputs at plant (*process modelling* function). Then, life cycle impact assessment of drinking water production is performed in a consecutive step (*environmental diagnosis* function). As shown in figure 2-1, different result categories are provided by a water treatment plant model. Indeed, a good overview of the plant's performances on technical, economic and environmental issues is essential for supporting the decision-making process.

The modelling approach for simulating a drinking water treatment plant is modular, i.e. a plant model is a network of sub-models, each representing a unit process. It makes it possible to configure the process chain in a flexible manner when simulating a water treatment plant. Different plant configurations and process sequences (i.e. flowcharts) can then be studied.

1.1 EVALEAU library

The unit process modules are stored in an Ecoinvent-like library named EVALEAU (figure 2-1). It is the bedrock of the tool and its development has been the core task of this research work. This section introduces the general concepts of this computational library while mathematical modelling of unit processes is detailed in chapter 3.

1.1.1 EVALEAU modules - modelling approach and results achieved

A module is the computer form of a physico-chemical model. The EVALEAU modules are deterministic models describing unit processes for conventional drinking water treatment. They are coded with the Python^{TM} programming language and they are mainly composed of energy and mass balance equations for process design and functioning. The EVALEAU modules are stored in the so-called EVALEAU library and classified in different process categories (e.g. disinfection, filtration processes, etc.).

The flexibility of the models has been strengthened in order to fit any engineering design and operating conditions related to project constraints. The tool allows accurate design of the processes from raw water quality and user-defined parameters, thus simulating a process chain within any specific project context. Accurate calculations of mass and energy balances (i.e. energy and chemical consumptions) are attempted in order to establish a predictive and reliable LCI of drinking water production, which makes this ecodesign tool more robust in return.

The principle of an EVALEAU module is described on figure 2-2 which summarizes the starting points for calculation, result categories and linkages with external software tools.

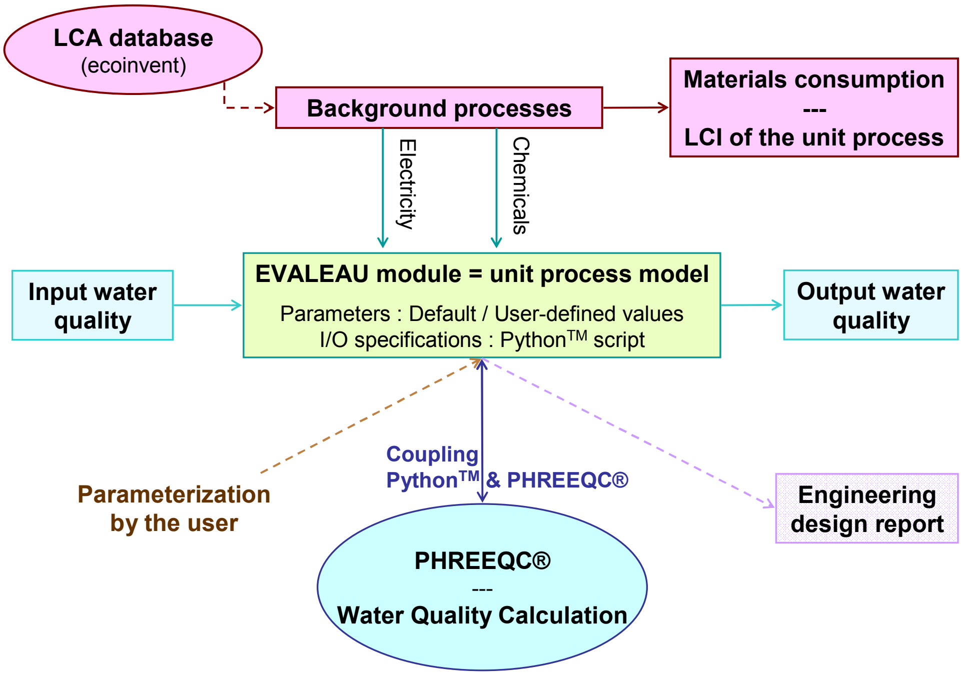


Figure 2-2. Principle of an EVALEAU module.

Next to the input water quality data, the parameters of a unit process model are the starting point for the calculations. It must be noted that input water quality is a constraint depending on the context of the project (i.e. local water sources) whereas most unit process parameters are technical specifications that can be modified (i.e. design and operating conditions). Three result categories are provided by the EVALEAU modules :

1. Output water quality data at the exit of the unit process
2. Chemical and energy consumptions
3. Basic engineering design report

The output water quality data is used as an input water quality data by the following module in the process chain or it is exported as a final result in the water quality database in case it is the last unit process of the treatment line (more explanations in the next section).

Chemical and energy consumptions are the basis for LCI/LCIA calculations. It must be noted that one can also calculate operational costs, by pricing these material consumptions.
Some basic engineering design facts and technical performances of the unit process are saved into a dedicated spreadsheet which takes the form of an engineering design report. This technical report is instructive and it allows appraising the technical feasibility of the project at early design stage, although it does not replace sound engineering judgement in late stages of plant design and construction.

1.1.2 Parameterization of the unit process models

The unit process models are generic and highly parameterized. The generic version of the models (as stored in the EVALEAU library) represents the average design and operating conditions of the corresponding unit processes. The high degree of parameterization enables the user to modify the generic version of the models in order to take account of the context of a specific project (e.g. specificities of the physical reality or project's requirements). It leads to very specific models, which are more representative of the case under study.

Model parameters can be technical design facts (e.g. surface hydraulic charge of a settler), operating conditions (e.g. velocity gradient in a mixing tank) and technical or legal constraints (e.g. disinfection requirements). Default values have been determined based on the literature, industrial guidelines or recommendations of water treatment experts.

The extensive parameterization allows deriving site-specific models from the generic version of the models. The underlying concept is that the user of the tool must make decisions about parameter values just as an engineer would have to make technical choices at the design stage. The rationale for such a modelling approach (i.e. genericity and high parameterization) is to make the parameterization of a plant model analogous to the activity of plant designing as carried out conventionally.

1.1.3 Linking with external and specialised software tools

Thanks to efficient programming, the EVALEAU modules can be linked to external and specialised software tools. The following example is presented for illustration but any software tools with open source code can be linked to the EVALEAU modules in order to make them more robust and thorough.

The tool uses PHREEQC® (PHREEQC website), geochemical software developed by the U.S. Geological Survey for more than twenty years. It is widely used for water quality modelling and chemical reaction simulation in aqueous phase. Linking the tool to PHREEQC® has been a major step in its development, since water quality can thereby be taken into account. In the context of drinking water production, health issues are central and water quality must be checked and validated as potable.

Resource water quality and drinking water quality as required by standards are different in each project. The technological solutions necessary to reach project requirements are multiple as well. Then, in every process model, in addition to mass and energy balances, the water's composition change through the process itself is calculated partly using the software PHREEQC®. The water quality and the chemical consumptions are precisely calculated along the modelled process chain. The accurate determination of required chemical doses makes the resulting predictive LCI more reliable, which is of the highest importance.

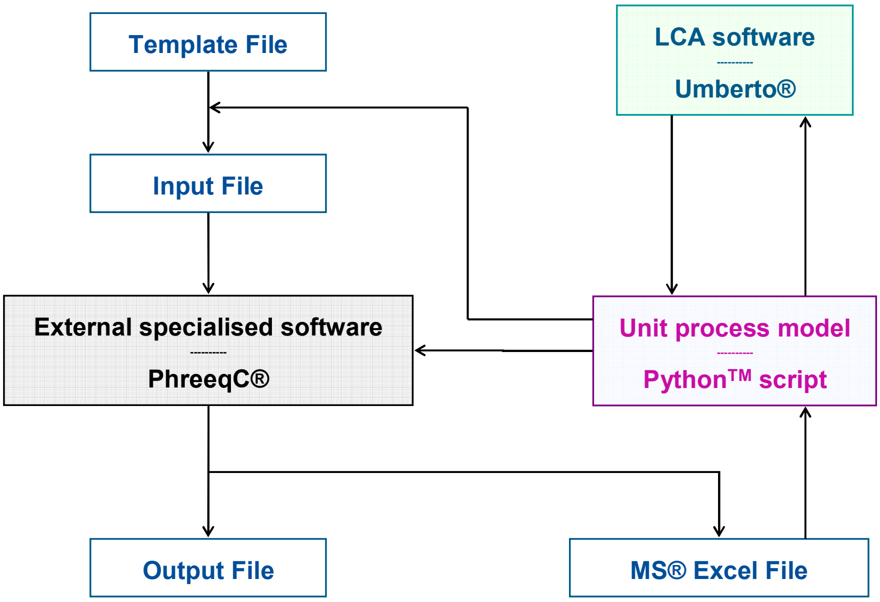


Figure 2-3. Coupling of Python^{TM} and PHREEQC® for chemical reaction simulation.

Figure 2-3 briefly describes how the linkage with the software PHREEQC® works. For each reactant likely to be introduced in the water during the treatment, a template file has been created. When this reactant is used during the modelling of a unit process, the corresponding Python^{TM} script opens the template file, modifies it according to the script coded instructions and saves it as an input file. Then, the Python^{TM} script launches the software PHREEQC®

and makes it simulate the chemical reaction defined in the input file previously created. The Python™ script finally gets the results back from PHREEQC® through an Excel spreadsheet.

Python™ scripting gives many opportunities to the programmers. Just as the tool has been linked to the software PHREEQC®, it can be linked to software dedicated to a particular industrial sector or to a specific application. This provides the LCA tool with benefits from previous research and modelling efforts by integrating complementary knowledge. It makes the modelling results more reliable and the tool better fitted for the intended applications.

1.2 Water quality database

The quality of every water flow is defined by a set of data representing a mathematical vector. This vector is composed of 170 quality data which define the water composition and it is presented in appendix 2-1. Ten categories of water quality data can be distinguished :

- General parameters (e.g. temperature, pH, complete alkalinity titration TAC)
- Radioactivity (e.g. total indicative dose, tritium)
- Organic matter (e.g. UVA, TOC)
- Pathogenic microorganisms (e.g. cryptosporidium, E. Coli, algae)
- Mineral and salt composition (e.g. Cl, Mg, total Ca and dissolved Ca)
- Nitrogen and phosphorus compounds (e.g. NH_4, NO_2, PO_4)
- Micropollutants (e.g. atrazine, benzene)
- Other compounds (in case where a rare pollutant is present in the source water)
- Disinfection by-products (e.g. trihalomethanes, haloacetic acids)
- Other reaction products (in case where a rare by-product is formed)

The development of a water quality database (figure 2-1) was then required to define the raw water quality in a case study and to check the water quality of the output flows (i.e. sludge and treated water). This water quality database is composed of three spreadsheets.

The first spreadsheet of the water quality database is dedicated to : 1/ the storage of data sets relative to the average water quality of different resources and 2/ the definition of the raw water quality in a case study as an input for the corresponding modelling scenario.
Data sets on water quality for numerous resources actually used by the industrial partner are made available. They are classified in different categories of water resources. At this point,

the database contains water quality data relative to twelve rivers, seven reservoirs, two lakes, four influenced ground waters and six not influenced ground waters. Average water quality for each resource category is calculated for indicative purpose only.

Indeed, the raw water quality of a case study must preferably be user-defined. In case no data is available for the raw water in a case study, average water quality of the resource category (e.g. rivers) can be used as an approximation but this is not recommended as the raw water quality is fundamental and determines the water treatment requirements. Raw water quality data is imported thanks to a specific module as an input for the plant model and this is a compulsory step.

The second spreadsheet concerns the treated water. In the framework of the EVALEAU tool, a modelling scenario always ends with a specific module for exporting the treated water quality in this spreadsheet in order to save it as a result. Drinking water standards are also defined in this spreadsheet and the treated water quality obtained by the modelling scenario must be compared with the ongoing regulations depending on the context of the plant under study. Specific guidelines (industrial or WHO guidelines) can be added as well.

The third spreadsheet concerns the produced sludge and its quality. There is no standard relative to sludge quality in drinking water treatment but it is saved as a result in order to evaluate the sludge's composition and its potential agricultural value for instance.

1.3 LCA database(s)

Among other things, a modelling scenario provides the energy and chemical consumptions of a drinking water treatment plant. The environmental impacts due to these material consumptions are calculated using an LCA database. It must be noticed that there are two different uses of LCA databases in the EVALEAU framework :

1. *Background processes*. The LCI of the production and transportation of materials are imported from an LCA database (figures 2-1 and 2-2). Their modelling is out of the scope of this research work.
2. *Life Cycle Impact Assessment*. LCIA evaluation methods from an LCA database are used to quantify the environmental impacts of drinking water production (figure 2-1).

The Ecoinvent database version 2.2 (Althaus et al. 2007, Althaus et al. 2010) is used in this version of the tool because it is the most widely used by LCA practitioners, but other LCA databases can be used as long as they are available within the software Umberto®.

1.4 Sensitivity analysis toolbox

1.4.1 Role of sensitivity analysis in the EVALEAU framework

In most LCA studies, sensitivity analysis is achieved without using any formal mathematical method. For instance, sensitivity analysis in LCA literature usually consists in studying the influence of the type of electricity supply or a simple parameter variation. Nevertheless, these sensitivity studies have limitations and mathematical formalism is required.

Numerous methodologies for sensitivity analysis exist in the literature (Saltelli et al. 2008). The global objective of a sensitivity analysis is to determine which inputs (i.e. variables and/or parameters) have the strongest influence on the results of the computational model under consideration. The interpretation of the results depends on the sought information and as a consequence, lessons learned from such mathematical methods are many and varied. Potential rationales for sensitivity analysis are introduced below (Saltelli et al. 2008) :

- *Prioritization of research efforts*. Determination of model parameters requiring additional research efforts (e.g. more precision required which in turn requires more measurements).
- *Model reduction*. Determination of insignificant model parameters that can be fixed as a constant or eliminated from the model under construction. This is often the first step towards *meta-modelling*.
- *Verification of model consistency*. Determination of weak assumptions potentially biasing the model's results.
- *Identification of interactions* between model parameters. Determination of crucial regions in the parameters' space.
- *Comprehension of the physical system*. Exploration of complex and large models that represent adequately a physical reality.

This is not an exhaustive list of possible reasons for performing sensitivity analysis on a computational model. Different manners for interpreting a sensitivity analysis and numerous applications exist in the literature. Nevertheless, the common thread is that they all follow from the determination of model factors that are most influencing the results. Nevertheless, sensitivity analysis is often used to strengthen the development of a model by indicating which parameters require additional research efforts, by simplifying the model's formulation and/or by checking the model's consistency.

In the EVALEAU framework, sensitivity analysis is originally applied and interpreted. It simply aims to identify the model parameters which have a significant influence on the results, which leads to a better comprehension of physical reality, assuming that the model is realistic enough. Once this postulate accepted, ***the influent model parameters represent action levers for reducing the environmental impacts, since they are engineering design facts or operating conditions defined by the user.***

The EVALEAU tool is addressed to water engineers who can take action on water treatment plants. Applying such mathematical analysis on a specific project at the design stage is enlightening since it enables water engineers to focus on the crucial technical choices and to better understand how the designed process system behaves. Therefore, sensitivity analysis is expected to effectively support the ecodesign activity within the EVALEAU framework.

1.4.2 Mathematical methods for sensitivity analysis

Numerous sensitivity analysis methodologies and their variants are made available in the literature for the modelling community. These methodologies differ in their principles and can be classified accordingly.

Local sensitivity analysis techniques are to be differentiated from global ones. Local sensitivity analysis allows studying the influence of the variation of one single parameter at a time, the others being fixed. On the contrary, global sensitivity analysis aims at studying the influence of model factors when they are all varying. The space of parameters is supposed to be entirely explored. The computational costs are increased compared to local techniques, but global techniques make it possible to detect interactions between model factors in non-linear or non-additive models.

Qualitative sensitivity analysis techniques are differentiated from quantitative ones. Qualitative techniques allow screening a few influential model factors within a model with a high number of factors. It enables the user to identify the model factors of higher interest but the results are only qualitative. Quantitative sensitivity analysis aims at assessing the variance of the model result(s) due to each model factor. The information brought by such sensitivity analysis techniques is substantial but the computational costs are increased.

Different types of mathematical methods for sensitivity analysis have been developed and the main categories are introduced below :

- *Screening methods* (e.g. the Morris method)
- *Regression-based methods* (e.g. the Latin Hypercube Sampling (LHS) method)
- *Variance-based methods* (e.g. the Fourier Amplitude Sensitivity Test (FAST) and the method of Sobol)

At the current stage of development of the EVALEAU tool, a Morris method algorithm has been coded. Even if variance-based approaches are more accurate and able to provide quantitative results, the Morris method offers a good overview of the key parameters of a model at a lower computational cost (Confalonieri et al. 2010; Hamby 1994). Besides, the interpretation of the Morris method is straightforward and graphical, which makes it easily comprehended by non-mathematicians. Campolongo et al. « recall the attention of the modelling community to the effectiveness of this method » (Campolongo et al. 2007). These are the reasons why the Morris method has been selected for implementation in the sensitivity analysis toolbox as a first step.

Nevertheless, the LCA tool could also be linked to SimLab, a free development framework for sensitivity and uncertainty analysis (SimLab website), if further sensitivity analysis methods are required. The tool would benefit from research and development efforts made by the community of sensitivity analysis experts.

1.4.3 The Morris method

The Morris method is a screening method which is also called the « elementary effects method » (Morris 1991; Campolongo 2007; Saltelli 2008). The objective is to determine qualitatively which parameters have an influence on the model result and which kind of influence they have (linear or not, interaction with another parameter). Key factors are then identified among the numerous factors of the model. It is widely recognised that it is one of the sensitivity analysis methods having the lowest computational costs.

In the Morris method, model parameters but also input variables can be considered. They are both referred as factors and *k* is their number. Each factor varies over *p* levels, i.e. the space of factors is discretized in *p* levels. The variation of the model result due to the variation of one factor is called an elementary effect (EE) (derivative-based approach). The elementary effect EE_i of the i^{th} factor can be expressed as below :

$$EE_i = \frac{y(x_1,...,x_{i-1},x_i \pm \Delta,...,x_k) - y(x_1,...x_k)}{\Delta} \qquad (2\text{-}1)$$

$$\Delta \in [\frac{1}{p-1};...;\frac{i}{p-1};...;\frac{p-2}{p-1}]$$

- *k* : number of model factors under study.
- *p* : number of levels.
- x_i is the value of the i^{th} factor and $(x_i + \Delta)$ is its value on the next (or previous) level.
- Recommendation : p even number and $\Delta = \frac{p}{(2*(p-1))}$.

A trajectory is a set of *(k+1)* points in the space of factors. The first point is randomly determined. Then, the factors are switched to a different level one-at-a-time, which creates a trajectory of (k+1) points in the k-dimensional parameters' space. Thus one trajectory allows calculating one elementary effect for each factor considered in the study.

The Morris method consists in generating *r* trajectories and running the corresponding model calculations. It is then possible to calculate *r* elementary effects for each factor. In the basic version of the Morris method, the mean μ of the elementary effects and the standard deviation σ are computed for each factors and used as sensitivity measures to evaluate the factors' influence on the model. The mean μ represents the global effect of a factor on the model's result while the standard deviation σ accounts for the non-linear effects of the factor (due to non-linearity or interactions with other factors).

This information is then summarized on the so-called Morris graph by plotting the mean μ on the abscissa and the standard deviation σ on the ordinate. Each factor of the model is then represented by one point. The farther a point is to the right of the graph, the stronger the influence of the corresponding factor on the model. The higher a point is on the graph, the more the influence of the factor is a non-linear one. The interpretation of the Morris graph is straightforward and that is what makes the method easy to understand for non-mathematicians.

Some variants of the Morris method have been proposed in the literature. For instance, the mean μ^* of absolute values of elementary effects can be used instead of the regular mean μ of elementary effects (Campolongo 2007). It better takes into account the global effects of model factors. The variance σ^2 of the elementary effects can also be used instead of their standard deviation σ. The standard deviation has the advantage to have the same dimension than the model's result but the variance is a direct measure of its dispersion.

In the EVALEAU framework, the mean μ^* and the variance σ^2 of the elementary effects are used as sensitivity measures for the Morris method. Parameter variation intervals are set by default applying ± 25% to the nominal value of the parameters, but these intervals can be modified by the user to avoid inconsistencies. The Morris method can be applied on LCIA results as well as on treated water quality results, thus enabling to detect the model parameters influencing the environmental impacts and/or the treated water quality.
Nevertheless, this method is related to only one result (e.g. one selected environmental impact category). It could be applied in parallel for different results in case different categories of results have to be investigated. For each selected result of the plant model, a Morris graph will be generated by the tool. Performing a sensitivity analysis on a plant model makes it possible to identify the most influential parameters and to prioritize the action levers.

2. Modelling approaches

2.1 Retrofit approach and predictive approach

There are two modelling approaches made available in the EVALEAU framework and the modules from the EVALEAU library can be classified accordingly. The main rationale for their development was the need for both a descriptive and a prospective approach regarding material consumptions.

When collecting inventory data on the field, the consumption of one chemical is most often due to a particular unit process and it can be attributed to it (e.g. coagulant is used as a reactant only during the coagulation process). On the contrary, the energy consumption is known at plant level but it is not possible to measure or assess accurately the contribution of each unit process to the global energy consumption.

As energy consumption cannot be measured on site for each unit process, it must be predicted by the EVALEAU modules regardless of the considered modelling approach. Therefore, energy consumptions are always calculated from related model parameters such as pumps' efficiency, velocity gradient in a mixing reactor, etc. Finally, the global consumption predicted by the plant model can eventually be compared to the global energy consumption measured on site for model validation (at least when the plant already exists).

For chemical consumptions, the situation is different because they can be measured and attributed to one unit process. In the retrofit approach, the chemical doses are user-defined parameters and that makes the retrofit models more descriptive regarding the inventory of chemical consumptions. In other words, this part of the inventory is not predicted but user-defined in return. The water quality is predicted and the modifications due to the addition of reactants are modelled based on the user-defined chemical dose.

In the predictive approach, the chemical consumptions are forecasted. Process performances are user-defined parameters in the predictive models (e.g. removal of one pollutant) and the required chemical dose to achieve this process objective is calculated based on water quality modelling. Therefore, the inventory (i.e. energy and chemical consumptions) is entirely forecasted in the predictive approach.

In fact, the water quality calculations in both modelling approach are the same but they are reversed. The retrofit approach allows calculating the resulting water quality from a user-defined chemical dose and the predictive approach allows calculating the chemical dose required to fulfil a user-defined process objective in terms of water quality.

In a conventional LCA, inventory data is globally measured/estimated at plant level and this is the starting point for LCIA calculations. In a retrofit LCA performed with the EVALEAU tool, the inventory is partly predicted (i.e. energy consumptions) and partly described thanks to measurements and/or estimations (i.e. chemical consumption) as in a conventional LCA. In a predictive LCA, the site inventory is entirely predicted, i.e. energy and chemical consumptions are all forecasted at the level of each unit process based on user-defined process performances and technical specifications.

Therefore, the retrofit approach is better adapted for studying a drinking water treatment plant which already exists or for studying the accuracy of water quality modelling. The predictive approach is clearly more instructive by its nature because it leads to prospective modelling scenarios. It is consequently the best suited approach for supporting process ecodesign.

2.2 Technical procedure for process ecodesign

In this section, a technical procedure is suggested for performing the ecodesign of drinking water treatment plants. It enables one to improve the environmental (and/or economic) performances of one plant by selecting the best suited unit processes or by taking action on targeted design facts and operating conditions.

Figure 2-4 represents the technical procedure for process ecodesign as proposed here and it provides an overview of the different steps which are :

1. Establishment of a ground modelling scenario as a basis for further investigations.
2. In-depth analysis of the ground modelling scenario.
3. Building alternative modelling scenarios searching for improvement opportunities.
4. Selection of alternative modelling scenarios truly improving the environmental and/or economic performances of the plant.
5. Deriving an optimal scenario from the ground scenario thanks to the lessons learned.

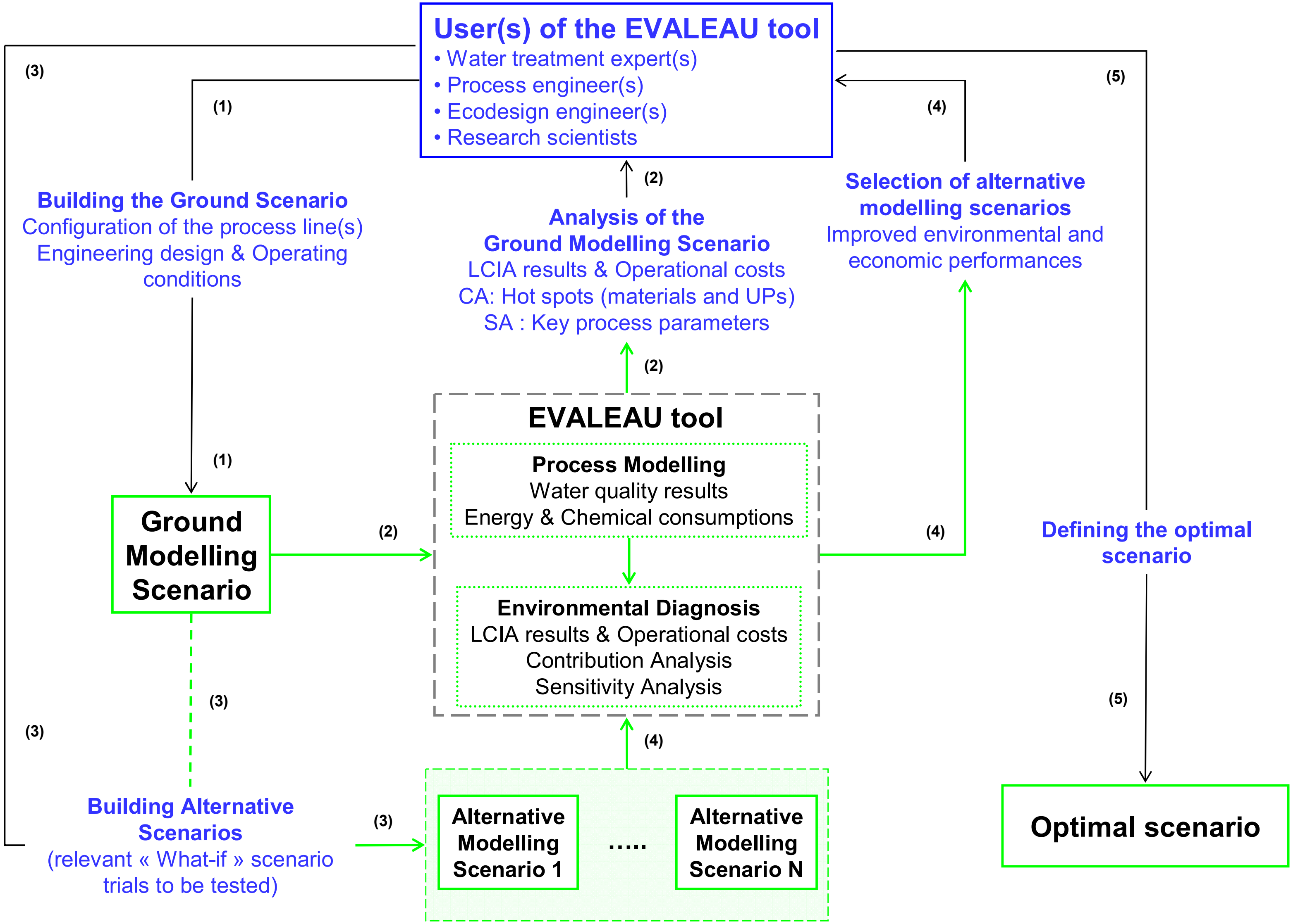


Figure 2-4. Technical procedure for process ecodesign.

The first step consists in establishing the ground modelling scenario. It is a crucial step for the ecodesign procedure since further alternative scenarios rely on this default scenario. It must be predictive since one prerequisite for process ecodesign is forecasting energy and chemical consumptions (clearly, a retrofit model does not comply with this constraint). Two different cases can be distinguished : 1/ the plant already exists and it must be re-designed or 2/ the plant does not exist and it must be designed prior to its construction.

In the first case, the ground modelling scenario must stick to the physical reality taking place on the field. In other words, the plant model must reproduce the actual functioning of the plant and its main characteristics. Besides, the configuration of an existing plant cannot be modified in most cases, so the establishment of the ground modelling scenario is consequently not an issue in this context.

In the last case, the engineering design work must be carried out from scratch. The EVALEAU tool is able to assist water engineers in this task but the establishment of the ground modelling scenario is not so obvious in this case. We recommend trying different configurations of the treatment line(s) in order to evaluate the relevance of the considered plant's configurations. More than one technical option (i.e. configuration of the plant) can eventually be taken into consideration and the technical procedure can be repeated with different ground modelling scenarios if doubts remain about the choice of processes' configuration within the plant. Expertise in water treatment is necessary in this context.

The second step of the ecodesign procedure aims at analysing this ground modelling scenario. Energy and chemical consumptions are predicted by the plant model. Treated water quality must be checked in order to validate the scenario. LCIA results and operational costs are calculated afterwards. A contribution analysis brings quantitative information about which material consumptions and which unit processes are most contributing to the environmental impacts of drinking water production within this plant. Hot spots are detected thanks to a contribution analysis and this is an indication about what needs to be tackled during the following ecodesign attempts. Sensitivity analysis detects the most influent process parameters, i.e. design facts and operating conditions that have a significant influence on the LCIA results. These are priority action levers on which the ecodesign work must focus.

In the third step, alternative scenarios are derived from the ground scenario based on indications provided by the previous step. They all introduce one difference at a time compared to the ground modelling scenario (i.e. one improvement opportunity studied per alternative scenario). They represent a set of « what-if » scenarios.

The fourth step consists in determining relevant improvement measures. The environmental and economic performances of the different plants modelled in the alternative scenarios are assessed. The alternative treatment solutions reducing environmental impacts and/or operational costs are considered appropriate within an ecodesign perspective and they are selected for the final step.

In light of the results provided by the « what-if » scenarios, selected measures must be gathered in one final scenario which is supposed to combine all their benefits. At this point, the resulting plant model is enhanced from both environmental and economic points of view.

This technical procedure for ecodesign is given as a guideline for process engineers and research scientists but it does not represent a complete methodology covering all the issues encountered at early design stage. Nevertheless, it addresses the lack of formal methodology in process ecodesign.

3. Conclusion

The framework of the EVALEAU tool relies on an LCA software used as a working environment. The software Umberto® has been selected 1/ for its ability to model process networks and 2/ for the modelling flexibility provided thanks to integrated scripting.

The EVALEAU library is the major component of the tool and it is composed of computational models for unit processes involved in drinking water treatment. The parameters of these models are mainly design facts and operating conditions. Besides, the high parameterization enables the user to derive case-specific models from generic models as stored in the library. There is supposedly a parallel between the parameterization of a plant model and the design work achieved by an engineer at early design stage. In addition, the models can be linked to external specialised software which makes the tool benefit from specific knowledge.

The water quality database has been developed 1/ to define the raw water quality and 2/ to check that the treated water complies with the regulatory standard.

The Ecoinvent database is now part of the EVALEAU framework but any other database can be implemented thanks to the working environment. The main uses of the LCA database are 1/ background process modelling and 2/ life cycle impact assessment.

The sensitivity analysis toolbox is an original feature of the EVALEAU tool. It supports the decision-making process and the ecodesign activity by tagging priority action levers. The Morris method is the only sensitivity analysis technique that has been scripted at this stage of development but further methods could be used if the tool is linked to the SimLab framework for uncertainty and sensitivity analysis.

Two modelling approaches are made available for the user in the library : the retrofit and the predictive approach. The retrofit approach is by definition better adapted for describing a drinking water treatment plant that already exists whereas the predictive approach is better suited for the design of a future plant.

A technical procedure for process ecodesign is finally proposed. It requires using different features of the tool and it provides a simple guideline on how to use this tool to perform ecodesign of process plants.

The unit process models themselves (as presented in chapter 3 and related appendix 3-2) are applicable only to drinking water treatment. Nevertheless, It was intended that the concepts embedded in the tool and presented in this chapter could be applied in other process industries As a matter of fact, the modelling approaches (e.g. genericity and high parameterization of the unit process models), the technical procedure for process ecodesign and the original use of sensitivity analysis can be applied to other types of process plant like a refinery for instance.

Object-Oriented Programming (OOP) played an important role in the development of this ecodesign tool. Python^{TM} programming strongly enhanced the modelling flexibility (e.g. by linking to external software). The tool is able to evolve because the source code is open so it provides a collaborative platform for researchers and engineers. Research achievements and methodological advances can be put into practice jointly in such framework.

Chapter 3.

Mathematical modelling of unit processes

Résumé du chapitre 3. Modélisation mathématique des procédés unitaires.

Le langage de programmation Python^{TM} a été sélectionné pour le développement des modèles de procédés unitaires. C'est un langage de Programmation Orienté-Objet (POO). Ce paradigme de programmation informatique est de plus en plus utilisé dans toutes sortes de domaines. Par exemple, Google^{TM} se base principalement sur ce langage pour développer ses applications, notamment pour sa capacité à faire le lien entre des applications de nature différente.

Python^{TM} est aussi de plus en plus utilisé dans la recherche scientifique. Sa flexibilité et sa facilité d'apprentissage sont ses atouts majeurs pour la recherche. De nombreuses bibliothèques logicielles pour le calcul numérique sont disponibles, ce qui rend ce langage d'autant plus pratique et robuste.

Etant donné la nature multidisciplinaire du projet EVALEAU et les besoins en termes de développement informatique, Python^{TM} a logiquement été sélectionné pour ce projet de recherche.

Les différents fichiers impliqués dans la modélisation d'un procédé unitaire et leur relation sont ensuite décrits en détail. Le script principal est celui qui matérialise à proprement parler le modèle. Les calculs y sont effectués, des fonctions et constantes y sont importées si nécessaire, et les procédures requises sont gérées par ce script (par exemple, pour la requête d'un calcul par un logiciel externe comme PHREEQC®).

Un script de second niveau définit des fonctions et des constantes sur lesquelles un modèle de procédé unitaire repose. Ce genre de script est rendu facilement accessible à l'utilisateur pour lui permettre d'ajuster et d'affiner les modèles génériques tels que sauvegardés dans la bibliothèque logicielle.

Le fichier « EVALEAU_Chemical_Objects » définit quant à lui des objets Python^{TM} représentant les réactifs rendus disponibles dans l'outil EVALEAU pour la simulation de réactions chimiques. Ces objets et leurs attributs sont explicitement détaillés dans une annexe dédiée.

Le fichier « EVALEAU_Functions » est un script qui revêt une importance majeure pour les modèles de procédés unitaires. En effet, les fonctions les plus largement utilisées y sont définies. Par exemple, toutes les fonctions relatives au pompage de l'eau et la fonction *Reactant_Addition* (permettant de simuler l'ajout d'un réactif dans l'eau à traiter et d'en déduire la qualité de l'eau obtenue) sont définies dans ce script. Deux fonctions pour calculer la dose nécessaire de réactif pour ajuster le pH, ou le titre alcalimétrique complet de l'eau, à une valeur cible définie par l'utilisateur ont aussi été créées. Une autre fonction permet de simuler le mélange de deux flux d'eau et la qualité du flux d'eau en résultant.

Mais la fonction *Coagulant_Dose_Calculation* est certainement la plus originale de toutes celles développées au cours du projet. En réponse au besoin mentionné dans la littérature d'une modélisation mécanistique du procédé de coagulation, des efforts particuliers ont été accomplis sur ce sujet. Un modèle, récemment développé, est donc repris et intégré dans le fichier « EVALEAU_Functions » pour la prédiction de la dose de coagulant nécessaire pour abattre une certaine quantité de DOC. Une extension du modèle est même proposée pour le compléter astucieusement, en prédisant l'abattement d'absorbance UV qui s'opère en parallèle lors de la coagulation.

Les modèles mathématiques sont finalement brièvement introduits et leur description exhaustive est effectuée dans une annexe technique dédiée par souci de transparence. Les catégories de procédés modélisés sont listées ci-dessous :

- Pompage de l'eau
- Ajout de PAC
- Coagulation
- Séparation des flocs
- Filtration sur média
- Désinfection - Oxydation
- Neutralisation - Reminéralisation
- Traitement des boues

Chapter 3. Mathematical modelling of unit processes.

As a first step, this chapter introduces the Python^{TM} programming language and its benefits. The different files which play a role in the modelling of unit processes are then presented and the generic Python^{TM} functions developed during the project are described. The mathematical models of unit processes considered for implementation in the EVALEAU library are finally introduced in the last section of this chapter and detailed in the affiliated technical appendix.

1. Introduction to the Python^{TM} programming language

The programming language selected for this research project is Python^{TM} (Python website), an Object-Oriented Programming (OOP) language. This programming paradigm has gained interest in the recent years.

Python^{TM} is particularly powerful and flexible, and is currently used for many kinds of software development. For instance, Google^{TM} is powered by Python^{TM} notably because of its ability to connect different types of computer applications (e.g. text files, videos, databases, etc). Indeed, Python^{TM} is often called a *glue programming language* since it is well adapted to make computer codes written in distinct programming languages work in combination.

Python^{TM} is also used in scientific research and this programming language has been adopted by scientists from different disciplines. Its greatest interest for research remains the ability to handle in a flexible manner both commercial software (e.g. Microsoft Excel) and/or any object-oriented programs (e.g. PHREEQC®).

In addition, numerous libraries are available for scientific computing like NumPy (NumPy website) or SciPy (SciPy website) and it is easily grasped by non-specialists in programming.

Considering the need for development in informatics and the multidisciplinary nature of the EVALEAU project, Python^{TM} has been selected as the main programming language for the interesting features detailed above. The scripts presented in the following sections are all coded with this programming language.

2. Python^{TM} files involved in the modelling of a unit process

2.1 Main script - Unit process model

The main script of a unit process model is the basis for all calculations and procedures. It constitutes the input/output specifications of the corresponding EVALEAU module. Mass and energy balances at process level are calculated. Files and external software tools are handled by procedures (i.e. routines) in accordance with modelling requirements.

This Python^{TM} file imports the input water quality data and the model parameters (as defined in the module specification window) from Umberto®. Warnings can be printed in a dedicated Umberto® window when some water compound is above a critical limit at the entrance of the unit process. For instance, high organic matter concentration in the water entering the disinfection step (thus leading to an important risk of disinfection by-products formation) is reported by a warning generated by the main script.

This script can also import functions and constants, characteristic of the unit process, from the corresponding second-level script and generic functions from a common file. Python^{TM} chemical objects are imported for simulating chemical reactions if required. This is further explained in the next sections.

Finally, the main script of a unit process model always ends up exporting the results to Umberto® (i.e. output water quality data and material consumptions) and creating the engineering design report in the form of a spreadsheet.

2.2 Second-level script - Complementary functions and constants

Functions and constants related to one particular unit process model are defined in this kind of script and imported by the main script. The second-level script is easily accessible to the user in order to provide him with the possibility to modify some functions and/or constants on which the model relies. This helps the model to reflect more precisely the physical reality of the case under study and this definitely enhances the modelling flexibility.

For instance, the energy required for sludge scraping at the bottom of a settler was not possible to determine based on calculations. A value has been found in the literature for evaluating this energy consumption. This default constant, as defined in the second-level script of the settling process, is $6.786.10^{-4}$ kWh/(m^3 of sludge) but the user can change this value according to measurements in the context of a given case study.

2.3 File « EVALEAU_Chemical_Objects » - Python^{TM} objects for chemicals

A computer *object* is an abstract concept. The exact definition differs according to the programming language, so it is introduced here with a general example for illustrative purpose. An object has attributes and methods and it is always part of a *class* (pattern from which the objects are instantiated). For example, a text file can be seen as an object. The text itself (a character string) and the file's directory would be attributes while the read, write and save functions would be methods of the object. Object-oriented programming is in fact a conceptual way of programming that involves interacting computer objects.

In this research project, Python^{TM} objects have been created in order to represent the chemicals that can be used during drinking water treatment. The file named « EVALEAU_Chemical_Objects » defines the chemicals made available in the form of Python^{TM} objects for simulation of chemical reactions. The Python^{TM} chemical objects (and their attributes) developed at this stage of the project are listed in appendix 3-1.

In summary, a Python^{TM} chemical object represents one chemical and some related attributes. The Python^{TM} chemical objects can be directly imported by any main script. In the majority of cases, these objects are used by the function *Reactant_Addition* (introduced in the section 3.5 of this chapter) for simulating a chemical reaction.

2.4 File « EVALEAU_Functions » - Generic functions

Some Python^{TM} functions are generic and intervene in the modelling of several unit processes (e.g. simulation of the addition of one reactant into the water to be treated). These functions are defined and scripted in a dedicated file named « EVALEAU_Functions » and they can be imported and used by any main script.

This file is intentionally made not easily accessible for the user because the few functions defined in it are quite complex and they are not supposed to be modified. Nevertheless, the file is not totally hidden and the source code is open.

3. Generic functions

3.1 Constant « Water_Density »

There is only one constant defined in the file « EVALEAU_Functions ». It is a generic constant used in many unit process models. The water density assumed to be constant and equal to 1000 kg/m3.

$$\text{Water\_Density} = 1000\ \text{kg/m}^3$$

This is a reasonable assumption in the context of drinking water production because the temperature of the water to be treated varies in a restricted range and the water density can therefore be considered constant.

3.2 Function « Water_Dynamic_Viscosity »

The function *Water_Dynamic_Viscosity* calculates the dynamic viscosity *Mhu* [Pa.s] of the water depending on its temperature *T* [K].

$$\text{Mhu} = \left(-9.8022 \cdot 10^{-9} \times \text{T}^3\right) + \left(9.1623 \cdot 10^{-6} \times \text{T}^2\right) + \left(-2.8693 \cdot 10^{-3} \times \text{T}\right) + 0.30168 \quad (3\text{-}1)$$

This equation is an interpolation, i.e. the result of a curve fitting of the water thermodynamic table data. So, the water dynamic viscosity is given as a function of the temperature and it is valid for any temperature included between 273.15 K and 313.15 K (i.e. between 0°C and 40°C) which are typical temperatures of water resources around the world.

3.3 Function « Chen »

The function *Chen* provides the most accurate approximation of the Colebrook equation for the explicit calculation of the Darcy friction factor *f* for water flowing in a pipe (Chen 1979, Clamond 2009).

$$\text{f} = \left[\frac{1}{-2 \times \log_{10}\left(\frac{\text{K}}{3.7065} - \frac{5.0452}{\text{Re}} \times \log_{10}\left(\frac{\text{K}^{1.1098}}{2.8257} + \frac{5.8506}{\text{Re}^{0.8981}} \right) \right)} \right]^2 \quad (3\text{-}2)$$

K is the relative roughness [no unit] of the pipe and $K = \frac{k}{d}$ where k is the absolute roughness [m] of the pipe and d its diameter [m]. Re stands for the Reynolds number [no unit].

3.4 Function « Water_Pumping_Global_Function »

The function *Water_Pumping_Global_Function* provides six results for a pumping/piping system : the total head loss [Pa], the electrical power for each pump [kW], the specific electricity consumption [J/m^3 of pumped water], the number of pipes to be installed in parallel [no unit], the water flow [kg/s] and the water velocity [m/s] in each pipe.

The function *Water_Pumping_Global_Function* contains six sub-functions for calculating the six main results. These sub-functions are : *Head_Loss*, *Power*, *Elec_Consumption*, *Pipe_Number*, *Pipe_Flow*, *Pipe_Velocity*.

The variables of the function *Water_Pumping_Global_Function* are listed below :

- Total water flow to be pumped Q [kg/s] (no default value).
- Height to be pumped H [m] (default value is 1 m).
- Pipe length *L_pipe* [m] (default value is 10 m).
- Pipe diameter *D_pipe* [m] (default value is 0.5 m).
- Pipe absolute roughness *ABS_K* [m] (default value is 0.0008 m, which is the value for worn cast iron pipes, commonly found in drinking water pumping systems).
- Efficiency of the pump(s) *NU* [dec.%] (default value is 0.8).
- Water density *rho* [kg/m^3] (default value is 1000 kg/m^3).
- Water dynamic viscosity *mhu* [Pa.s] (default value is 0.001 Pa.s).

Number of pipes and water velocity

The pipe section area S is calculated based on the diameter *D_pipe* and assuming that it is a round pipe. Then, knowing the water flow Q, the program calculates the water velocity in the pipe *Pipe_Water_Velocity*.

$$\mathrm{Pipe\_Relative\_Roughness} = \frac{\mathrm{ABS\_K}}{\mathrm{D\_pipe}} \qquad \text{[no unit]} \qquad (3\text{-}3)$$

$$\mathrm{S} = \pi \times \left(\frac{\mathrm{D\_pipe}}{2} \right)^2 \qquad [\mathrm{m}^2] \qquad (3\text{-}4)$$

$$\text{Pipe\_Water\_Velocity} = \frac{Q}{\text{rho} \times S} \qquad [\text{m/s}] \qquad (3\text{-}5)$$

Then, the maximum water velocity in a pipe *V_max* must be determined. The limit could be a technical one (given by theoretical calculation or pump manufacturer recommendation) or a legal one.

French legislation is used in order to provide an order of magnitude of the legal limit *V_max_legal* concerning the maximum water velocity in a pipe (French legislation relative to water pumping stations). The French legal limit is different for suction pipes and discharge pipes. It is assumed that the piping system is composed of suction pipes and discharge pipes of the same length. So, the maximum water velocity used as a reference in this model is equal to the mean maximum water velocity of the two kinds of pipes. Finally, it is summarized by the following logical equations :

If $\text{D\_pipe} \leq 0.15$ then $\text{V\_max\_legal} = 1.5$ [m/s] (3-6a)

If $\text{D\_pipe} > 0.15$ then $\text{V\_max\_legal} = 1.9$ [m/s] (3-6b)

The technical limit *V_max_tecnical* concerning the water velocity in a pipe under pressure can be determined by the equation 3-7 (Masson 2005; Karassik et al. 2010). The maximum water velocity *V_max* is finally set to the minimum between the technical and legal limits.

$$\text{V\_max\_technical} = \sqrt{\frac{\text{D\_pipe} \times 1000}{50}} \qquad [\text{m/s}] \qquad (3\text{-}7)$$

The minimum water velocity *V_min* in a pipe is 0.6 m/s (Masson 2005). If *Pipe_Water_Velocity* is lower than *V_min*, it means that the user gave a value for *D_pipe* too high for the flow to be pumped. In such cases, the script warns the user because the water velocity in the pipe(s) is lower than the minimum dredging velocity.

At this point, the water velocity in one pipe and the corresponding number of pipes can be determined by iteration. Based on the water flow to be pumped *Q*, the program has calculated the water velocity in one single pipe (equation 3-5). If it is greater than the maximum water velocity *V_max*, the program adds one pipe to the piping system and calculates again the water velocity. The calculation is iterated until the water velocity *V_water* reaches a reasonable value (i.e. *V_water* < *V_max*). The result is a number of pipes *Number_of_pipes* and a certain water velocity *Pipe_Water_Velocity* in those pipes.

Given the values *Number_of_pipes* and *Pipe_Water_Velocity*, the function focuses on one single pipe and the results for the global pumping/piping system follow from the single pipe results.

Darcy friction factor

If the flow in the pipe(s) is turbulent (i.e. if the Reynolds number *Re* is higher than 4000), the calculation of the friction factor *f* is obtained thanks to the Colebrook equation. The Chen approximation is used here (the *Chen* function has been previously defined with the equation 3-2). So, the Reynolds number *Re* is calculated and then the friction factor *f*.

$$\mathrm{Re} = \frac{\mathrm{rho} \times \mathrm{Pipe\_Water\_Velocity} \times \mathrm{D\_pipe}}{\mathrm{mhu}} \qquad \text{[no unit]} \qquad (3\text{-}8)$$

$$\text{If } \mathrm{Re} \geq 4000 \text{ then } \mathrm{f} = \mathrm{Chen}(\mathrm{Pipe\_Relative\_Roughness}, \mathrm{Re}) \qquad \text{[no unit]} \qquad (3\text{-}9a)$$

$$\text{If } \mathrm{Re} < 4000 \text{ then } \mathrm{f} = \frac{\mathrm{Re}}{64} \qquad \text{[no unit]} \qquad (3\text{-}9b)$$

Total head loss

The total head loss of the pumping process *Total_Head_Loss* is due to the height to be pumped on one hand (*Head_Loss_Height*) and to friction in the pipe(s) on the other hand (*Head_Loss_Pipe*). The head loss due to friction is calculated with the Darcy-Weisbach correlation (equation 3-11). Adding both types of head loss allows calculating the total head loss.

$$\mathrm{Head\_Loss\_Height} = 9.81 \times \mathrm{rho} \times \mathrm{H} \qquad \text{[Pa]} \qquad (3\text{-}10)$$

$$\mathrm{Head\_Loss\_Pipe} = \mathrm{f} \times \frac{8 \times \mathrm{L\_pipe}}{\mathrm{rho} \times \pi^2} \times \frac{\mathrm{Pipe\_Water\_Flow}^2}{\mathrm{D\_pipe}^5} \qquad \text{[Pa]} \qquad (3\text{-}11)$$

$$\mathrm{Total\_Head\_Loss} = \mathrm{Head\_Loss\_Height} + \mathrm{Head\_Loss\_Pipe} \qquad \text{[Pa]} \qquad (3\text{-}12)$$

Electrical power of each pump

$$\mathrm{Pump\_Power} = \frac{\mathrm{Pipe\_Water\_Flow} \times \mathrm{Total\_Head\_Loss}}{\mathrm{rho} \times \mathrm{NU}} \qquad \text{[W]} \qquad (3\text{-}13)$$

Specific electricity consumption

$$\text{Electricity\_Consumption} = \frac{\text{rho} \times \text{Pump\_Power}}{\text{Pipe\_Water\_Flow}} \qquad [\text{J/m}^3] \quad (3\text{-}14)$$

Finally, the function *Water_Pumping_Global_Function* returns the six main results (total head loss, electrical power for each pump, specific electricity consumption, number of pipes, water flow and water velocity in each pipe). The sub-functions *Head_Loss*, *Power*, *Elec_Consumption*, *Pipe_Number*, *Pipe_Flow*, *Pipe_Velocity* return only one result through the global function. It must be noted that the function *Elec_Consumption* returns the specific electricity consumption with a different unit from the one returned by the function *Water_Pumping_Global_Function* ([kWh/kg of pumped water] instead of [J/m^3 of pumped water]) in order to stay consistent with other calculations performed in the main scripts.

3.5 Function « Reactant_Addition »

The function *Reactant_Addition* simulates a chemical reaction in aqueous phase due to the addition of one reactant into the water to be treated. The software PHREEQC® is used for such simulations. Depending on the Python$^{\text{TM}}$ chemical object corresponding to the reactant under consideration, this function returns the pH, the total hardness TH, the complete alkalinity titration TAC and the mineral composition (i.e. salt concentrations and precipitates, see appendix 2-1) of the water resulting from the chemical reaction.

The arguments of the function *Reactant_Addition* are listed below :

- Mineral composition *Salts_Conc* in the water before reactant addition, in the form of a Python$^{\text{TM}}$ dictionary, i.e. a list of variables in this case (both names and values).
- Temperature and pH of the water before reactant addition (which are included in the *Salts_Conc* dictionary for sake of simplicity).
- Mixing proportion between the water and the reactant *Chem_Treatment_Ratio*, which is equivalent to the chemical dose to be injected into the water.
- Python$^{\text{TM}}$ object *Chemical_Object* corresponding to the chemical used as a reactant.

The calculations are not performed by the Python$^{\text{TM}}$ script itself. As described in paragraph 1.1.3 of chapter 2, the function only manages the calculation procedure by 1/ modifying the template file in order to get the adequate input file for PHREEQC®, 2/ launching the software PHREEQC® to perform the calculations and 3/ getting back the results.

In order to obtain the appropriate PHREEQC® input file, the mineral composition, the pH and the temperature of the water are re-defined in the template file as well as the mixing ratio between the water and the reactant. The chemical composition of reactants is already defined in their template file and they are assumed to be standard chemicals with fixed chemical composition.

Then, the Python™ function *Reactant_Addition* launches the software PHREEQC® and finally gets back the results, i.e. the complete alkalinity titration TAC, the total hardness TH, the pH and the mineral composition of the water after reaching the new chemical equilibrium.

This generic function is fundamental and it is used by many unit process models. Indeed, it plays a major role in water treatment simulation regarding water quality modelling and/or prediction of required chemical doses.

3.6 Function « pH_Adjustment »

This Python™ function aims at calculating the required chemical dose (acid or base) to adjust the pH of the water to a targeted value. The arguments of the function *pH_Adjustment* are detailed below :

- Initial pH of the water *Initial_pH* before the operation.
- Targeted pH of the water *Target_pH* after the operation.
- Mineral composition of the water *Salts_Concentration* before the operation.
- Python™ object *Acid_Python_Object* defining the acid possibly used.
- Python™ object *Base_Python_Object* defining the base possibly used.
- Convergence tolerance *Epsilon* for the iterated calculations (default value is $1e^{-3}$).
- Maximum number of iterations *Nmax* to avoid infinite loops (default value is 100).
- Minimum chemical dose *MinDose* (default value is $1e^{-12}$).

The calculation of the required chemical dose to adjust the pH is based on the dichotomy method. This is done in three steps:

1. Determination of which kind of chemical is required (acid or base) by comparing the initial pH and the targeted pH.
2. Determination of an acceptable interval for the dichotomy method, i.e. a too low dose and a too high dose, thus ensuring that the right chemical dose is in this interval (use of the function *Reactant_Addition* for calculating the resulting pH).
3. Application of the dichotomy method by iterating calculations until determining the appropriate chemical dose (use of the function *Reactant_Addition* again).

Finally, this Python^{TM} function returns the required acid and base doses (one of them is obviously null), the mineral composition, the pH, the total hardness TH and the complete alkalinity titration TAC of the water after pH adjustment.

3.7 Function « TAC_Adjustment »

The function *TAC_Adjustment* is very similar to the function *pH_Adjustment*. Indeed, the principle is exactly the same, except that the targeted value concerns the complete alkalinity titration TAC instead of the pH. The complete alkalinity titration TAC is calculated from the following equation.

$$\mathrm{TAC} = 2 \times \left[\mathrm{CO_3^{2-}}\right] + \left[\mathrm{HCO_3^-}\right] + \left[\mathrm{OH^-}\right] - \left[\mathrm{H^+}\right] \qquad (3\text{-}15)$$

Equation 3-15 shows that the TAC is increased 1/ when the pH is increased or 2/ when carbonate ions CO_3^{2-} and/or bicarbonate ions HCO_3^- are added to the water.
As a first step, the function *TAC_Adjustment* determines whether the TAC of the water to be treated needs to be increased or decreased depending on the targeted value (user-defined parameter), thus selecting the appropriate reactant. Then, it calculates the quantity of reactant required to adjust the TAC to the targeted value.

3.8 Function « Flows_Mixing »

The function *Flows_Mixing* is used to simulate the mixing of two water flows. The principle is very similar to the function *Reactant_Addition*, at least when considering the case of diluted liquid reactants in the function *Reactant_Addition*. Indeed, in this type of case, both functions consist in simulating the mixing of two aqueous solutions. So the function *Flows_Mixing* is explained here by comparing it with the function *Reactant_Addition* since they are analogous.

In the function *Reactant_Addition*, the mineral composition and the pH of the water flow are re-defined in the PHREEQC® template file and the concentration of the reactant stays unchanged. This allows creating the adequate PHREEQC® input file for simulating the mixing of the reactant and the water flow under consideration (i.e. for simulating the chemical reaction).

In the function *Flows_Mixing*, the mineral composition and the pH of both water flows are re-defined in a dedicated PHREEQC® template file in order to generate the adequate input file. Their mixing ratio must also be provided as an argument for the function.

Finally, the complete alkalinity titration TAC, the total hardness TH, the pH and the mineral composition of the resulting water flow are returned by the function *Flows_Mixing*.

3.9 Function « Coagulant_Dose_Calculation »

As mentioned in chapter 1, modelling and design of the coagulation process are still an issue for water scientists (Dudley et al. 2008). Most of the coagulation models used in industry are empirical and require extensive measurement data for calibration. This research work intends to bypass this problem and the modelling objectives state that mechanistic models with minimum calibration requirements must be preferred to empirical and statistical ones (chapter 1). Therefore, the modelling of the coagulation process has been carried out accordingly and a mechanistic model was sought following a broad literature review.

The model selected for implementation in the EVALEAU framework (through the function *Coagulant_Dose_Calculation* presented here) is the one developed by Kastl et al. (Kastl et al. 2004; Kastl et al. 2008). This model was initiated by the research work of Edwards and Tseng (Edwards 1997; Tseng and Edwards 1999).

The reliability of this coagulation model has been proved and it is already used in practice since 2004 (van Leeuwen et al. 2009). Six drinking water treatment plants located in Australia actually use one version of this model, embedded in a software named mEnCo®, for coagulant dose determination. The authors also apply it successfully at the design stage of water treatment plants and this is of the highest interest since it is a major objective of the EVALEAU project.

The authors have formulated a mechanistic model (equation 3-16) which is valid in the pH range [5.0-7.0]. The model allows calculating the DOC remaining in the coagulated water depending on 1/ the raw water DOC, 2/ the type of coagulant (aluminium or iron based coagulants), 3/ the coagulant dose and 4/ the pH at which the coagulation process is operated.

$$\mathrm{DOC}_{\mathrm{Coagulated\_Water}} = \mathrm{f}\ (\mathrm{DOC}_{\mathrm{Raw\_Water}}, \mathrm{Coagulant\_Type}, \mathrm{Dose}, \mathrm{pH}) \qquad (3\text{-}16)$$

- $DOC_{Coagulated\_Water}$: DOC in coagulated water
- DOC_{Raw_Water} : DOC in raw water
- *Coagulant_Type* : type of coagulant (aluminium or iron salt)
- *Dose* : dose of metal ion (Al or Fe)
- *pH* : pH of the coagulation process

This coagulation model relies on one postulate which represents its main originality. The authors proposed to consider three distinct fractions of DOC : the non-polar fraction f_{nonpolar}, the humic (and fulvic) acids fraction f_{ha} and the non-sorbable fraction $f_{\mathrm{nonsorbable}}$.
The non-polar fraction f_{nonpolar} of DOC represents the dissolved organic compounds that are adsorbed independently from the coagulation pH. The humic acids fraction f_{ha} represents the dissolved organic compounds that are adsorbed depending on the coagulation pH. Indeed, the associated form of these acids is adsorbed on flocs unlike the dissociated form and this explains why these compounds are adsorbed on flocs depending on the pH of the operation. Finally, the third fraction of DOC represents the non-sorbable organic compounds.

Some assumptions are stated by the authors. In fact, most of them were already stated in the research work of Edwards (Edwards 1997). These assumptions are listed below :

- DOC removal is mainly due to adsorption onto metal hydroxide flocs formed during the coagulation process.
- DOC is removed by adsorption following a Langmuir isotherm.
- Physical properties of the organic matter to be removed do not depend upon the pH.
- The variation of DOC concentration in a given water resource is due to dilution or concentration of DOC, the three fractions of DOC being constant.
- The maximum sorption capacity remains constant in the pH range tested for developing the model.

The model relies on parameters, which are coagulant and water dependent. They must be ideally calibrated by minimum jar-test experimentation. They are introduced below :

- a : Maximum sorption capacity [mgDOC/meq metal].
- b : Sorption coefficient [L/mgDOC].
- f_{ha} : Humic acids fraction of DOC [dec.%].
- $f_{nonpolar}$: Non-polar fraction of DOC [dec.%].
- pKa : Dissociation constant of humic acids [no unit].
- k : Relative adsorption constant [no unit].

It must be noted that the relative adsorption constant k was close to 1 in all cases studied by the authors, which means that humic acids and non-polar fractions have the same adsorption activity on flocs. The relative adsorption constant k is therefore assumed to be equal to 1 and it is not considered by the authors as a parameter to be calibrated for this adsorption model.

The mathematical model can then be described by the equation system presented below.

Sum of the three fractions of DOC in raw water

$$\mathrm{f_{ha}} + \mathrm{f_{nonpolar}} + \mathrm{f_{nonsorbable}} = 1 \tag{3-17}$$

Acid-base equilibrium of humic acids

$$\mathrm{Ka} = \frac{\left[\mathrm{A^-}\right]_{\mathrm{liq}} \times \left[\mathrm{H^+}\right]_{\mathrm{liq}}}{\left[\mathrm{HA}\right]_{\mathrm{liq}}} \tag{3-18}$$

Different forms of humic acids in the liquid and solid phases

$$\mathrm{DOC_{ha,0}} = [\mathrm{HA}]_{\mathrm{sol}} + [\mathrm{HA}]_{\mathrm{liq}} + [\mathrm{A^-}]_{\mathrm{liq}} \tag{3-19}$$

Langmuir isotherm equation for the compounds of the humic acids fraction

$$\frac{[\mathrm{HA}]_{\mathrm{sol}}}{\mathrm{D}} = \frac{\mathrm{a} \times \mathrm{b} \times [\mathrm{HA}]_{\mathrm{liq}}}{1 + \mathrm{b} \times \left([\mathrm{HA}]_{\mathrm{liq}} + \mathrm{k} \times \mathrm{DOC_{nonpolar,liq}}\right)} \tag{3-20}$$

Langmuir isotherm equation for the compounds of the non-polar fraction

$$\frac{\mathrm{DOC_{nonpolar,0}} - \mathrm{DOC_{nonpolar,liq}}}{\mathrm{D}} = \frac{\mathrm{a} \times \mathrm{b} \times \mathrm{k} \times \mathrm{DOC_{nonpolar,liq}}}{1 + \mathrm{b} \times \left([\mathrm{HA}]_{\mathrm{liq}} + \mathrm{k} \times \mathrm{DOC_{nonpolar,liq}}\right)} \tag{3-21}$$

- $f_{nonsorbable}$: Non-sorbable fraction of DOC [dec.%]
- $[H^+]_{liq}$: Concentration of hydrogen ions H^+
- $[A^-]_{liq}$: Concentration of the dissociated form of humic acids A^- in the coagulated water (liquid phase)
- $[HA]_{liq}$: Concentration of the associated form of humic acids HA in the coagulated water (liquid phase)
- $[HA]_{sol}$: Concentration of the associated form of humic acids HA adsorbed on flocs in the coagulated water (solid phase)
- DOC_0 : Total DOC in raw water
- $DOC_{Coagulated\_Water}$: Total DOC remaining in coagulated water (liquid phase)
- $DOC_{ha,0}$: fraction of DOC induced by humic acids in raw water (f_{ha} . DOC_0)
- $DOC_{nonpolar,0}$: fraction of DOC induced by non-polar compounds in raw water (f_{np} . DOC_0)
- $DOC_{nonsorbable}$: fraction of DOC induced by non-sorbable compounds in raw and coagulated waters ($f_{nonsorbable}$. DOC_0)
- $DOC_{nonpolar,liq}$: DOC induced by non-polar compounds in coagulated water (liquid phase)
- D : coagulant dose [mEq/L of coagulant salt].

Resolving this equation system allows calculating the remaining DOC in coagulated water $DOC_{Coagulated\_Water}$ as expressed in the equation 3-22 :

$$DOC_{Coagulated\_Water} = DOC_{nonsorbable} + [HA]_{liq} + [A^{-}]_{liq} + DOC_{nonpolar,liq} \tag{3-22}$$

This coagulation model has been implemented in the EVALEAU framework through the function *Coagulant_Dose_Calculation*. Nevertheless, it must be noted that the calculations are reversed with regard to the model as formulated by Kastl et al. because the objective is to determine the coagulant dose required to remove a certain proportion of DOC (i.e. DOC removal is a process objective within a design perspective). Indeed, a certain coagulant dose can be determined based on a DOC removal objective or vice versa. The equation system is the same in both cases. The four arguments of this Python^{TM} function are :

- *pH* : Coagulation pH [no unit].
- *Input_DOC* : DOC of the input water [mg/L].
- *Input_UVA* : UVA of the input water [m^{-1}].
- *DOC_removal* : DOC removal objective [dec.%].

The parameters of the function *Coagulant_Dose_Calculation* are also provided as arguments (for sake of simplicity in the code) and they are listed below :

- *Max_Sorption_Capacity* : Maximum sorption capacity [mgDOC/mEq coagulant salt]
- *Sorption_Coefficient* : Sorption coefficient [L/mgDOC]
- *HA_Fraction* : Humic acid fraction in DOC [dec.%]
- *NP_Fraction* : Non-polar fraction in DOC [dec.%]
- *HA_pKa* : Dissociation constant of humic acids [no unit]

Average parameter values from the work of Kastl et al. are set as default values for all parameters depending on the coagulant salt (Al or Fe) (Kastl et al. 2004). The authors of the model argue that the minimum number of jar-tests for calibration is 8 but they recommend more jar-tests to improve the accuracy of model fitting. On-site measurements are then needed for calibration.

The parameters *Max_Sorption_Capacity* and *Sorption_Coefficient* are water and coagulant dependent. They are not likely to be changed by any unit process. They are defined by their default values in the second-level script corresponding to coagulation and they can be modified if their calibration is carried out.

The parameters *NP_Fraction*, *HA_Fraction* and *HA_pKa* are not defined in the second-level script corresponding to coagulation but in a dedicated file. This Python^{TM} file, named « OM_Information », is part of the water quality database (i.e. it is located in the same directory as the three spreadsheets described in chapter 2 paragraph 1.2). The reason is that these parameters are not coagulant dependent, they are only water dependent.

Besides, the values of the parameters *NP_Fraction* and *HA_Fraction* are likely to be changed by some unit processes. It happens when the organic matter is oxidised or partly removed. So, any unit process removing UVA and/or DOC changes the numerical values of organic matter fractions (f_{ha}, $f_{nonpolar}$ and $f_{nonsorbable}$). The concerned unit process model must calculate the new values of the parameters so that it can take into consideration the related effects on the performances of the coagulation process taking place afterwards. For instance, when an oxidation process is placed at the beginning of the process chain, one typical objective is to remove UVA in order to enhance the coagulation step that comes next. In such a case, the parameter's values are redefined in the Python^{TM} file « OM_Information » so that this issue is duly addressed in the modelling of a drinking water treatment plant.

Finally, the results obtained by the function *Coagulant_Dose_Calculation* are presented here. The function returns three different results required for the calculations in the main script of the coagulation models. They are listed below :

- The coagulant dose *Coagulant_Dose* required for fulfilling the DOC removal objective.
- The maximum DOC removal due to the characteristics of the dissolved organic matter of the water under consideration.
- The resulting UVA removal *UVA_Removal* obtained simultaneously.

When removing DOC by coagulation, one also removes UVA at the same time. Indeed, the presence of UVA is due to a fraction of dissolved organic compounds which are then part of the compounds responsible for the presence of DOC in water. Thus the coagulation process removes DOC and UVA at the same time, but not necessarily in the same proportions. UVA removal is not initially considered in the model developed by Kastl et al. but we propose to calculate this performance of the process from the same model.

The dissolved organic compounds responsible for the presence of UVA in natural waters are mostly the humic (and fulvic) acids (WTP manual 2001). As the model calculates the quantity of humic acids adsorbed $[HA]_{sol}$ on the flocs formed during the coagulation process, the removal of UVA [dec.%] is then assimilated to the removal of humic acids (equation 3-23).

$$\text{UVA\_Removal} = \frac{[\text{HA}]_{\text{sol}}}{\text{DOC}_{\text{ha},0}} \qquad (3\text{-}23)$$

It must be noted that the calculation of UVA removal during clarification in the Water Treament Plant model developed by the US EPA (WTP manual 2001) is based on the equations of Edwards (Edwards 1997) like the coagulation model of Kastl et al. presented here. Results from the methods we propose here have been compared with results from the Water Treament Plant model on a few cases. They are very similar (the difference is at most 3%) which is logical since the original equations are the same. So, the calculation of UVA removal that we propose to integrate in this coagulation model seems to be consistent but more efforts are required to properly validate this completion of the coagulation model.

4. Mathematical models for unit processes

The mathematical models for unit processes are introduced and explicitly formulated in the appendix 3-2 for sake of clarity. This appendix describes in detail the mathematical models developed during the EVALEAU project. These models concern only unit processes involved in conventional drinking water treatment.

The categories of unit processes, presented in the appendix 3-2, are listed below. The unit process models themselves are further listed in the sections of the appendix corresponding to their process category.

- Water pumping
- PAC addition
- Coagulation
- Flocs separation
- Media filtration
- Disinfection - Oxidation
- Neutralisation - Remineralisation
- Sludge treatment

This appendix can be seen as a user manual of the EVALEAU tool since it provides fully detailed explanations about the unit process models made available in the EVALEAU library.

5. Conclusion

Object-Oriented Programming is a relevant paradigm for computer programming and it is currently being adopted by a rising number of scientists from various disciplines. During this research project, Python^{TM}, known as a glue programming language, was used successfully to create a multidisciplinary framework.

The unit process models, developed and stored in the computational library, are based on a few Python^{TM} files. The basis for a unit process model is the so-called main script. It makes the connection between the different files involved in the modelling of one unit process and manages the calculation procedure (e.g. call of external software). The second-level script (one at the most for each unit process model) defines functions and constants on which the unit process model relies. Besides, the files named « EVALEAU_Functions » and « EVALEAU_Chemical_Objects » are of the highest importance, since generic functions and objects are defined in these scripts.

The generic functions have been described in detail in this chapter. The research work has particularly focused on the coagulation modelling through the development of the generic function *Coagulant_Dose_Calculation*. Indeed, it was imperative to base the calculations as much as possible on mechanistic models and the literature review on water treatment simulation comes to the conclusion that coagulation needs to be studied further. An existing recent mechanistic model was adopted. Furthermore, we propose an extension of the model by : 1/ integrating it in a global chemical equilibrium model for water, 2/ enabling one to calculate not only the DOC removal but also the UVA removal, based on the same equation system.

The mathematical models, briefly listed in this chapter, are explicitly formulated in the appendix 3-2. This appendix presents the modelling work in its entirety and can be seen as the user manual of the EVALEAU tool.

Chapter 4.

An integrated « Process Modelling-Life Cycle Assessment » tool for the assessment and design of water treatment processes

A pilot study

Résumé du chapitre 4. Outil intégré « Modélisation de Procédés - Analyse de Cycle de Vie » pour l'évaluation et le dimensionnement de procédés de traitement de l'eau. Une étude de cas pilote.

Une rapide revue de la littérature scientifique permet de rappeler les tenants et les aboutissants d'un outil tel que celui développé et présenté dans cette thèse.

L'outil EVALEAU est ensuite décrit succinctement au début de ce chapitre pour rappel. Les concepts embarqués et les approches de modélisation associées sont de même introduits.

L'approche modulaire, générique et fortement paramétrée pour la modélisation d'usines de production d'eau potable est aussi rappelée. Son importance est évidemment primordiale à l'heure d'appliquer l'outil en pratique. En effet, il y a une analogie entre le paramétrage des modèles grâce à l'outil EVALEAU et le travail de dimensionnement d'une usine de production d'eau potable.

L'analyse de sensibilité et l'utilisation originale qui en est faite sont aussi discutées. L'application de la méthode de Morris dans l'étude de cas est censée apporter des informations précieuses pour l'écoconception de l'usine et pour la recherche d'opportunités d'amélioration.

L'usine étudiée se situe dans la région parisienne et utilise la Seine comme ressource. La chaîne de procédés pour le traitement de l'eau est assez complexe, tout en étant représentative d'un traitement conventionnel d'eau potable. L'inventaire de données est disponible de sorte que les résultats issus de la modélisation peuvent être comparés aux données du terrain (qualité de l'eau, consommations de réactifs et d'énergie). Il faut noter que le traitement des boues et leur épandage est négligé dans cette étude par manque d'information. Le transport des réactifs est quant à lui exclu intentionnellement des frontières du système. En effet, le but de cette étude pilote n'est pas de réaliser une analyse de cycle de vie précise et complète, mais plutôt de chercher à valider des modèles de procédés unitaires et plus généralement l'approche de modélisation proposée dans ce travail de recherche. L'unité fonctionnelle choisie est « 1 m^3 d'eau potable en sortie d'usine ».

Les résultats concernant la qualité de l'eau sont satisfaisants. Les différentes recommandations (légales ou industrielles) sont respectées et les résultats sur la turbidité et l'absorbance UV sont assez proches des valeurs mesurées sur site.

Les consommations de réactifs et d'électricité, prédites par le modèle de l'usine, sont très proches des consommations réelles sur site. Les erreurs de prédiction sont inférieures à 10% quelle que soit la consommation considérée, ce qui est tout à fait satisfaisant. Ceci est d'une importance majeure, puisque c'est sur la base de ces consommations calculées que les impacts environnementaux sont évalués par la suite.

Les résultats d'impacts environnementaux, obtenus avec la méthode Impact 2002+, sont en conséquence en très bonne correspondance avec ceux obtenus par l'analyse de cycle de vie conventionnelle (basée sur l'inventaire de données recueillies sur site).

L'analyse de contribution montre que les procédés unitaires contribuant le plus à la catégorie d'impact « Climate Change » sont le pompage (30%) et la pré-ozonation (34%), et dans un moindre degré la coagulation (15%), l'inter-ozonation (12%) et la filtration sur charbon actif en grain (8%).

Le graphe de Morris (relatif à la catégorie d'impact « Climate Change ») obtenu après application de la méthode sur le modèle de l'usine montre clairement que quatre paramètres de procédés sont plus influents que les autres. Tous sont des paramètres des deux étapes d'ozonation. Ces paramètres sont l'efficacité de transfert de l'ozone dans l'eau et le pourcentage d'oxygène pur dans le gaz utilisé pour la production d'ozone. Les leviers d'action prioritaires pour réduire les impacts générés par la production d'eau potable dans cette usine sont donc identifiés grâce la méthode de Morris.

Chapter 4. An integrated « Process Modelling-Life Cycle Assessment » tool for the assessment and design of water treatment processes - A pilot study.

Abstract

Purpose

The application of Life Cycle Assessment (LCA) to the design of water treatment plants is hampered by: i) a large diversity of unit processes, ii) the high variability of the operation conditions in relation with the water quality input, iii) the range of possible technical solutions to fulfil the treatment needs. For a consistent prospective assessment, the LCA should be based on the simulated functioning of the unit processes rather than on average data, as it is most often the case when no real data are available. Here, a novel, integrated and flexible « Process Modelling–Life Cycle Assessment » (PM-LCA) tool for design and LCA of water treatment technologies is presented.

Methods

The tool (EVALEAU) was developed in Umberto® (v5.5) using the Python^{TM} language for code scripting. A library of Unit Process (UP) modules was built. Each module is a detailed and highly parameterized model of a specific water treatment process, which is further linked with the software PHREEQC® for water chemistry calculation. Input data are: water composition, design, operation parameters, including literature or user-defined values. The modules are linked to Ecoinvent datasets (v2.2) for background processes. By combining the modules, water treatment chains can be designed and evaluated in Umberto® with a high level of detail and specifications. A sensitivity analysis toolbox (Morris method) was included for the identification of the process parameters mainly affecting the impact results.

Results

The tool was successfully applied to the test bed case of an existing drinking water plant located in the Paris region. The conventional LCA results, based on average recorded data, were compared with the results obtained using the PM-LCA tool. Modelling results for technical parameters were also compared with data collected on site. An overall good agreement between simulations and real data was obtained, proving the relevance of the developed tool. Sensitivity analysis indicated that ozone production and transfer into water are the main technological parameters influencing climate change (taken as example since it is of high interest for stakeholders), which have therefore to be fine-tuned.

Conclusions

The EVALEAU tool successfully solves the challenge of linking LCA results to the related engineering design choices, from the assessment and eco-design perspectives. The concepts and methodologies embedded within the tool provide the user with complementary views of the designed system, in terms of potable water quality, design and operation parameters and environmental impacts generated over its life cycle.

Key words

Life Cycle Inventory, Life Cycle Assessment, water treatment, process modelling, eco-design, sensitivity analysis, drinking water.

1. Introduction

Nowadays, Life Cycle Assessment (LCA) methodology is increasingly used to evaluate the environmental performances of processes, products and services and potentially represents a powerful tool for eco-design. As suggested by Azapagic et al. (1999, 2006), the integration of environmental criteria through LCA for instance, at the very early stages of process design is essential in the life cycle optimization of the designed system, focusing both on the foreground and background processes. Nevertheless, it still needs the development of adapted integrative methods and tools.

Indeed, life cycle inventories are traditionally based on average data (material and energy inputs and outputs) collected on site or estimated from literature or from modelling studies performed prior to the LCA study. This approach has recognized shortcomings when applied on processes characterized by highly variable design and operation parameters. This is the case of pollution treatment technologies, e.g. water treatment, which are composed of a chain of unit processes (UP) linked together by the functional unit (the water flow to be treated). Raw water undergoes subsequent quality changes across the chain of UPs, until the targeted output quality is reached. Water treatment technologies are characterized by: 1) different types of raw water treated (sea, rivers, groundwater, specific effluents, sewage, etc.) and the variability of their properties (local composition variations, flow rates, seasonal or other time related constraints, etc.), making each treatment plant unique and site specific; 2) highly adaptable operation conditions in response to the raw water quality fluctuations (variation of energy and material input/output); 3) many possible technical solutions (i.e. types of UPs and their combinations) in the design phase; 4) variability of UP's operating conditions (physic-chemical parameters)which are most often chosen based on economic considerations. As for most of the UPs there are only limited Life Cycle Inventory (LCI) data available, currently it is not possible to set up databases considering points 1) to 4). As a result, the application of LCA to water treatment is hampered and in most of the cases the LCA results are not relevant for the comparison of different technologies or for the identification of environmental hot spots.

The water quality and the operation parameters determine the required energy and material consumptions. Therefore, the LCI is dependent on the technological specifications and project constraints. Consequently, the building of a highly parameterized LCI is mandatory to properly evaluate the environmental impacts of water treatment chains. Moreover, the use of LCA as a tool for eco-design requires a predictive and prospective LCI, which has to take into account the elements of points 1) to 4).

In the past decade, significant efforts have been made in order to cope with the challenge of integrating environmental criteria into the design of process-based plants. Sugiyama et al. (2008) suggested a framework for decision-making support on process design, integrating technical, economic and environmental aspects and a similar approach was proposed by Khan et al. (2001). However, the application of these concepts in the industrial practice remains difficult and process design is often considered as a preliminary step to LCA instead of being fully integrated in a coherent framework (Bojarski et al. 2008, Iosif et al. 2010, Kniel et al. 1996, Vince et al. 2008a). The indirect environmental impacts due to off-site pollutant emissions of background processes were taken into consideration by Bernier et al. (2011) by linking a power plant model with Ecoinvent-like modules, corresponding to the background processes involved. Chen et al. (2004) went a step further and proposed a fully integrated framework linking the ASPEN software for process modelling and Excel to carry out the LCA, with applications to the chemical industry. The automated connection between those tools and databases makes it possible to get the different results in parallel and not consequently, proving a better understanding of the design alternatives on the LCA results. Nevertheless, the approach of Chen et al (2004) cannot be applied to all types of industrial processes, as for example the depollution technologies, because of the lack of appropriate modelling tools. Concerning conventional LCA studies (based on site inventories) on potable water production, a state of the art was presented recently (Igos et al., 2012) and therefore this subject is not detailed here. The most of the available studies focused on membrane technologies for desalination and very few approached the conventional processes (Vince et al. 2008; Raluy et al. 2005; Friedrich 2002; Sombekke et al. 1997).

A certain number of exposed bottlenecks have been successfully solved through the development of a fully integrated « Process Modelling – Life Cycle Assessment » (PM-LCA) tool for water treatment technologies. The tool named EVALEAU fulfils two functions: *process modelling - design aid* and *environmental diagnosis*.

In this paper, the principles and methods used to develop the tool are described, then its validation is presented and discussed through a test bed case.

2. Methods

2.1 EVALEAU tool development

The developed PM-LCA tool, hereafter named EVALEAU, is aimed at covering the specificities of water treatment technologies and has to fulfil at a minimum the following requirements:1) calculate the LCA results of different water treatment (foreground) processes according to the ISO 14040-44 standards, using conventional LCI databases for the background processes and recognized LCIA methods; 2) allow easy combination of UPs in different treatment chains, in order to assess a variety of different technologies; 3) account for the influence of design and operation parameters on the foreground LCI; 4) allow easy modification of the default values of process parameters (user-defined values) for calculating the corresponding LCI in order to evaluate the LCA results for different working conditions of the plant, and 5) automatically identify the hot spots, i.e. the process parameters having the major influence on LCA results.

In order to fulfil the first requirement, the software Umberto® v5.5 (http://www.ifu.com/en) has been chosen as working environment because of its capability to resolve complex flow networks. The inventory modules are uploaded from LCI database Ecoinvent (Weidema et al. 2009), for energy suppliers, chemicals, transports, etc., or are defined by the user through specific scripts, for the specific UPs of water treatment. The integrated scripting capability of Umberto® was exploited to create a complementary library of independent modules dedicated to the different UPs of water treatment technologies, which allowed complying with the second requirement. The library allows building the foreground process chain (i.e. EVALEAU modules for the water treatment chain) which is further linked to the required background processes (i.e. Ecoinvent modules for electricity and chemicals production). The principle of the developed tool and of the LCI calculation is schematized in figure 1.

The modules stored in the EVALEAU library are parameterized models, written in Python^{TM}, which calculate chemicals and energy consumptions and substance emissions at the level of each UP. In addition, each UP model provides the technical design and operation data necessary to link the UPs in the whole process network and to assess the process efficiency. The Water Quality Data (WQD) is a set of 168 criteria including generic parameters (temperature, pH, turbidity, etc.), organic matter parameters (UV absorbance, dissolved organic carbon, etc.), pathogenic micro-organisms, inorganic compounds, micro-pollutants, reaction products. The WQD template is stored in an Excel file, directly available (reading and writing) to the Python^{TM} scripts and has to be fed by the user with specific data concerning the raw water of the case under study. A sensitivity analysis tool relative to the model parameters was implemented as well in order to fulfil the fifth requirement.

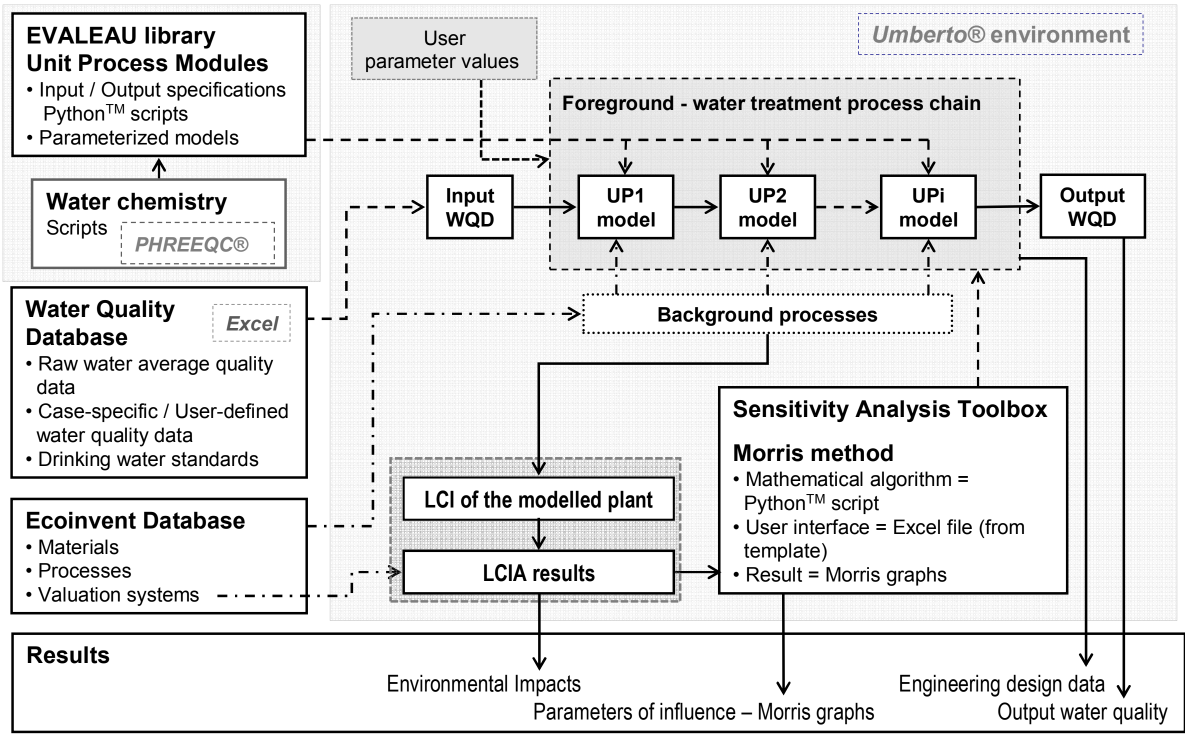


Figure 4-1. Principle of the EVALEAU tool - automatic linkages between different software tools, main tasks and results.

In the Umberto environment (figure 1), the UP modules are first linked each other to build the water treatment chain (foreground level) and then linked to the appropriate Ecoinvent (currently used database) background modules. At the level of a UP module, the input data are: i) water quality data, being issued from the raw WQD file or calculated by the previous module, ii) specific parameters of the process (user values or default values). This model architecture ensures specific inventory calculation at the level of each UP, of the complete plant and of the plant's life cycle, thus satisfying the third requirement.

Besides the LCI, the UP models calculate engineering design data as well - a brief overview of the UP design and its overall efficiency, which are mandatory from an ecodesign perspective (e.g. electric power to be installed, water velocity in pipes, etc.). They are currently stored in an automatically created spreadsheet (engineering design data report), together with the intermediary and output WQD. The results obtained from the tool are: i) energy and chemicals consumptions at the level of each UP and complete LCI, ii) LCIA results, iii) output water quality, iv) engineering design data, and v) sensitivity analysis results.

To sum up, EVALEAU is a PM-LCA tool. Its main components are the computational library of UP models, the sensitivity analysis toolbox, a set of water quality data (WQD), output spreadsheet data (WQD, engineering design report and their linkages. It fully benefits from Umberto environment and capabilities. It allows flowchart building for any water treatment plant and calculation of material and energy input/output at plant (*process modelling* function). It performs *environmental diagnosis* of the modelled plant.

2.1.1 UP modelling and parameterization

The UPs are traversed by the water flow which undergoes changes at the level of each UP. At the level of a given UP, the pollutant abatement is achieved by chemical reactions (like precipitation, coagulation, oxidation, etc.) and/or separation processes (settling, filtration, etc.). The water quality can also be corrected by adding specific substances for mineralization, softening, etc. All these processes have to be characterized using chemical reaction and/or separation efficiency models. Chemicals and energy consumption in the water treatment processes is a function of the input water quality (i.e. the nature and quantity of pollutants) and of the treatment performance objective (output water quality). A literature review of existing models for water treatment processes has been carried out in order to select the best available UP models. The selected models are reference models in their respective domain and have been developed by recognized scientific organization (for example the WTP modelling approach developed by the US EPA for assessing Disinfection By-Products formation (WTP manual 2001)). An additional selection criterion was the good agreement of the models with industrial practices.

The models consist mainly of a set of equations defining energy and mass balances, for steady state functioning conditions. The efficiency of separation operations and kinetic performances were used for each type of UP and related equipment (for example a given type of settler, filter, etc.), using literature and constructor specifications as default values.

In order to model the chemical reactions in aqueous solutions the geochemistry software PHREEQC® (Parkhurst and Appelo 1995) was used, because of the completeness of water chemistry models and databases included, and of its wide scientific recognition. A library of PHREEQC scripts for each UP was built, to be used by the corresponding Python^{TM} script. Concerning the microbiology, results of the European project Microrisk (Smeets et al. 2006) were used in terms of mean elimination capacity of pathogen per UP. For the disinfection UP, conventional models were used combining hydrodynamics and imposed residual dose of oxidant.

The flexibility of the tool is ensured by the high parameterization of the UP models. The adjustable process parameters are a set of data that define: engineering design choices (e.g. pipe diameter, pump efficiency, device hydrodynamics), technical and productivity constraints (e.g. height to be pumped, filter area and backwashing schedule), and legal constraints (e.g. CT=(contact time)x(residual oxidant concentration), which is a disinfection requirement criterion) or pollutant abatement requirements.

The models stored in the EVALEAU library are generic and their parameters are set to default values, collected from literature, guidelines or expert recommendations. They are representative of hypothetical average working conditions of the unit processes. Defining the parameter values enables the user to modify the generic version of the model and to get a very specific model, more representative of the case under study. The comprehensive parameterization of the UP models allows to adapt to specific situations, which is a key feature of EVALEAU tool. The modelling strategy used allows therefore fulfilling the fourth and fifth tool requirements.

2.1.2 Sensitivity analysis

The highly parameterized modelling approach generates LCI results for a high number of parameter datasets (about 100 for a conventional plant model). As a result, it is very difficult to assess their influence on the results, and to identify the engineering design and operation choices which mostly affect the LCIA results per impact category. This shortcoming was resolved by integrating sensitivity analysis relative to the model parameters, using the Morris approach (Morris 1991, Campolongo et al. 2007).

In the Morris method, model parameters but also input variables can be considered. They are both referred as factors and k is their number. The space of factors is discretized in p levels; each factor varies over the p levels. The variation of the model result due to the variation of one factor is called an elementary effect (EE) (derivative-based approach). The variation of one factor is realised as follows. The first point is randomly determined. Then, the factor value is switched to a different level, which creates a trajectory of (k+1) points in the k-dimensional parameters' space. Thus one trajectory allows calculating one elementary effect for each factor. The Morris method consists in generating r trajectories and running the corresponding model calculations. It is then possible to calculate r elementary effects for each factor. The procedure is repeated for each factor. In the basic version of the Morris method, the mean of the elementary effects and the standard deviation are computed for each factor and used as sensitivity measures to evaluate the factors' influence on the model.

This method was selected since it is easily understandable, it has low computational costs and it works almost on every kind of model. The method provides a graph which can be interpreted without considering the details of the mathematical method. Each model parameter is represented by a point and, depending on its position on the graph; qualitative information about the parameter influence can be deduced. The more a parameter is influent, the more its position will be on the right of the graph. The less linear is the parameter's influence, the higher the point will be on the graph. The sensitivity analysis points out the key parameters to be further studied for eco-design.

2.2 Test bed case

The case study of a drinking water production plant, situated on the Seine river in the Paris region, has been used to prove the reliability of the tool while illustrating the concepts and methods implemented. The treatment chain is quite representative of conventional drinking water production and is composed of the following operations (figure 2): pumping, pre-ozonation, coagulation/flocculation/settling, clarification by biolite filtration, inter-ozonation, granular activated carbon (GAC) filtration and disinfection by chlorine.

First, average site data from yearly recordings were used to carry out a conventional LCA (see Igos et al. (2012)) for detailed discussion of the LCA results). The site inventory reference year is 2007, the average production rate during the reference year was 1525 m3/h. The available site data include: electricity consumption for the whole plant, quantities of purchased reactants and GAC. So, the LCI of the plant is based on total yearly consumptions, specific detailed electricity/reactants consumption by unit process being not available.

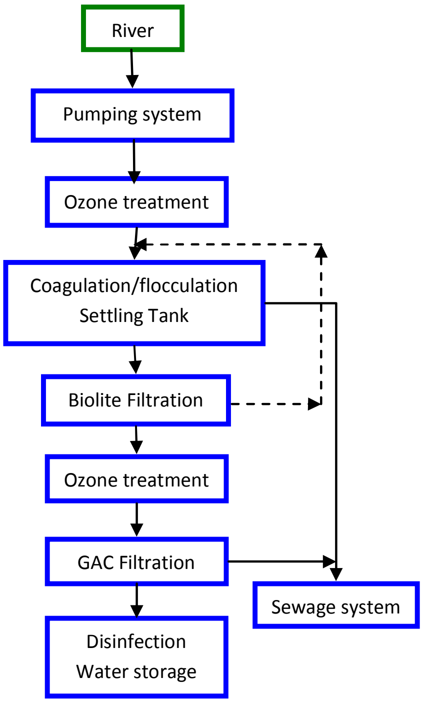


Figure 4-2. Flowchart of the studied plant

Second, process modelling was coupled with the LCA approach within the EVALEAU tool. This approach allows representing the plant's flowsheet as it actually is: the chain of UPs is simulated using the respective modules from the EVALEAU library, further adapted to the site conditions, as explained in the following. The ozonation operations use air as feed gas for ozone production and take place in two different contactors, because of the different objectives, respectively enhancing the coagulation efficiency (pre-ozonation) and oxidizing the small organic molecules for a better adsorption in the GAC filters before disinfection. Aluminium sulphate is used as coagulant, polymers are added for flocculation. Coagulation/flocculation/settling take place in a compartmented device, equipped with scrappers. The filtration operations run by gravity in open devices, equipped with fixed beds of appropriate granular media. Backwashing is realized with water and compressed air. The biolite washing effluent is returned to the coagulation step whereas sludge from the settler and GAC washing effluent are sent to a separate treatment site. As no data were available on sludge treatment, this UP was not considered neither in the conventional LCA nor the

PM-LCA, and this is a limitation of the presented case study. Model development for sludge treatment (sludge from potable water plants) is an ongoing work. The disinfection using sodium hypochlorite is the last operation realized in the stocking reservoir. There is no intermediary pumping as water flows inside the plant by gravity. In this work the focus is on the calculation of the foreground inventory data using the EVALEAU tool, by simulating the operating conditions of the plant. The raw water quality (used at the model input) is known from mean values recorded over many years including the reference year.

For both the conventional LCA and the PM-LCA, the functional unit chosen is “1 m3 of drinking water at plant”. Water quality has been checked in the modelling scenario for ensuring that legal limits and industrial guidelines for potable water were respected. Plant construction and decommissioning are not included; they are out of the scope of the EVALEAU tool and library at the present stage of development. Tap water distribution is out of scope as well. Both the conventional LCA and the PM-LCA were carried out using Umberto® 5.5 and Ecoinvent 2.2 (using the same background processes), and relying on the Impact 2002+ methodology (Jolliet et al. 2003) for LCIA. As the background conditions are the same, any divergence between the LCA and the PM-LCA results has to be ascribed to the foreground processes.

3. Results and discussion

3.1 Test bed case for the validation of the PM-LCA tool

The foreground water treatment process has been built in Umberto by linking the appropriate UP modules loaded from the EVALEAU library and by defining appropriate values for the process parameters. All the models used are briefly described in the Electronic Supplementary Material (ESM) along with the respective parameters and their values (ESM -table 1. The first result obtained from the process simulation is the water quality at the treatment chain output and at the output of the different UPs (Table 1). Only a few data obtained by site measurements are available for the UPs and concern only the major parameters that have a great importance for the evaluation of treatment efficiency, such as the UV absorbance and turbidity. It was found that the simulated values are in relatively good agreement with the measured values or with the limits imposed by the current regulations.

Table 4-1. Measured and modelled water quality parameters.

Parameter	Average measure *or imposed limit*	Simulation	Observations
Settled water UV absorbance [m^{-1}]	3.22	3.70	error 14.9%
Settled water turbidity [NTU*]	*<2*	0.57	In the range
Biolite filtration turbidity [NTU*]	0.13	0.095	error -26.9%
Potable water pH	*6.5 – 8.5*	7	In the range
UV absorbance [m^{-1}]	1.26 *(<1.5)*	1.31	error 3.9 %
Turbidity [NTU*]	*<0.3*	0.016	In the range
Total Hardness [French Degree**]	*15 - 25*	19	In the range
Al total [mg/L]	*<0.1*	0.0033	In the range
TOC [mg/L]	*<1.5*	1.2	In the range

* NTU: Nephelometric Turbidity Units

** 1 French Degree = 1 part / 100,000 calcium carbonate

Imposed limits are written in italic

The estimation of the chemicals and the electricity consumptions is not straightforward due to the high variability in time of the raw water quality. A consistent estimation of these data is however mandatory. Field data for chemicals and electricity consumptions at plant are used to calculate average values over the reference year. They are compared with simulation results in Table 2. It is observed that the relative difference does not exceed 10%, and therefore the modelling approach is considered as consistent. It is worth mentioning that the water industry know-how about consumption forecasting does not seem to provide better estimates than our modelling.

Table 4-2. Summary of the measured and modelled on-site consumptions.

Inventory item	Real on-site consumption	Modelled consumption	Error
Electricity [kWh/m^3]	0.896	0.824	-7.99%
Polymer [g/m^3]	0.174	0.170	0.05%
Sodium hypochlorite [g/m^3]	5.92	5.50	-7.06%
Aluminum sulfate [g/m^3]	62.9	62.8	0.17%
GAC [g/m^3]	6.00	6.59	9.80%

Details on plant inventory and the corresponding data sets (Ecoinvent2.2) used for background processes are presented in ESM-table 2. Calculated detailed inventory by UP (simulation results with EVALEAU tool) is given in ESM-table 3.

As the LCIA results per inventoried substance are linearly dependent to the LCI, it is expected to have similar LCIA results for the two LCA approaches. Figure 3a confirms this expectation, showing the good agreement between the LCIA results obtained from the conventional LCA and from the PM-LCA. The results were obtained using the Impact2002+/Endpoint methodology, with European normalization, as currently implemented in Umberto®5.5.

The relative difference is even lower than for the LCIs (+2.25% for climate change, -6.01% for ecosystem quality, -2.79 for human health, -5.43% for resources). The rationale is that the damage factors in LCIA are very different from one substance to another and the individual

LCIA results are finally aggregated per impact category, thus reducing the discrepancies between the conventional LCA and the PM-LCA results.

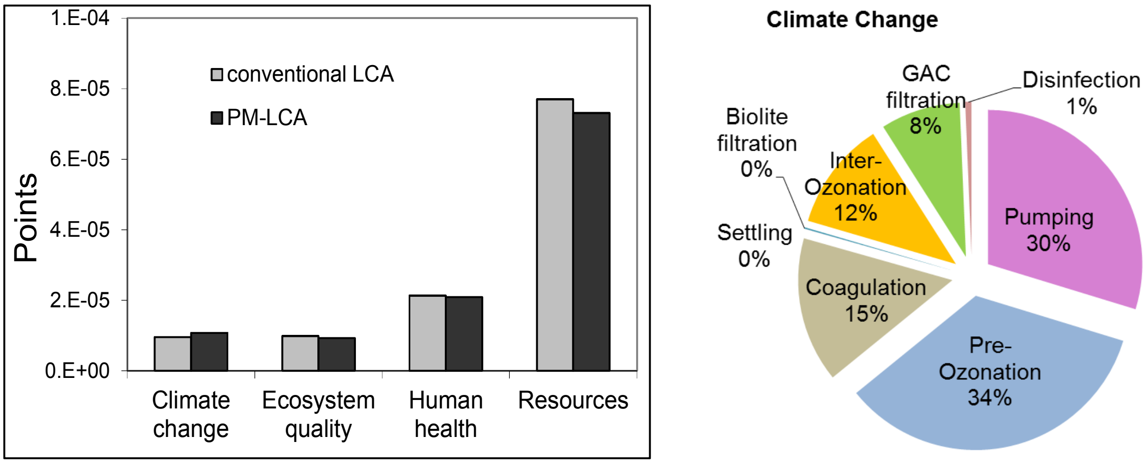


Figure 4-3. LCIA results obtained from conventional LCA and from PM-LCA (a, left) and UP contribution to the "Climate change" impact category (b, right).

Detailed LCIA results for the studied plant are not fully presented here since this is not the objective of the present work. The conventional-LCA application and results for the same plant are also presented in extenso in Igos et al. (2012). The following evaluation results are presented in ESM: detailed endpoint results for the midpoint impact categories (ESM-figure 2) for the whole plant life cycle; UPs' contribution analysis based on endpoint categories (ESM-figure 3); UPs' contribution analysis on several midpoint impact categories (calculated ad endpoint) (ESM-figure 4).

An analysis of the midpoint impact categories (normalized at endpoint; Humbert et al., 2005) have shown that "non-renewable energy", "respiratory effects" and "terrestrial ecotoxicity" have the most important scores within their endpoint category, "resources", "human health" and "ecosystem quality" respectively (ESM-figure 2). Climate change (the fourth endpoint category) is also one of the remarkable impacts. These results are explained by the fossil fuels consumption for electricity production, electricity being intensively used at plant. Fossil fuels utilisation generates the other observed major impacts: climate change, respiratory effects, ecotoxicity. The contribution analysis on all impact categories revealed similar behaviour, i.e. the dominance of ozonation processes followed by pumping and in lesser extent by coagulation operation (figures 2-4 in ESM). Focusing on the climate change for illustrative purpose (figure 3b), the two ozonation processes are the main contributors (46%), followed by the pumping station. This result is explained by the intensive use of electricity.

3.2 Sensitivity analysis

The Morris method implemented in EVALEAU can be applied to all the impact categories. Again, for sake of simplicity and for testing purposes, only the parameters' influence on the climate change category was analysed here and the results are presented in figure 4. A set of 18 parameters, with defined ranges of variations, was chosen as relevant for sensitivity analysis of the whole plant model. For example, for the ozonation operations the chosen parameters are: the ozone transfer efficiency (%), the pure oxygen fraction in the feed gas (% mol) and the ratio T10/T, which is a ratio characterizing the hydrodynamics of the device by comparing the time needed to get 10% of a tracer out of the reactor and the theoretical hydraulic residence time.

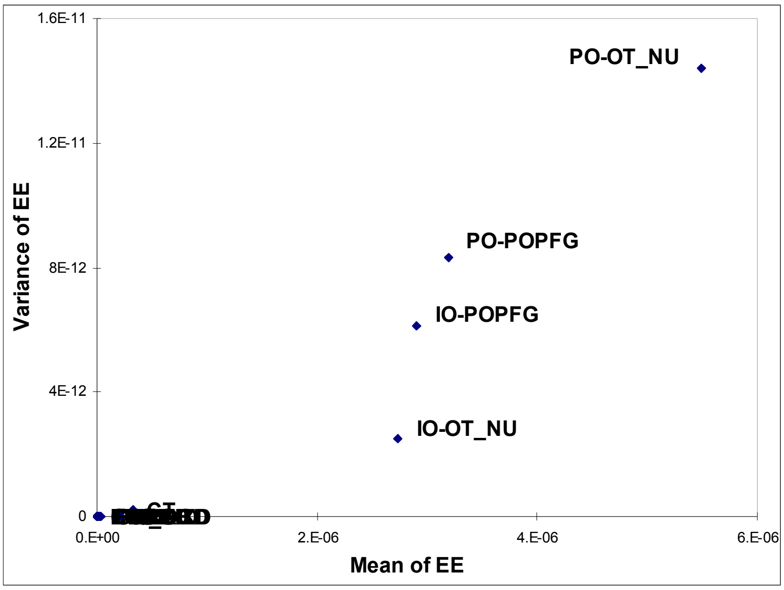


Figure 4-4. Morris graph relative to the "Climate change" results for the whole plant model.

The variation of a result due to the variation of one parameter at a time is called elementary effect (EE on the Morris graph). The mean of the EEs is represented on the abscissa and the variance on the ordinate. An influent parameter will lead to a high EE's mean, while a non-linear influent parameter will lead to a high EE's variance. The Morris graph resulting from sensitivity analysis applied to the water treatment plant identified two main parameters, relative to the two ozonation processes ('PO' for pre-ozonation, 'IO' for inter-ozonation): the ozone transfer efficiency (“OT_NU”) into the contact reactors and the proportion of oxygen in the gas used for the ozone production (“POPFG”). So the Morris method indicates that the operation conditions of the two ozonation processes are the main lever actions for improving the plant’s environmental performance with respect to the chosen impact category. Both operating parameters intervene in the energy-consumption calculation for the ozone production at plant. The improvement of the ozone production technology and of the ozone/water contactor is therefore the main priority action in the aim of decreasing the energy consumption and the related impacts.

4. Conclusions

The concepts and methodologies embedded within the developed PM-LCA tool, named EVALEAU for water treatment, provide the user with complementary views of the designed system. The modelling principle which consists in parameterizing a generic model to get a project-specific model enables the user to cope with high variability of water treatment processes and water quality. The tool allows to address the project constraints and to test the engineering design choices, thus providing useful support to eco-design. Sensitivity analysis of the model parameters suing the Morris method is an original feature of the tool as well and provides a significant added value to plant operators. EVALEAU successfully solve the problem of linking LCA results with the related engineering design choices and operation parameters. To our knowledge, it is the first fully-fledged integrated PM-LCA tool for environmental assessment and design of processes, specifically developed and targeted to the water industry.

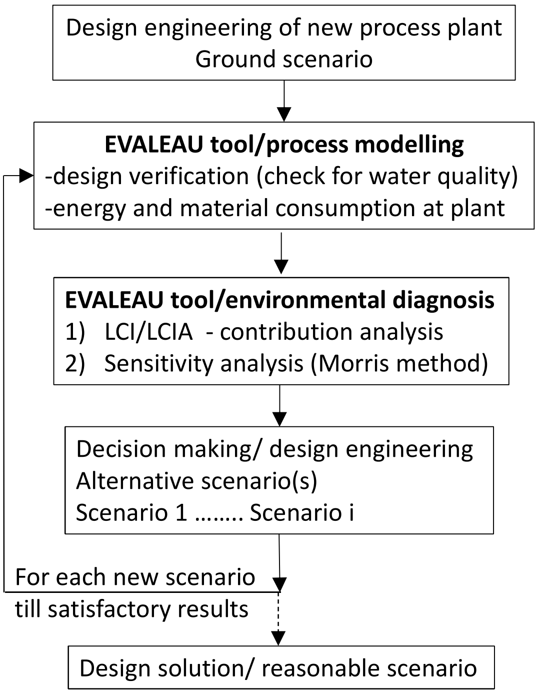


Figure 4-5. Use of EVALEAU tool for eco-design of water treatment processes.

The EVALEAU tool could be used in an eco-design process (figure 5) since it combines two functions: *process modelling-design aid* and *environmental diagnosis*. In the design engineering of a new plant, it can be used for the verification of the initial technological choices (“ground scenario”) against the produced water’s quality requirements, by using the *process modelling* function of the tool. Then, the *environmental diagnosis* function provides two complementary features: i) LCIA and contribution analysis, ii) sensitivity analysis on process parameters with respect to the selected impacts. The results supplied by the EVALEAU tool allow therefore identifying and assessing relevant design options (“alternative scenarios”), relative to the replacement of UPs for instance, or to the modification of design and operation parameters, of reactants, etc. The tool shall be consistently applied to all the selected scenarios, for technological verification followed by environmental diagnosis. The eco-design process could be iterated until an optimal solution is found following the chosen criteria (environmental but also economic and technical).

The test bed case presented in this paper uses only part of the UP modules existing in the EVALEAU library, which covers most of the UPs processes based on physic-chemical mechanisms, currently used for potable water production and waste water treatment. The application case shows the reliability of the models used for describing the UPs: i) the plant’s model, with appropriate parameter values, is able to reproduce the water quality transformation in the treatment chain, the water being the functional flow, and ii) the PM-LCA tool generates relevant LCI/LCIA results when compared to conventional LCA results.
During the development of the tool, special attention was given to the software architecture, in order to anticipate further developments. The tool has the necessary flexibility to integrate future expert recommendations as well as novel technologies. The user can introduce additional functionalities through the integrated scripting (e.g. integrating optimization algorithm to choose the best set of parameter values). The robustness of the tool also benefits from the linking with external, specialized and well recognized software as PHREEQC® for complex aqueous chemistry modelling.

Chapter 5.

Detailed case study of a drinking water treatment plant

Résumé du chapitre 5. Etude de cas détaillée d'une usine de production d'eau potable.

Une étude de cas détaillée est présentée dans ce chapitre. L'usine étudiée est localisée en région parisienne. Sa capacité de production est importante (225 000 m^3/j), même si la production journalière dans l'étude (pour l'année 2006) était moindre, à savoir 114 000 m^3/j. La chaîne de traitement mise en œuvre dans cette usine est relativement complexe puisqu'elle est composée de trois lignes de procédés en parallèle et de plusieurs boucles de recirculation.
Cette usine a été sélectionnée sur deux critères: 1/ son importante capacité de production et 2/ la connaissance approfondie de son fonctionnement. Ceci a permis de disposer de données de qualité d'eau et d'inventaire de données fiables. La procédure pour l'écoconception de procédés est appliquée sur cette usine afin de l'illustrer par un exemple concret.

L'approche rétrospective est utilisée pour valider la modélisation des calculs concernant la qualité de l'eau. En effet, en se basant sur la qualité de l'eau brute et sur les doses de réactifs réellement consommées (données issues de l'inventaire de données), l'incertitude sur la modélisation de la qualité de l'eau peut être estimée. Des équations spécifiques à cette usine ont été développées par l'exploitant (i.e. Suez Environnement) et celles-ci ont été reprises et intégrées dans les modèles de procédés unitaires composant le modèle de l'usine.
Sept paramètres de qualité d'eau sont pris en compte dans l'étude : la turbidité, l'absorbance UV (UVA), le carbone organique total (TOC), le pH, le résiduel total d'aluminium, les bromates et la concentration totale de trihalométhanes. Les valeurs de ces paramètres obtenues par la modélisation sont comparées à celles issues de mesures sur site (ou issues de recommandations industrielles) pour les eaux décantée, filtrée et traitée. La qualité de l'eau traitée est aussi comparée à celle imposée par la législation en vigueur. Les résultats montrent que la modélisation de la qualité est fiable au regard des objectifs.

L'approche prédictive est ensuite appliquée en reprenant la modélisation de la qualité de l'eau validée lors de l'étape précédente. Un modèle prospectif, reproduisant la réalité du terrain, est établi afin de créer un scénario de base pour la procédure d'écoconception menée par la suite.

Les impacts environnementaux générés par la production d'eau potable dans cette usine sont calculés selon la méthode d'Analyse de Cycle de Vie (ACV). L'unité fonctionnelle est « 1 m^3 d'eau potable produit ». Les phases de construction et de démantèlement de l'usine sont exclues des frontières du système. Le pompage en entrée et en sortie (jusqu'au château d'eau), le traitement de l'eau, le traitement et l'épandage des boues sont pris en compte tout comme le transport et la production des matériaux (excepté le transport du GAC et de la chaux).
Les consommations de réactifs et d'électricité sont prédites avec une bonne précision (15% d'erreur maximum) avec un bémol pour la consommation de soude. Les résultats d'ACV sont en accord avec les résultats de l'ACV conventionnelle (basée sur les données d'inventaire), l'erreur sur le score total étant de 12.5% (Recipe). Les deux catégories d'impact contribuant le plus au score total sont "Climate Change" (46.6%) and "Fossil Depletion" (36.7%).

Des analyses de contribution et de sensibilité sont alors menées sur ce scénario de base. La consommation de PAC est la principale source d'impact (32.6% de l'impact "Climate Change" et 38.7% de l'impact "Fossil Depletion"), l'électricité ne contribuant qu'à hauteur de 20-25% selon l'impact. Les graphes de Morris relatifs aux différentes catégories d'impact montrent que deux paramètres opératoires semblent être les leviers d'action prioritaires : les objectifs d'abattement de la DOC des procédés de coagulation et d'ajout de PAC.

Des scénarios alternatifs sont ensuite testés à la recherche d'opportunités pour réduire les impacts environnementaux. La première alternative est de jouer sur les objectifs d'abattement de DOC dans les procédés de coagulation et d'ajout de PAC. La deuxième consiste à utiliser de l'oxygène pur pour produire l'ozone au lieu de l'air. La troisième teste l'utilisation de chaux à la place de la soude et d'eau de javel à la place du chlore en fin de traitement. Certaines solutions alternatives de traitement s'avèrent intéressantes pour réduire les impacts (utilisation de la chaux) mais les objectifs environnementaux et économiques sont conflictuels pour chaque scénario testé.

Finalement, un épisode pluvieux est simulé en changeant la qualité de l'eau brute. Sans entreprendre de changements sur le fonctionnement de l'usine, l'UVA et le TOC posent problème en sortie d'usine. Pour pallier cela, les conditions opératoires sont modifiées (abattement du DOC), ce qui entraine une nette augmentation des impacts environnementaux générés par la production d'eau potable (+138% sur l'impact "Climate Change").

Chapter 5. Detailed case study of a drinking water treatment plant.

An in-depth analysis of a drinking water treatment plant is presented in this chapter in order to put into practice the unit process models of the EVALEAU library (chapter 3 and related appendix 3-2) as well as the concepts and the modelling approaches previously described (chapter 2). It illustrates how the tool could be effective and it provides an overview of some outcomes that could be expected by the user. A better understanding of the plant's performances (regarding technical, economic and environmental issues) is supposed to be brought by the modelling scenarios. The technical procedure for process ecodesign, introduced in paragraph 2.2 of chapter 2, is tested in this pilot study. A plan of actions to reduce both environmental impacts and operational costs will be proposed in case there are ecodesign opportunities.

Both global modelling approaches of the EVALEAU tool are tested in this case study : the retrofit approach and the predictive approach.

Concerning chemical consumptions, the retrofit approach is descriptive and it makes more sense to apply it to existing plants where the average chemical doses are well-known. Even if it is not the most instructive, this approach makes it possible to validate the water quality results separately from the other result categories (i.e. potential errors could come only from water quality modelling). Using site-specific equations and source data from the field as a starting point for the calculations (i.e. measurements of raw water quality and average chemical doses), the retrofit modelling scenario should lead to water quality results similar to on-site measurements for the produced water exiting the plant.

The predictive approach is suited for designing a plant prior to its construction or for exploring improvement opportunities within an existing one. As a first step, a ground modelling scenario is established by reproducing the existing plant's design and operating conditions (step 1 of the procedure for process ecodesign). It is adjusted in terms of water quality objectives (i.e. technical performances of unit processes) and it is then expected to reproduce the actual functioning of the processes as occurring on the field. The ground modelling scenario must serve as a basis for further investigations.

Once this ground modelling scenario has been established and validated, the case study is performed according to the following objectives :

- *Contribution analysis*. It gives information about which are the unit processes generating environmental impacts and which are the chemicals and/or energy consumptions responsible for these (step 2 of the procedure for process ecodesign).
- *Sensitivity analysis of the plant model on LCIA results*. The mathematical method followed is the Morris method (chapter 2). The Morris graphs provide qualitative information about key parameters of the plant model for each considered impact category (step 2 of the procedure for process ecodesign).
- *Alternative treatment solutions*. While respecting drinking water standards, the predictive approach enables the user to try alternative treatment options (i.e. plant design and operating conditions) and to observe their effects on the economic and environmental performances of the plant (steps 3 and 4 of the procedure for process ecodesign).
- *Deterioration of the raw water quality*. For instance, a rain event is a temporary deterioration of raw water quality but it may affect the functioning of the plant and therefore its performances. Knowledge about potential repercussions caused by this kind of event is essential even more when the plant is frequently submitted to water quality disturbance. Future modifications of raw water quality due to a changing context of the plant could be anticipated by an analogous study.

Each of the objectives presented above could be achieved separately based on the ground modelling scenario. However, contribution analysis and sensitivity analysis should be preferably performed prior to the "what-if" scenario trials since they enable the user to focus on the processes and parameters having the most influence on the results of the plant model.

Firstly, the water quality modelling is validated with the retrofit approach. Then, the plant is hypothetically re-designed with the predictive approach and correspondence with field reality is checked. The last sections of the case study are dedicated to better understanding the behaviour of the plant model, exploring areas of improvement and bringing quantitative responses with "what-if" scenarios.

1. Description of the drinking water treatment plant

The plant to be studied was selected mostly on 2 criteria: 1/ a high production capacity and a large amount of potable water produced during the reference year; 2/ a thorough knowledge about the functioning of the plant. The first reason is to be able to assume the stability of the functioning of the plant and the relevance of the average chemical and energy consumptions. The second reason is to allow validating modelling results from different points of view (technical facts, water quality, mass and energy balances).

The required data are available for model parameterisation and for model validation as well. As it is one of the first studies performed with the EVALEAU tool, it is better to do it on a well-known plant where every difficulty has been overcome. A deep understanding of what is at stake within the plant is crucial to check the consistency of the results and the behaviour of the plant model. The selected plant has been studied in details for years. Our work benefits from these previous studies and from fruitful discussions with researchers and plant operators. Several technical documents and spreadsheet reports were provided by them.

The drinking water treatment plant is located in the region of Paris and it uses the Seine River as source water. The maximum production capacity is 225 000 m^3/day. The reference year of the case study is 2006, i.e. site inventory is relative to chemical and energy consumptions over the year 2006. The average drinking water production was 114 106 m^3/day during the reference year.

The process chain is relatively complex because it involves different unit processes, 3 separate treatment lines and several loops (figure 5-1). At the same time, it is representative of a conventional water treatment system for drinking water production. The process chain begins with a pre-treatment line (addition of sulfuric acid H_2SO_4 at 96%, pure gaseous chlorine Cl_2, PAC and coagulation with aluminium sulphate at 8.5% Al_2O_3). Then it splits into three process lines: 30% of the water goes to process line 1, 30% to process line 2 and 40% to the third. The process line 1 follows the process sequence : settling - GAC filtration - ozonation. The process lines 2 and 3 follow the process sequence : settling - sand filtration - ozonation - GAC filtration. The settling technology is different in these process lines. The settler of process line 3 relies on more advanced technology and it produces a concentrated sludge able to skip the sludge settling step. The final treatment line is composed of two unit processes : chlorination for disinfection (with pure gaseous chlorine Cl_2) and pH adjustment with soda (NaOH at 50%) for water taste. Sludge treatment is also handled on-site by thickening, liming and dehydrating with a filter-press. The treated sludge is finally spread on agricultural soils and the sludge overflow is sent to a sewer.

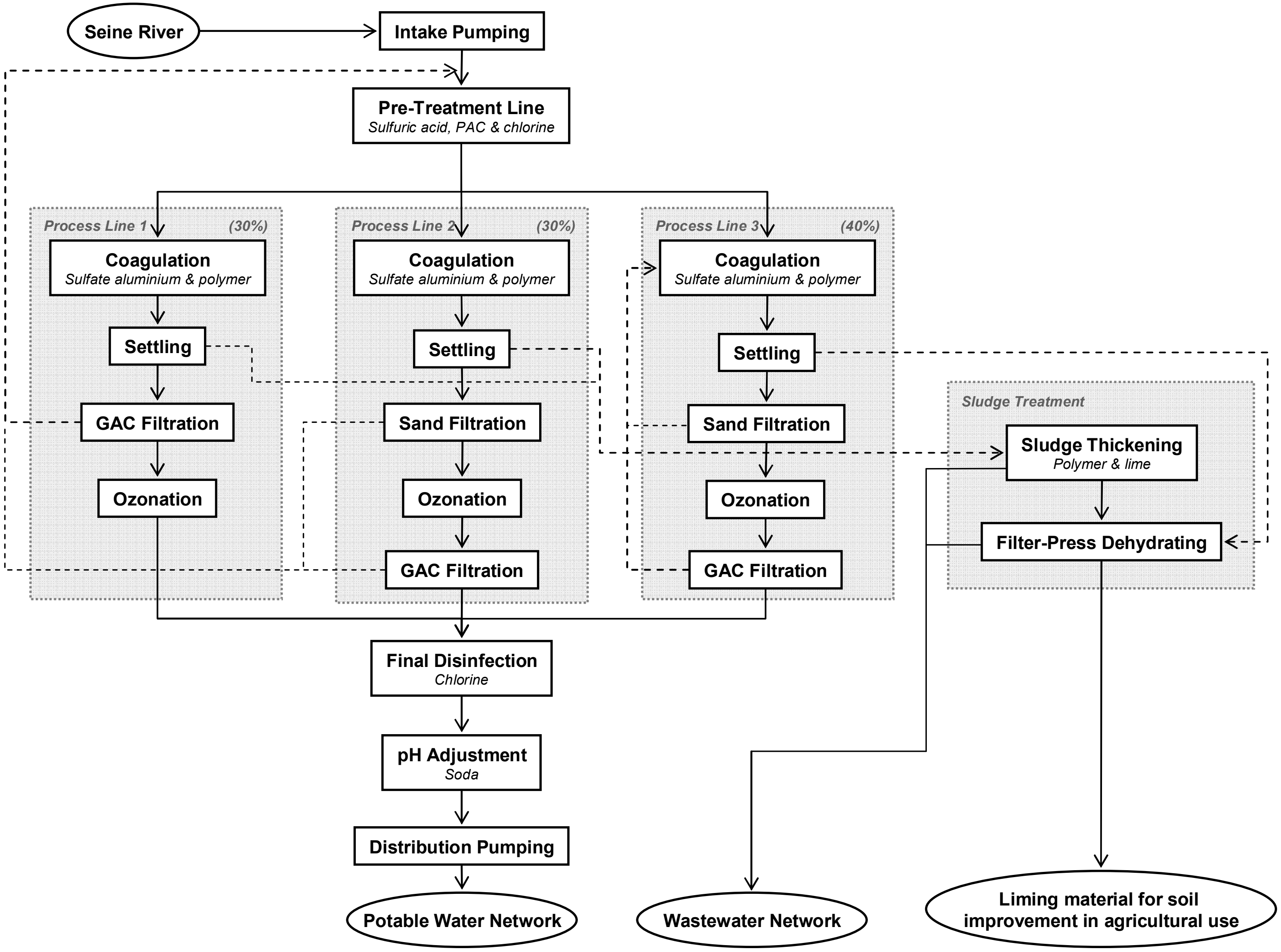


Figure 5-1. Flowsheet of the studied plant.

2. Retrofit approach - Validating the water quality modelling

Within the retrofit approach, the main objectives are 1/ to calculate energy consumptions based on technical design facts and 2/ to model the water quality obtained at the level of each unit process based on field data (i.e. average chemical doses over the reference year). In this case study, the retrofit modelling scenario is aimed at validating water quality calculations. As a consequence, this section focuses on the second objective and the first one is disregarded since it will be further studied in the next sections of this chapter (i.e. no LCA is performed in this section of the study). Water quality is investigated by comparing modelling results with on-site measurements or guidelines in order to assess the accuracy of the unit process models.

Field data are mandatory for performing this part of the study and they have been collected by the industrial partner (i.e. CIRSEE laboratory of Suez Environnement). They are required 1/ for reproducing the plant flowsheet in the EVALEAU framework; 2/ for parameterising the unit process models by setting the engineering design parameters (e.g. hydraulic residence time in a reactor) and by setting chemical doses in the concerned unit processes; 3/ for calculating and validating the water quality parameters.

Therefore, collected field data are: 1/ description and engineering design of the studied plant; 2/ site inventory (i.e. electricity and chemical consumptions over the reference year); 3/ average quality parameters of the raw, settled, filtered and treated waters.

These data allow building the modelling scenario on the one hand and validating the water quality calculations on the other hand.

2.1 Reproducing the plant flowsheet

For this purpose, the main source of information is an internal document of Suez Environnement which is a technical audit of the plant (CIRSEE 2002). It describes in detail the plant and the unit processes with technical facts. The process chain and the global configuration of the plant are deduced from this document. The flowsheet is then built under the Umberto® working environment. The figure 5-2 shows the retrofit modelling scenario in Umberto® graphical user interface.

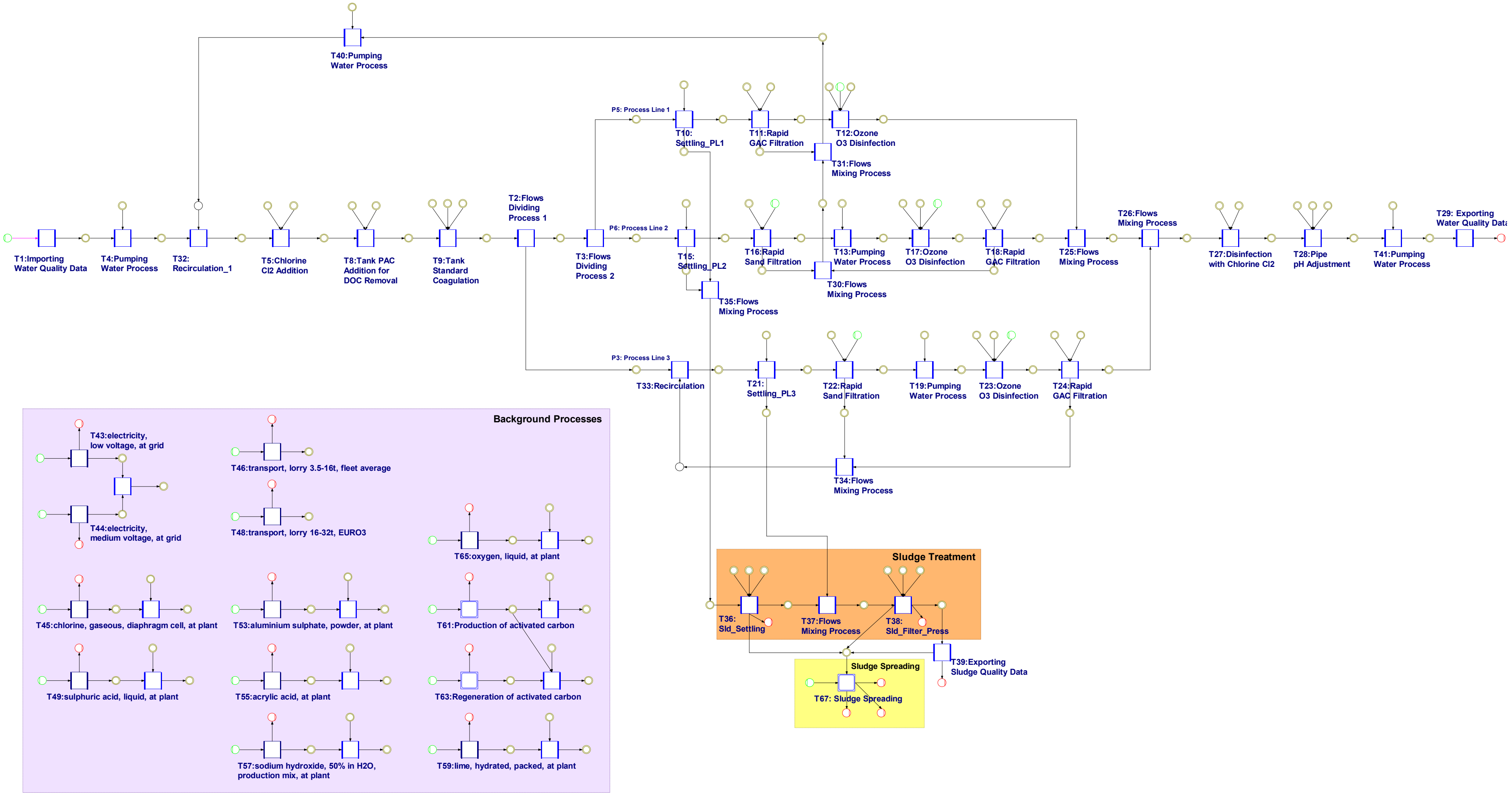


Figure 5-2. View of the modelling scenario in Umberto® graphical user interface.

To actually build the scenario, unit process models must be imported from the EVALEAU library (blue squares on figure 5-2) and connected by material flows (grey circles on figure 5-2). It leads to a network of modules that are interconnected and represent the water treatment plant. At this point, the process models are in their generic form (as stored in the library).

2.2 Parameterisation of the unit process models

Once the global configuration of the plant has been established, the unit process models must be parameterised to stick to the field reality in order to better represent the functioning of the plant. Design facts describing the unit processes are found in the technical audit of the plant (e.g. filtration cycle duration, GAC regeneration scheduling, heights to be pumped, surface hydraulic charge in the settlers, etc.). Average chemical doses are calculated as the ratio between purchased quantities of chemicals and the amount of treated water over the reference year. The required information comes from spreadsheet reports provided by the operators of the plant.

Appendix 5-1 gives the whole parameterisation data set for the retrofit modelling scenario. All parameters of every unit processes are given with their default value and their case-specific value if different. At this stage of the study, the plant model is parameterised and the retrofit scenario is able to model water quality along the process chain.

2.3 Water quality modelling

In the generic models of the EVALEAU library, some physical and/or chemical phenomena occurring in water treatment are not well modelled for lack of knowledge despite a broad literature review on these issues (chapter 3). As a consequence, technical performances of unit processes are sometimes badly assessed (e.g. UVA removal during chlorination). This limitation can be overcome by developing site-specific equations and by implementing them in the code of the concerned unit process models. It strongly enhances water quality modelling for the plant under consideration.

In case no site-specific equations have been developed, the range of expected values for process performances can be useful as a last resort. In other words, setting an arbitrary value that underestimates the process performances (in terms of pollutant removal for instance) allows one to stay coherent with the functioning of the process while avoiding mistakes like considering that the produced water is potable although it might not be.

Within the studied plant, the main issue about water quality is the organic matter, that is to say DOC (or TOC) and particularly UVA. The problem is not the quantity of organic matter that must be removed but its recalcitrance to treatment. Site-specific equations have been developed for some unit processes in order to predict their technical performances concerning organic matter removal. On-site measurements indicate the range of values that could be expected for the other processes.

This knowledge has been re-used and the corresponding codes have been implemented in the modelling scenario so that it fits better the actual functioning of the processes. UVA and DOC removals have been studied for the following unit processes: 1/ pre-chlorination; 2/ PAC addition; 3/ coagulation; 4/ GAC filtration; 5/ ozonation; 6/ post-chlorination (disinfection).

2.3.1 Pre-chlorination

No empirical equations have been developed for this process but a range of values for UVA removal is available. UVA removal varies from 10% to 20% so the corresponding process performance has been set to 10% by default in the pre-chlorination model. It might be underestimated but at least the process model is coherent (there is UVA removal during chlorination) and it is cautious regarding the final water quality to be calculated. DOC is not removed during chlorination.

2.3.2 PAC addition

An empirical equation has been developed to better estimate the UVA removal. It is valid for PAC doses which are below 30 g/m^3 (real doses are never higher than 20 g/m^3 according to the plant audit). As the organic matter responsible for the presence of UVA is normally adsorbed more easily than the rest of it, DOC removal is estimated as 75% of UVA removal.

$$\mathrm{UVA\_Removal} = -2.67 + 11.04 \times \mathrm{PAC\_Dose}^{0.56} \qquad (5\text{-}1)$$

$$\mathrm{DOC\_Removal} = 0.75 \times \mathrm{UVA\_Removal} \qquad (5\text{-}2)$$

- PAC_Dose : g/m^3
- $UVA\_Removal$ and $DOC\_Removal$: %

2.3.3 Coagulation

No empirical equation is used on site. DOC and UVA removal are calculated with the regular approach of the coagulation model (as described in chapter 3). It requires calibrating five parameters (Kastl et al. 2004). It could work with the average values coming from the work of Kastl et al. but it is much better to use site-specific parameter values. These parameters have been calibrated by processing jar-test results with Matlab scripts.

Table 5-1. Parameters of the coagulation model.

	Maximum sorption capacity	Sorption coefficient	Humic acid fraction	Non polar fraction	Humic acid pKa
Average value	4.06	182	0.245	0.258	4.4
Site-specific value	4.11	209	0.250	0.290	4.3

2.3.4 GAC filtration

Empirical equations have been developed for calculation of UVA and DOC removal during GAC filtration. The form of the equations is the same for both calculations of UVA and DOC removal and for each process line but with different values for empirical coefficients.

$$\text{Removal} = a + b \times \ln(\text{SFV}) \pm \varepsilon \qquad (5\text{-}3)$$

- *Removal* : removal of organic matter in % (DOC or UVA removal)
- *SFV* : Specific filtered volume, i.e. volume of filtered water (in m^3) by 1 m^3 of GAC since last GAC regeneration of the filter under consideration

Table 5-2. Empirical coefficients required for the calculation of UVA and DOC removal during GAC filtration.

	UVA coefficients			DOC coefficients		
	a	b	ε *	a	b	ε *
Process line 1	150.11	-12.98	15	127.81	-11.35	-
Process line 2	125.18	-9.61	5	147.78	-12.25	-
Process line 3	183.68	-16.06	10	173.78	-15.67	-

* Error due to calibration / experimental measurement.

The empirical coefficients for calculation of UVA and DOC removal in each process line are presented in table 5-2. Organic matter removal during GAC filtration depends directly on the cumulated amount of filtered water (i.e. the variable SFV in equation 5-3) and thus it depends indirectly on the filtration cumulated time. This is why the scheduling of GAC regeneration is important to make this process work efficiently. As simulations are steady-state within this case study, the previous empirical equations have been integrated over the adsorption cycle which is user-defined through parameterization.

The adsorption cycle begins with the use of newly regenerated GAC (or simply new GAC) and ends when the GAC is sent out of the plant for regeneration. Its duration is approximately two years. The regeneration cycle is the period when the GAC is regenerated, which is done outside the water treatment plant. Its duration is approximately two weeks. The expression « regeneration cycle » is often mistakenly used by plant operators and water engineers to designate the duration between two regenerations of one filter's GAC, that is to say the adsorption cycle.

In addition, it must be noted that a mechanistic model for adsorption (e.g. Langmuir or Freundlich adsorption isotherm) should have been developed instead of such an empirical equation as the one developed for this water treatment plant (i.e. equation 5-3).

2.3.5 Ozonation

An empirical equation has been developed for calculation of UVA removal and it is common to the three process lines (equation 5-4). This equation is used instead of the one defined in the generic version of the ozonation model which was inspired by the WTP model (WTP manual 2001). DOC is not removed during ozonation.

$$\mathrm{UVA\_After} = 0.601 - 0.018 \times \theta + 0.416 \times \mathrm{UVA\_Before} \pm 0.2 \qquad (5\text{-}4)$$

- *UVA_After* : UVA value after ozonation (m^{-1})
- *UVA_Before* : UVA value before ozonation (m^{-1})
- θ : Temperature (°C)

2.3.6 Post-chlorination

The situation is the same as for pre-chlorination : no empirical equations were developed for calculation of UVA removal but a range of values was available. UVA removal in this disinfection process is comprised between 10% and 20% as well, so UVA removal is estimated as 10%.

2.4 Results

Seven water quality parameters are major issues for this water treatment plant. These parameters are turbidity, pH, UVA, TOC, Al residual, Bromate and TTHM. As a consequence, validation of water quality modelling focuses on these seven parameters.

The EVALEAU tool allows calculating the water quality of every water flow within the plant. It is more difficult to measure all these different water quality data on the field and only few measurement results exist. In addition to on-site measurements, values from industrial guidelines (CIRSEE 1999) will be used for comparison with the results of water quality modelling and for checking the consistency of their order of magnitude.

Measurements of raw water quality data were made daily from 1993 to 2004 and they were saved in a water quality database. The reference year (2006) is not comprised in this period but it is assumed that the quality of the Seine River has not drastically changed since then. Average values of raw water quality data over this period (1993-2004) are used in this case study as a starting point for the water quality calculations.

Within the plant, the considered water quality data are measured at different points of the process lines mainly for on-line monitoring. These measurements were saved weekly in a distinct database. Average values of these water quality data at intermediate points of the treatment line and over this same period are also used in this case study in order to validate water quality calculations.

For settled waters, there are no on-site measurements and only 2 recommended values from the industrial guidelines. They concern turbidity and Al residual.

For filtered waters (resulting from first stage filtration), on-site measurements (for each process line) and recommended values from the guidelines are available concerning again turbidity and Al residual.

For the treated water, there is more information available. On-site measurements are provided for all the studied water quality data except for the final pH whose value is an experts' estimation. Treated water pH is regularly measured on site but it is not recorded in any water quality database. Legal limits and industrial objectives are also provided for most of the studied water quality data.

In this section of the study, the modelling results are compared to on-site measurements, industrial guidelines and/or legal limits in order to check if the water quality is well modelled along the process chain.

2.4.1 Settled waters

The modelling results are compared to industrial guidelines. They are presented in table 5-3 for turbidity and in table 5-4 for Al residual.

Based on table 5-3, the turbidity of the settled waters calculated by the plant model seems to be in accordance with the guidelines. As the turbidity values are comprised in the expected range, the water quality modelling can be considered acceptable.

Table 5-3. Compared results for turbidity of the settled water.

Settled water turbidity (NTU)	Guidelines recommendations	Modelling results
Process line 1	0.5 – 3.0	1.02
Process line 2	0.5 – 3.0	1.01
Process line 3	0.5 – 3.0	1.03

For Al residual, the legal limit, guidelines and on-site measurements concern the total amount of Al residual (and not only the dissolved Al residual). The dissolved Al residual is problematic because it cannot be removed by settling and filtration steps coming after coagulation unlike the particulate Al residual. Dissolved Al residual can appear in the settled waters if the coagulation-settling steps do not work correctly.

Normally, it occurs when the coagulation is operated at a wrong pH when the solubility of Al is higher ($pH < 6.0$ or $pH > 7.5$). Coagulation pH measurements are mandatory to definitely validate modelling of Al residual but no pH measurements were made in the coagulation reactor. According to the modelling scenario, the pH is 6.7 which is in the correct range. Therefore, the coagulation process is supposed to work correctly.

Table 5-4. Compared results for Al residual in the settled water.

Settled water Al residual (mg/L)	Guidelines recommendation (Total Al)	Modelling results (Dissolved Al)	Modelling results (Total Al)
Process line 1	< 0.1	0.000764	0.113
Process line 2	< 0.1	0.000764	0.113
Process line 3	< 0.1	0.000757	0.116

Based on table 5-4, the results of the water quality modelling are coherent with typical values encountered on the field. The guidelines' recommendation is not strictly respected but modelled Al residual in the settled water is close to the recommended value. Besides, the concentration of dissolved Al residual is very low which means that the coagulation process is well operated. As most of the Al residual is not dissolved, it will be possible to remove it during the following filtration steps. At this point, the water quality modelling for Al residual is acceptable.

2.4.2 Filtered waters

The results of water quality modelling are compared to the guidelines' recommendations and average on-site measurements. This is presented in table 5-5 for turbidity and in table 5-6 for Al residual.

The turbidity values for modelled and real filtered waters are in accordance with the recommendations from the guidelines. The order of magnitude is good but the modelling scenario is predicting filtered water turbidity that is more than twice the real one for process line 2.

Table 5-5. Compared results for turbidity of the filtered waters.

Filtered water turbidity (NTU)	Guidelines recommendation	On-site measurements	Modelling results
Process line 1	< 0.2 (95% of the samples) < 0.5 (always)	0.12	0.170
Process line 2		0.08	0.169
Process line 3		0.18	0.172

On-site measurements for raw and filtered waters are not necessarily made at the same time. No information was available on the delay time between different on-site measurements. The problem is that the water quality of the Seine River can rapidly change for an independent reason (e.g. turbidity increases during a rain event) and the situation can be completely different between two measures. In addition, raw water quality data were measured daily while water quality data at intermediate points were measured only weekly. As a consequence, there is no direct correlation between measurements in raw water and at intermediate points of the treatment line. This remark can be made in general for all water quality measurements presented in this case study. This bottleneck must be kept in mind when analysing results on water quality as it can explain such inconsistency as the one observed on filtered water turbidity of process line 2.

According to the plant model, the recommended value for Al residual (i.e. total Al residual) is respected in the three process lines. The order of magnitude of modelling results is good compared to on-site measurements, which means that the plant model is consistent and logical from a qualitative point of view. Nevertheless, the modelling results are not accurate since on-site measurements of Al residual are double or quadruple, so they should not be considered for water quality control for instance.

Table 5-6. Compared results for Al residual in the filtered waters.

Filtered water Al residual (mg/L)	Guidelines recommendation (Total Al)	On-site measurements (Total Al)	Modelling results (Dissolved Al)	Modelling results (Total Al)
Process line 1	< 0.1	0.04	0.000764	0.0196
Process line 2	< 0.1	0.06	0.000764	0.0195
Process line 3	< 0.1	0.07	0.000757	0.0201

The most important source of discrepancies between calculated and measured Al residual comes from the chemical model implemented in PHREEQC®. During coagulation, aluminum precipitates in the form of aluminum hydroxide $Al(OH)_3$. Aluminum hydroxide phases can have different allotropic forms (from amorphous to crystalline) and hence different solubility products. Moreover, the solubility product values strongly depend on temperature (they decrease with temperature increase). It is expected that in the conditions of coagulation reactor, Al precipitates rather as a microcrystalline or amorphous phase. Currently a microcrystalline phase $Al(OH)_3$(mc) is considered in the model, which has a mean solubility product situated between gibbsite (the less soluble form) and amorphous (the most soluble).

Calculation trials carried out for all the three phases and for different temperature values yield the results presented in table 5-7. The equilibrium pH calculated by the model is 6.71 for all trials.

Occasional on-site measurements of Al concentration reported on table 5-6 are unfortunately not accompanied by the corresponding pH and temperature values. However, analyzing the calculation results in table 5-7, we conclude that there is better correspondence in the case of the microcrystalline phase. Considering a temperature of 15°C, the concentration estimated by interpolation is 0.02 mg/L, which is of the same order of magnitude as the site measurements. Furthermore, the final value for Al residual in treated water is 0.02 mg/L as will be shown later in the study (table 5-8). At the end of the treatment, the water has been settled and filtered in two different steps and the remaining Al residual is almost entirely dissolved in water because Al precipitates have been removed by separation processes (i.e. settling and filtration steps). Then the dissolved Al concentration calculated by the chemical model for a temperature of 15°C (which is close to the real water temperature) and the Al residual in treated water are in agreement.

Table 5-7. Dissolved Al concentration in retrofit scenario, coagulation/settling process. Influence of solid phase type and temperature on Al solubility.

Phase		0°C	25°C	60°C
Gibbsite	Log K *	9.39	7.74	4.13
	Al (mg/L)	8.3e-4	1.9e-5	4.6e-9
Al(OH)3(mc)	Log K *	11.02	9.35	7.50
	Al (mg/L)	3.8	7.6e-4	1.1e-5
Al(OH)3(am)	Log K *	12.52	10.58	8.41
	Al (mg/L)	4.0	0.19	8.7e-5

* K for dissolution/precipitation reaction : $Al(OH)_3 + 3H^+ = Al^{3+} + 3H_2O$ (Thermoddem database website)

One remaining problem is that PHREEQC® does not take into account temperature and the equilibrium constant is always the one of standard conditions (25 °C). The dissolved Al residual is therefore underestimated by the EVALEAU models because of this approximation.

One concludes that the chemical model could be improved provided that more investigations are led on site to measure complete sets of parameters and ideally for identifying the nature of Al precipitates.

The modelling results about Al residual should be considered with caution as dissolved Al residual is underestimated by the plant model and they cannot be trusted on the field for water quality control for example.

2.4.3 Treated water

Modelling results and on-site measurements for the seven water quality data of interest are presented in table 5-8 for the treated water, together with their value in the raw water. The aim is to estimate the error on the final values as well as the error on the corresponding removals. Table 5-8 also provides information on legal limits that must be respected as well as legal recommendations and industrial objectives. This legal information is relative to French legislation as the studied plant is located in France (French drinking water standard).

When analysing these results, one should bear in mind that the treated water is the final product of a process chain composed of several unit processes. The consequence is that modelling errors induced by one unit process model can be propagated over the process chain. It makes it difficult 1/ to know which unit process models generate errors and 2/ to obtain good results on the last calculated value within the treated water flow.

The turbidity modelling along the process chain is relatively good. Even if the error between the modelling result and average on-site measurement is 41.5%, the turbidity removal is very well calculated (the error is only 0.33% on turbidity removal). Both on-site measurement and modelling result are below the legal limit at the exit of the plant (1.0 NTU) and close to the industrial objective (0.1 NTU).

Modelling results concerning organic matter (i.e. UVA and TOC) are good. This is a positive consequence of having site-specific equations developed for this plant. The modelling of UVA and TOC is performed precisely enough to be considered valid and this is a key result as they are limiting factors in this context. Indeed, organic matter removal (and particularly UVA removal) is a major issue within this plant.

The pH is an experts' estimation and not a measurement. The targeted value in treated water must be above 7.5 and the recommended value is defined by the equation 5-5. Unfortunately, the saturation pHs must be calculated from the water quality (complete alkalinity titration TAC and salt concentrations) and it was not possible to calculate it with on-site measurements so it was estimated by water treatment experts.

$$\mathrm{pH} = \mathrm{pH}_{\mathrm{saturation}} + \varepsilon \tag{5-5}$$

- pH : recommended pH value in treated water.
- $pH_{saturation}$: saturation pH.
- ε : constant in the range [0.1; 0.3].

Table 5-8. Treated water quality : on-site measurements, modelling results, legal information and industrial objectives.

	Raw water	Treated water				Legal and industrial information		
	On-site measurements (A)	On-site measurements (B)	Modelling results (C)	Error on final value (D)	Error on removal (E)	Legal limits*	Legal recom-mendations*	Industrial objectives**
Turbidity (NTU)	15.0	0.12	0.070	-41.5 %	0.33 %	1.0	0.5	0.1
UVA (m^{-1})	5.66	1.18	1.02	-13.6 %	3.57 %	-	-	1.3
TOC (mg/L)	3.0	1.13	1.21	7.1 %	-4.28 %	-	2.0	1.3
pH	8.0	7.7 ***	7.17	-6.9 %	-	-	6.5 - 8.5	-
Al residual (mg/L)	0.0	0.0200	0.00855	-57.2 %	-	-	0.2	0.1
Bromate (µg/L)	0.0	< 5	0.993	In the range	-	10.0	-	-
TTHM (µg/L)	0.0	14.3	8.58	-40.0%	-	100.0	-	-

* French drinking water standard;

** CIRSEE 1999;

*** Experts' estimation for typical pH value in treated water.

$$D = \frac{C - B}{B} \qquad (5\text{-}6)$$

$$E = \frac{\frac{(C - A)}{A} - \frac{(B - A)}{A}}{\frac{(B - A)}{A}} = \frac{(C - A)}{(B - A)} - 1 \qquad (5\text{-}7)$$

Experience shows that the range of values obtained on the plant for treated water pH is 7.5-7.8. Discussions have been held with the industrial partner to decide which value must be set for the targeted pH. The value of 7.7 seems realistic even though it is in the high range. The choice was made to set a value in the high range to overestimate soda consumption at the end of the treatment rather than underestimate this chemical consumption.

The pH in treated water calculated by the plant model is not good enough since it is below 7.5. Water chemistry is modelled along the process chain by using PHREEQC® and there are some limitations. Only one form is defined for each salt precipitates in PHREEQC® subprograms ($Al(OH)_3$, $CaCO_3$, $Fe(OH)_3$, MnO_2 and SiO_2) and temperature is not taken into account despite its influence on water chemistry equilibrium.

The results on Al residual in treated water is a consequence of what has been discussed previously for Al residual in filtered waters. The plant model underestimates the Al residual but the order of magnitude is good and it is in accordance with legal and industrial objectives.

TTHM and Bromate concentrations are calculated with the WTP modelling approach which is empirical (WTP manual 2001). The empirical coefficients were not calibrated for the plant under study and default values from the WTP model were used. Nevertheless, the order of magnitude obtained by the plant model is good which provides an interesting means for detecting problems that might appear when trying alternative treatment solutions.

2.5 Conclusion

This part of the study aims at estimating the relevance of water quality modelling. The retrofit approach is not used to present LCA results (or any other result category) since it is more appropriate to assess environmental impacts generated by drinking water production in the next sections.

After careful consideration of water quality modelling results, it can be concluded that :

1. Removals of pollutant of interest are well modelled.
2. Precision on final values is not completely satisfactory except for UVA and TOC (because site-specific equations have been developed).
3. The order of magnitude makes sense for all water quality data.

In case where site-specific equations have been developed, the relative water quality modelling is accurate and the plant model simulates the functioning of the processes in good agreement with field reality. Otherwise, default equations of generic models from the EVALEAU library lead to less precise results on water quality but the order of magnitude is still satisfactory for the purpose of the study. One objective within this modelling approach is to check qualitatively that the produced water is potable in order to ensure that the studied system is correctly delivering the required functional unit. Finally, the plant model can be considered to provide valid water quality modelling in the context presented previously.

3. Predictive approach - Establishing the ground modelling scenario

The principle of the predictive approach is to design a drinking water treatment plant while considering environmental issues through LCA. Energy and chemical consumptions required to obtain drinking water are predicted based on technical design facts and process/treatment objectives. Environmental impacts and operational costs are calculated afterwards.

As the studied plant already exists, the plant flowsheet stays unchanged (figure 5-2) compared to the retrofit scenario. The differences come from the unit process models which are the predictive ones instead of the retrofit ones. The interest lies in establishing a ground modelling scenario reproducing the field reality while being predictive. It must serve as a basis for further investigation with “what-if” scenario trials.

3.1 Differences between the retrofit and the predictive scenarios

3.1.1 Parameterisation of the unit process models

For establishing the ground modelling scenario, the unit process models must be parameterised in order to reproduce the real functioning of the plant. In the studied case, technical and engineering design facts must stay unchanged in the predictive scenario because they cannot be changed on the field. Only operating conditions can be modified when re-designing a plant.

In this study, the fact that the plant already exists creates a constraint : technical and engineering design facts relative to equipment sizing must stay unchanged. They cannot be considered as potential action levers for improving the performances of the plant in this context.

The difference with the retrofit approach is related to process and treatment objectives. Here, the treatment objective (e.g. pollution removal) is user-defined and the corresponding reagent consumption is calculated. For instance, within the unit process “pH adjustment by soda addition” at the end of the water treatment line, the defined process objective is a targeted pH of 7.7 (instead of defining the soda dose like in the retrofit approach). This is how energy and chemical consumptions are predicted depending on treatment and process objectives.

The exhaustive data set for the parameterisation of the predictive modelling scenario is presented in appendix 5-2. We notice that the parameters involved in energy calculation remain unchanged with respect to the retrofit approach.

3.1.2 Modelling of the coagulation process

In the retrofit scenario, it is considered that aluminium sulphate and sulphuric acid are injected in the water because site inventory indicates a consumption of both chemicals. It is called enhanced coagulation, that is to say coagulation boosted by the addition of acid. Indeed, by adding an acid into water, more DOC can be removed with the same quantity of coagulant.

In the case of the studied plant, sulphuric acid is used by operators to deal with two kinds of problem :

1. The pH of the raw water is too high (important risk of Al residual in the treated water).
2. The temperature of the Seine River is very low because of a period of intense cold. Thus the coagulation kinetics is slowed down and coagulation is enhanced with addition of sulphuric acid to compensate the low water temperature.

Both problems rarely happen. In the predictive scenario presented here, it has been considered that the coagulation process is not enhanced by acid addition. There are two reasons for that :

1. It is what it really happens on the field when the working conditions are regular ones (CIRSEE 2002);
2. In this case study, we have considered that the environmental and economic performances of the plant are better with no acid addition. Numerical experiments have been conducted considering a coagulation pH varying between 6.0 and 7.0. The optimum coagulation pH both in terms of operational costs and LCIA results is obtained with no addition of sulphuric acid (appendix 5-3). Standard coagulation leads to better environmental and economic performances than enhanced coagulation in regular working conditions.

Enhanced coagulation is only put into practice in specific contexts occurring rarely (i.e. a few weeks over the year). As the predictive modelling scenario presented in this section aims at simulating the functioning of the plant in nominal working conditions, it is considered that coagulation is not enhanced by the addition of acid.

3.2 Characteristics of the conventional and predictive LCA studies

In this section, the characteristics of the conventional and predictive LCA studies are presented. LCIA results will be presented in the next section for sake of comparison and model validation together with other result category (treated water quality and material consumptions). In next paragraphs, the goal and scope of both types of LCA study are explained, the system boundaries are explicitly defined and the assessment of environmental impacts and operational costs during the LCIA phase is briefly introduced.

3.2.1 Goal and scope definition

In the following LCA calculations, the functional unit is defined as “1 m^3 of drinking water at plant” and the reference year is 2006. Construction and decommissioning of the plant are excluded from the system boundaries. The literature review (Friedrich 2001; Raluy et al. 2005). as well as a specific research work achieved during the EVALEAU project (Igos et al. 2012) confirmed that these life phases can be neglected for a drinking water treatment plant as mentioned in chapter 1. Indeed, these life phases represent around 10% of the total environmental impacts generated over the life cycle of the plant. Then, the operation phase represents around 90% of the total environmental impacts and this life phase is the only one considered in the next LCA calculations.

The operation phase takes into account intake pumping, water treatment, the first stage of distribution (i.e. pumping to water towers), sludge treatment and sludge spreading. The transportation of chemicals is comprised in the system boundaries, except for hydrated lime and GAC, since their transportation distance was unknown.

Use of water resources in LCA methodology is badly accounted for and it is a major knowledge gap that many have tried to bridge in the last few years (Boulay et al. 2011a; Boulay et al. 2011b; Milà I Canals et al. 2008; Pfister et al. 2009). It is a crucial issue closely related to LCA on water treatment systems. For instance, comparing desalination in a coastal area with surface water treatment and long-distance transfer requires considering the use of different water resources to be consistent (Muñoz et al. 2010; Raluy et al. 2005b). This is one of the reasons why LCIA evaluation methods must take into account environmental impacts due to water withdrawals. In this research work, the aim is to focus on drinking water production seen as one element of the process industry. Issues related to water in LCA will not be tackled if they do not concern the process viewpoint. Accounting for water use in LCA will not be taken into consideration as it is out of the scope of this research project. Nevertheless, this is not an important limitation for this case study since the "what-if" scenarios do not consider the use of alternative water resources and only alternative treatment solutions are investigated based on the actual water resource.

3.2.2 Life Cycle Inventory

In the conventional LCA study, energy and chemical consumptions are calculated as the ratio between purchased quantities over the reference year and the total amount of drinking water produced in the same period. The results are average chemical doses and energy consumptions which are relative to the functional unit and expressed in g/m^3 or kWh/m^3. The information required for establishing these mass and energy balances is available in the technical plant audit and in specific spreadsheet reports provided by the industrial partner (CIRSEE 2002).

In the predictive LCA study, average chemical doses and energy consumptions are forecasted by the unit process models developed and presented in chapter 3. In the case study presented here, these process models are modified according to the results of the previous section, i.e. the site-specific equations are integrated in the predictive models to improve the accuracy of water quality modelling.

At this point, mass and energy balances have been established and the corresponding LCI still needs to be calculated. Background processes for material production and transportation are modelled thanks to the Ecoinvent database (version 2.2) for this purpose.

3.2.3 Life Cycle Impact Assessment

The Recipe method (both MidPoint and EndPoint levels) has been selected since it is an evaluation method widely recognised by the LCA community (Goedkoop et al. 2009). Different evaluation methods are used in chapter 4 and 5 (Impact 2002+ in chapter 4 and ReCiPe in chapter 5). The rationale is to illustrate the flexibility provided by the tool and the full integration of process modelling and LCA tool (i.e. PM-LCA tool). Besides, no justification clearly indicates an evaluation method more adapted for this case study.

Operational costs only take into account purchase of energy and chemicals. Human labour, taxes and maintenance are not part of the operational costs as considered in this case study.

3.3 Results

3.3.1 Water quality

Results on water quality modelling are briefly presented in table 5-9. Building a predictive scenario which reproduces the functioning of the plant is a prerequisite. The treated water quality modelled with the predictive approach must be as similar as possible to the real one. As it is shown by table 5-9, this constraint is respected.

It can be observed that the treated water quality is not identical in the retrofit and predictive scenarios (tables 5-8 and 5-9). This is due to the coagulation process which is modelled differently in the two scenarios. When coagulation is enhanced by acid addition, the pH is lowered and UVA is better removed because water compounds responsible for UVA are better adsorbed with a lower pH.

The DOC removal objective during the coagulation process is the same in both scenarios but the coagulation pH is not. Indeed, the coagulation process is enhanced by acid addition in the retrofit scenario unlike in the predictive one. As a consequence, DOC is removed with the same efficiency unlike UVA. Treated water UVA is higher in the predictive scenario as a result. There is more Al residual (both total and dissolved Al residual) because more aluminium sulphate (i.e. coagulant) has been used to remove the same quantity of DOC. TTHM is more present in treated water as well because their precursors (i.e. water compounds responsible for UVA) have been less removed so TTHM formation is increased during ozonation and chlorination steps taking place after coagulation. Bromate formation is also increased since there is less UVA removed and thus a higher ozone demand.

Table 5-9. Results of water quality modelling within the predictive approach for treated water.

	Raw water	Treated water			
	On-site measurements (A)	On-site measurements (B)	Modelling results (C)	Error on final value (D)	Error on removal (E)
Turbidity (NTU)	15.0	0.120	0.070	-41.7 %	0.34 %
UVA (m^{-1})	5.66	1.18	1.16	-1.69 %	0.45 %
TOC (mg/L)	3.0	1.13	1.20	6.19 %	-3.74 %
pH	8.0	7.70 *	7.70	0.0 %	-
Al residual (mg/L)	0.0	0.0200	0.0109	-45.5 %	-
Bromate (µg/L)	0.0	< 5	1.87	In the range	-
TTHM (µg/L)	0.0	14.3	8.91	-37.6 %	-

* Experts' estimation for typical pH value in treated water.

Nevertheless, the treated water quality modelled by the predictive scenario respect the regulatory standards (table 5-8), it is close to on-site measurements and to the treated water quality modelled by the retrofit scenario.

3.3.2 Chemical consumptions

Chemical consumptions predicted by the plant model are compared in table 5-10 to the real ones in order to evaluate the accuracy of their prediction and more generally the relevance of the predictive modelling approach.

It is considered that coagulation is not enhanced by acid addition and consumption of sulphuric acid is null as a consequence. Consumption of aluminium sulphate (i.e. coagulant) is predicted with satisfactory accuracy (prediction error is 15.4%) even more considering the industrial know-how about forecasting coagulant consumptions.

PAC consumption is almost perfectly predicted but this is normal since the empirical equation developed for this plant is used in the model. With the same process objective as the actual water treatment (DOC removal of 16.5%), the predictive model logically calculates the same PAC consumption.

Table 5-10. Real and predicted chemical consumptions over the reference year.

	Real consumptions (g/m^3)	Predicted consumptions (g/m^3)	Prediction error
Sulfuric acid (96%)	7.17	0.0	-100 %
Soda (50%)	23.2	52.6	127 %
Chlorine (100%)	1.39	1.21	-13.4 %
PAC	4.30	4.31	0.144 %
Aluminium sulphate (8.5% of Al_2O3)	87.5	101	15.4 %
Flocculant for water	0.145	0.143	-1.12 %
Hydrated lime (94%)	7.93	7.02	-11.5 %
Flocculant for sludge	0.0270	0.0240	-11.1 %
New GAC	1.09	1.27	16.3 %
Regenerated GAC	2.05	2.20	7.06 %

Hydrated lime and flocculant used for sludge treatment are underestimated by approximately 11%. In fact, sludge production is underestimated in upstream unit processes (e.g. settling) and that is the reason why the chemicals used for sludge treatment are less consumed in the modelling scenario. The true prediction error is not due to the unit process models involved in sludge treatment (i.e. sludge settling and sludge filter press) but is certainly due to the coagulation and/or settling unit process models. However, an error of 11% is still acceptable all the more since sludge treatment is not contributing a lot on LCIA results (this will be confirmed later in this study).

GAC consumption (new GAC or regenerated GAC) depends on the scheduling of GAC regeneration and GAC replacement. In the plant audit, there are recommendations on GAC regeneration scheduling which have been used as technical design facts for the modelling scenario. This is a default scheduling that must be adapted on the field for many reasons and the plant operators are likely to change it. For instance, if the GAC is not saturated at the end of the adsorption cycle (i.e. if it is still efficiently adsorbing pollutants), the decision can be made to extend the adsorption cycle in progress and delay the GAC regeneration. Thus the plant model is predicting different GAC consumptions. Besides, adsorption cycle duration is about two or three years which is more than the period considered for site inventory (i.e. one year), so the average values for GAC consumption are less reliable than the other material consumptions.

Chlorine consumption is underestimated by 13.4%. This is a satisfactory result, considering that there are two chlorination processes in the process sequence and one of them is at the end of the water treatment line. The final chlorination model may suffer the consequences of prior process model errors.

Another explanation for the difference between actual and modelled chlorine consumptions is about algal bloom. The pre-chlorination is a pre-oxidation step. It is normally supposed to partly remove UVA and it is operated with a chlorine dose of 0.5 g/m^3 but when an algal bloom arises, the chlorine dose is raised to 3.0 g/m^3. This is not taken under consideration in the predictive modelling scenario which considers regular working conditions and this is why the actual chlorine consumption is higher than the predicted one. In fact, the prediction error may be better than 13.4% if one compares the predicted consumption with the actual one excluding the algal bloom situations. Unfortunately, it has been impossible to evaluate the quantity of chlorine used on site to cope with algal blooms.

Soda addition for pH adjustment is the last unit process of the treatment line and soda consumption is overestimated. There are mainly three explanations :

- This unit process model may suffer the consequences of prior process model errors concerning water chemistry modelling (physical form of the salt precipitates not representative enough, temperature not taken into account for water chemistry equilibrium in PHREEQC® calculations)
- The targeted pH value for this process has been estimated as 7.7 but it is an estimation in the high range which induces an overestimation of the pH gap to be compensated by soda addition.
- No direct correlation on water quality measurements in the raw water and at different points of the treatment.

3.3.3 Energy consumption

Energy consumption only involves electricity. Table 5-11 shows the electricity consumptions estimated by the plant operators at different steps of water treatment and the corresponding predicted consumptions. Indeed, the plant model makes it possible to estimate electricity consumptions for each unit process. On the contrary, only the global electricity consumption is accessible on the field but the contribution of some processes to the global consumption is only known approximately. The following estimations have been deduced from the electrical power installed on site for these specific processes.

Table 5-11. Electricity consumptions over the reference year : operators' estimation and modelling results.

	Operators estimation (kWh/m^3)	Predicted consumptions (kWh/m^3)
Intake pumping	0.055	0.052
Ozonation processes	0.055	0.087
Other processes	0.055	0.070
Distribution pumping	0.385	0.394
Total	0.550	0.602

The electricity consumptions generated by the intake pumping and by the distribution pumping seem to be well predicted by the plant model (table 5-11). Discrepancies could be explained by the presence of valves and elbows in the pipes, the difficulty in determining the roughness of fifty year old pipes, etc.

The electricity consumption of the ozonation processes calculated by the unit process models is higher than the operators' estimation. Normally, during ozonation, there is an immediate ozone demand (i.e. ozone that reacts instantaneously with some water compounds) and slow ozone demand which reacts with a first-order kinetic (Roustan et al. 1998). The quantity of ozone that reacts in a contact reactor is the sum of the immediate ozone demand and the proportion of ozone that can react in the time allocated due to the hydraulic residence time in the contactor. In addition, the ozonation processes are operated with a targeted ozone residual at the exit of the contact reactors. Then, the required ozone dose is the sum of the ozone that reacts in the contactors and the targeted ozone residual. The total ozone demand is not necessarily satisfied. No kinetics is taken into account in the ozonation model as stored in this version of the EVALEAU library, it is assumed that the ozone demand is totally satisfied. The ozone dose to be injected is overestimated, and so is the electricity consumed to produce it.

The other processes also consume electricity and their consumption is overestimated by the plant model in comparison with operators' estimations. The most probable explanation is relative to the mixing in the pre-treatment reactor. In fact, PAC and coagulant are added in the same reactor (at different points). The mixing is operated with a very high velocity gradient : 2000 s^{-1} instead of 500 – 1000 s^{-1} in a common coagulation reactor (Degrémont 2007). The mixing duration is very short (almost instantaneous) but the mixing must be achieved correctly. As the duration of the mixing is very short, the mixing power is raised. The mixing duration was not available and it was not measurable because it is below 5s or 10s. In this case study, it has been decided to estimate this mixing duration by the minimum duration that could have been measured (about 5s) and as a consequence, it leads to an overestimation.

The total electricity consumption (average value over the reference year) is compared with the predictive model result in table 5-12. The modelling result is satisfactory since the error is 11.1% and it is validated.

Table 5-12. Total electricity consumption over the reference year : real and predicted consumptions.

	Real consumptions (kWh/m^3)	Predicted consumptions (kWh/m^3)	Prediction error
Total	0.542	0.602	11.1 %

Then, based on this list of chemical and energy consumptions, the environmental impacts generated by the drinking water production within this plant can be evaluated.

3.3.4 LCIA results

All chemicals were present in the Ecoinvent database (version 2.2) except the flocculant and the activated carbon (production and regeneration). The Ecoinvent modules (or specific EVALEAU modules) used in this LCA study are presented in table 5-13.

The flocculant is a commercial product named ASP25. It has been assimilated to acrylic acid which is its main component.

The activated carbon LCI does not exist in any LCA database. It is an issue that has been discussed recently by the LCA community because activated carbon is widely used in the chemical industry. Based on the work of Meier which provides energy and chemical consumptions for activated carbon production and regeneration (Meier 1997), two specific EVALEAU modules ("activated carbon production" and "activated carbon regeneration") have been built for the purpose of evaluating the environmental impacts of GAC and PAC consumptions. The energy and chemical inventory from Meier (1997) for production and regeneration of activated carbon is presented in appendix 5.4. No other data set relative to the production of activated carbon has been found in the literature.

Table 5-13. List of Ecoinvent modules used in the LCA study for background process modelling.

Background process	Ecoinvent module
Production of electricity (type 1)	electricity, medium voltage, at grid
Production of electricity (type 2)	electricity, low voltage, at grid
Production of gaseous chlorine	chlorine, gaseous, diaphragm cell, at plant
Production of sulphuric acid	sulphuric acid, liquid, at plant
Production of coagulant	aluminium sulphate, powder, at plant
Production of flocculant (ASP25)	acrylic acid, at plant
Production of soda	sodium hydroxide, 50% in H2O, production mix, at plant
Production of hydrated lime	lime, hydrated, packed, at plant
Production of PAC	Not present in database – specific EVALEAU module
Production of GAC	Not present in database – specific EVALEAU module
Regeneration of GAC	Not present in database – specific EVALEAU module
Sludge spreading	slurry spreading, by vacuum tanker
Transportation (mode 1)	transport, lorry 3.5-16t, fleet average
Transportation (mode 2)	transport, lorry 16-32t, EURO3

Two different voltages for electricity supply are taken into consideration. The proportion of low voltage electricity over the reference year was 30% and the rest was medium voltage electricity.

An Ecoinvent-like module has been developed for assessing the environmental impacts generated by sludge spreading. The spreading operation is modelled with an Ecoinvent module and the pollutant emissions to soil and water has been examined in this study by a dedicated module specifically developed for this case study. The concentrations of pollutant in the sludge have been incorporated in this module to take into account their environmental impacts during the LCIA step.

Transportation distances were known for every chemical except for hydrated lime and GAC. Their transportation is inevitably neglected in this study. The transportation distance and mode (transportation mode is defined in table 5-13) for the other chemicals are listed below in table 5-14.

Table 5-14. Distance and Ecoinvent module for transportation of each chemical.

	Sulfuric acid	Soda	Chlorine	PAC	Coagulant	Flocculant
Transportation distance (km)	34	238	50	210	372	445
Transportation mode	2	2	1	2	2	1

Finally, after considering the production and transportation of materials (i.e. chemicals and electricity), the LCIA results are calculated. Results obtained with the evaluation method Recipe MidPoint (Goedkoop et al. 2009) are presented in table 5-15. The predicted environmental impacts correspond quite well with the ones calculated by a conventional LCA for most MidPoint impact categories.

Table 5-15. LCIA results with the evaluation method Recipe (MidPoint) : conventional and modelled approaches.

	Conventional LCIA	Predicted LCIA	Prediction error
Agricultural land occupation (m^2.a)	0.00309	0.00356	15.4 %
Climate change (kg CO_2-Eq)	0.212	0.238	11.9 %
Fossil depletion (kg oil-Eq)	0.0713	0.0816	14.4 %
Freshwater ecotoxicity (kg 1,4-DCB)	0.00144	0.00218	50.8 %
Freshwater eutrophication (kg P-Eq)	0.233	0.260	12.0 %
Human toxicity (kg 1,4-DCB)	0.104	0.124	18.8 %
Ionising radiation (kg U235-Eq)	0.650	0.728	12.0 %
Marine ecotoxicity (kg 1,4-DCB)	0.00158	0.00184	16.6 %
Marine eutrophication (kg N-Eq)	0.233	0.260	12.0 %
Metal depletion (kg Fe-Eq)	0.0118	0.0118	0.0824 %
Natural land transformation (m^2)	3.70 1e-05	4.21 1e-05	13.6 %
Ozone depletion (kg CFC-11-)	2.24 1e-08	2.42 1e-08	8.01 %
Particulate matter formation (kg PM10-Eq)	0.000324	0.000335	3.54 %
Photochemical oxidant formation (kg NMVOC)	0.000556	0.000589	5.88 %
Terrestrial acidification (kg SO2-Eq)	0.000971	0.000974	0.241 %
Terrestrial ecotoxicity (kg 1,4-DCB)	7.80 1e-05	3.41 1e-05	-56.3 %
Urban land occupation (m^2.a)	0.00105	0.00103	-2.20 %
Water depletion (m^3)	1.05	1.01	-4.16 %

In order to facilitate the interpretation of the LCIA results, the Recipe method at the EndPoint level (Goedkoop et al. 2009) is used to provide aggregated results. In addition, it allows estimating the contribution of each Midpoint impact category to the corresponding EndPoint impact category and to the total EndPoint score. The results obtained are presented in tables 5-16 and 5-17 and on figure 5-3.

Table 5-16. Compared LCIA results with the evaluation method Recipe (EndPoint).

	Conventional LCIA	Predicted LCIA	Prediction error
Ecosystem Quality (Points)	0.00414	0.00461	11.3 %
Human Health (Points)	0.00915	0.0102	11.4 %
Resources (Points)	0.00749	0.00858	14.4 %
Total (Points)	0.0208	0.0234	12.5 %

Table 5-17. Contribution of each Midpoint impact category to the corresponding EndPoint impact category and to the total EndPoint score according to the predictive model.

Impact category	Contribution to EndPoint category	Contribution to total EndPoint score
Ecosystem Quality		
Agricultural land occupation	1.98 %	0.39 %
Natural land transformation	2.39 %	0.47 %
Marine ecotoxicity	0.00 %	0.00 %
Terrestrial acidification	0.28 %	0.06 %
Terrestrial ecotoxicity	0.21 %	0.04 %
Climate change, ecosystems	93.5 %	18.4 %
Freshwater ecotoxicity	0.03 %	0.01 %
Urban land occupation	0.99 %	0.19 %
Freshwater eutrophication	0.64 %	0.13 %
Human Health		
Particulate matter formation	16.9 %	7.38 %
Photochem. oxidant form.	0.0 %	0.0 %
Climate change, human health	64.6 %	28.2 %
Ionising radiation	2.32 %	1.01 %
Human toxicity	16.1 %	7.04 %
Ozone depletion	0.01 %	0.01 %
Resources		
Metal depletion	0.06 %	0.02 %
Fossil depletion	99.9 %	36.7 %

The errors on predicted LCIA results with the Recipe EndPoint method are less than 15% for all EndPoint impact categories (table 5-16). The modelling approach seems to be adapted to perform ecodesign based on LCA. Alternative treatment solutions can then be studied taking into account environmental performances as well.

Table 5-17 quantifies the contribution of each MidPoint impact category to the corresponding EndPoint category and to the total EndPoint score. The "Climate Change" impact category is responsible for 93.5% of the impact on "Ecosystem Quality" and for 64.6% of the impact on "Human Health". The "Fossil Depletion" impact is responsible for 99.9% of the impact on "Resources".

The "Climate Change" and "Fossil Depletion" impact categories are those that contribute most to their respective EndPoint categories. As a consequence, they are the main impact categories contributing to the total EndPoint score. "Climate Change" and "Fossil Depletion" impacts represent respectively 46.6% (=18.4%+28.2%) and 36.7% of the total EndPoint score.

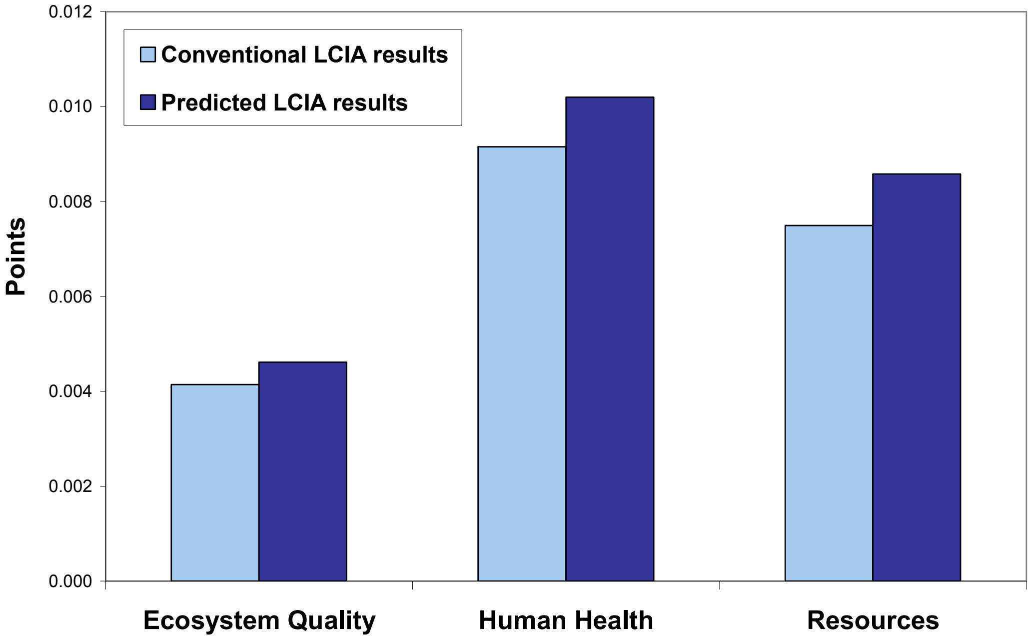


Figure 5-3. Compared LCIA results (Recipe EndPoint).

The predictive modelling scenario was then validated regarding the water quality, electricity and chemical consumptions and LCIA. The scenario, developed and described in this section, is considered as the ground modelling scenario within this case study and it will be further used to create alternative scenarios.

3.4 Conclusion

The predictive approach has been applied in this case study. The plant design relative to equipment sizing and the process sequence are unchanged since the plant already exists. The process objectives are user-defined and the coagulation model has been modified in order to reproduce the regular functioning of the plant. The treated water quality obtained by the predictive approach is close to the real one and it complies with the regulatory standard.

The predictive plant model makes it possible to forecast energy and chemical consumptions as well as LCIA results. It can be concluded that :

1. Energy and chemical consumptions are well predicted (except soda consumption).
2. LCIA results obtained with the Recipe method are well predicted (which is a consequence of point 1).
3. The two impact categories contributing the most to the total EndPoint score are “Climate Change” (46.6%) and “Fossil Depletion” (36.7%).

This predictive plant model reproduces the regular functioning of the plant and it is therefore considered reliable. This ground modelling scenario will serve as a basis for further detailed analysis and for creating alternative scenarios in order to search for improvement opportunities.

4. Contribution analysis and sensitivity analysis

In order to guide further ecodesign attempts, contribution analysis and sensitivity analysis are performed on the plant model. The contribution analysis can determine which unit processes and/or material consumptions are most influencing the LCIA results while sensitivity analysis can determine key process parameters. It makes the behaviour of the plant model more understandable and it automatically tags key process parameters as priority action levers on the field. Contribution and sensitivity analyses provide simple guidelines for improving the performances of the plant.

4.1 Contribution analysis

A deeper understanding of the performances of the plant is possible by investigating the contribution of materials and/or unit processes to the generated environmental impacts. Results of the contribution analysis presented on figures 5-4 and 5-5 are relative to the MidPoint impact categories "Climate Change" and "Fossil Depletion". These environmental impact categories have been selected because they contribute most to the total EndPoint score (table 5-17).

4.1.1 Contribution analysis of materials

The figure 5-4 shows the contribution of each material consumption (i.e. electricity and chemicals) to the "Climate Change" and "Fossil Depletion" environmental impacts. According to the literature, electricity consumption at plant is often the major source of environmental impacts in drinking water production (Friedrich 2002). In this case study, electricity consumption is only responsible for 25.2% on "Climate Change" and for 19.6% on "Fossil Depletion". There are two explanations :

1. The production of drinking water within this plant requires more chemicals than in other plants.
2. The French electricity mix is used in this case study because the plant is located in the Paris area and this electricity mix generates reduced "Climate Change" and "Fossil Depletion" impacts compared to other countries' electricity mix. This is a consequence of the high proportion of nuclear energy in the French electricity mix.

Chlorine, flocculant and hydrated lime consumptions are responsible for negligible contributions to the considered impact categories. Other chemical consumptions contribute much more to the "Climate Change" and "Fossil Depletion" impacts : PAC, GAC and to a lesser degree soda and aluminium sulphate.

Therefore, improvement opportunities for this plant could consist in reducing the electricity consumption and the PAC, GAC, soda and coagulant consumptions.

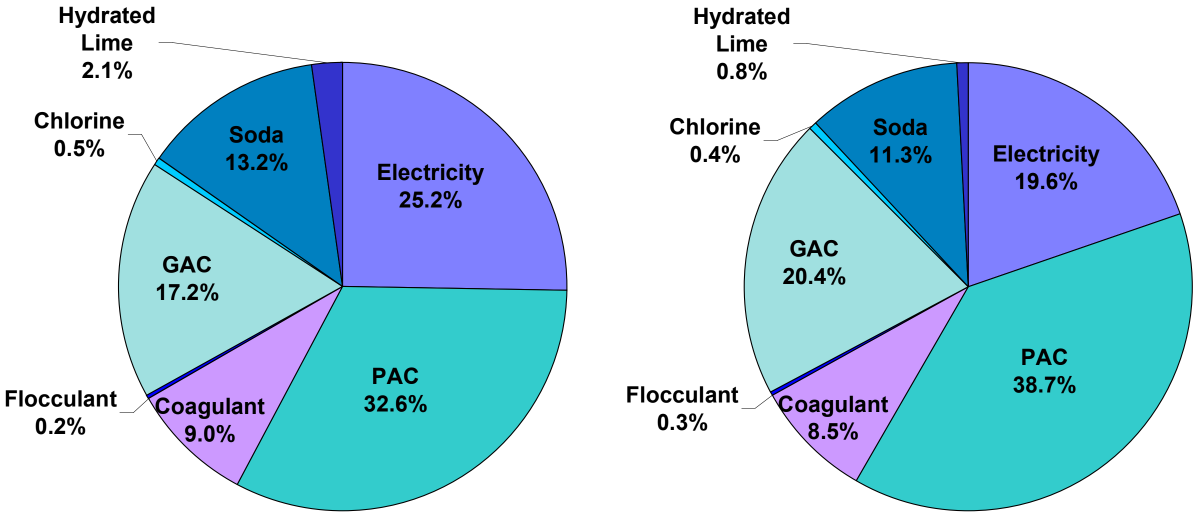


Figure 5-4. Contribution of material consumptions to the MidPoint impact categories "Climate Change" (left) and "Fossil Depletion" (right).

It must be noticed that the two graphs in figure 5-4 are very similar. The contributions of material consumptions to each impact category are almost the same. These impact categories are mainly due to the consumption of non-renewable energy sources in background processes. Only results concerning "Climate Change" impacts will be presented in the next sections of the study since they are almost the same for "Fossil Depletion" impacts and they do not provide additional insights. The "Climate Change" impact category is selected because 1/ it is the impact category that contributes most to the total EndPoint score and 2/ its interest for decision-makers and stakeholders is growing.

4.1.2 Contribution analysis of unit processes

The figure 5-5 shows the contribution of each unit process (by process line/category) on the MidPoint impact category "Climate Change". Previous results presented on figure 5-4 are confirmed by figure 5-5. Operations like PAC addition, coagulation, GAC filtration and pH adjustment are the unit processes contributing the most to the “Climate Change” impact because of their chemical consumptions (respectively PAC, aluminium sulphate, GAC and soda).

Another unit process making an important contribution is the distribution pumping step. It generates an electricity consumption of 0.394 kWh/m^3 out of 0.602 kWh/m^3. It represents 65.4% of the total electricity consumption which in turn contributes for 25.2% of the “Climate Change” impact. Then, the contribution of the distribution pumping to “Climate Change” is about 16.4% which is significant. The problem is that the pumping station is already optimised (i.e. the efficiency of the pumps is already maximised) and the topography of the plant’s location can obviously not be changed so the height to be pumped is fixed. As a consequence, there is no improvement opportunity relative to the distribution pumping (and to any pumping step in general).

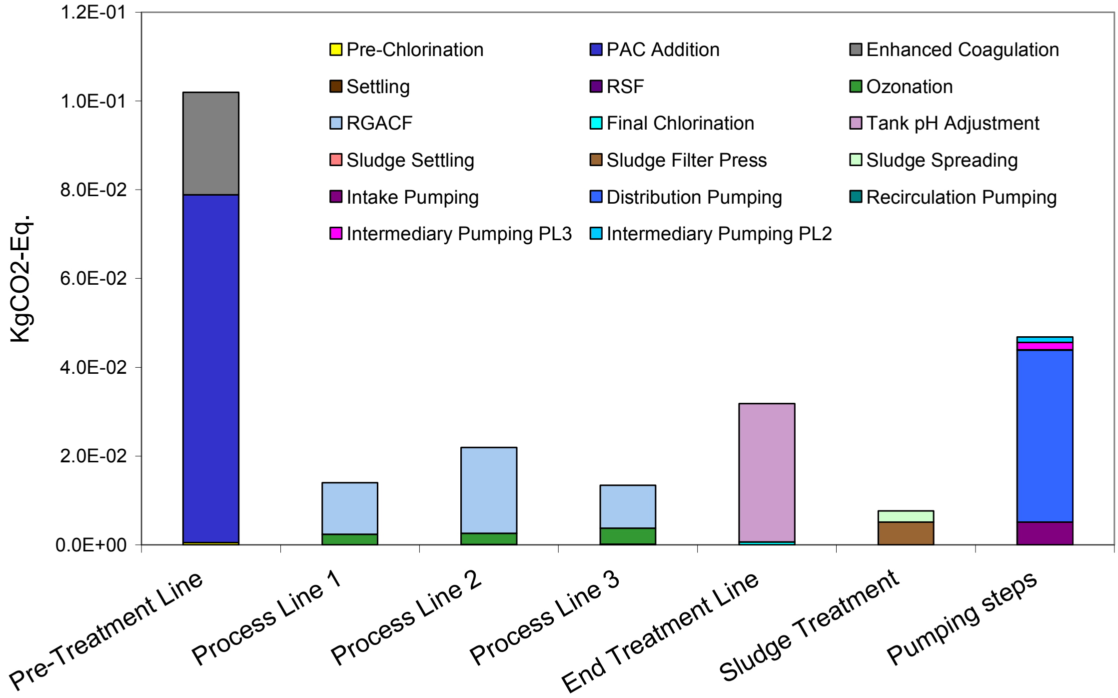


Figure 5-5. Contribution of unit processes to the MidPoint impact category “Climate Change”.

Hereafter the study focuses on chemical consumptions. The environmental impacts relative to chemical consumptions are due to : 1/ their off-site production and 2/ their transportation. The plant operators cannot really act on the off-site production of the chemicals but they may be able to replace one chemical by a less polluting one. Concerning the transportation of chemicals, they can select a supplier closer to the plant's location to reduce the related environmental impacts. The contribution of the chemical transportation to the environmental impacts is estimated for the current situation. It is presented in table 5-18 in order to evaluate if it is a potential action lever for reducing the environmental impacts.

Table 5-18. Contribution of chemical transportation to the environmental impacts (Recipe).

	Climate Change ($kgCO_2$-Eq)	Climate Change contribution	Total score (Points)	Total Score contribution
Chemicals transportation	0.00945	3.97 %	0.000935	4.00 %

The contribution of chemical transportation is only about 4% while the total contribution of chemical consumptions is about 75% (production and transportation). Thus the transportation of chemicals is a negligible source of environmental impacts compared with their off-site production.

In order to really reduce environmental impacts, one should reduce chemical consumptions as much as possible or use alternative chemicals. Smarter combination of chemical doses is also another possibility to reduce the environmental impacts, e.g. increasing one chemical dose may allow reducing another one which has more environmental impact.

4.2 Sensitivity analysis

The Morris method is applied on the predictive plant model, with the aim of detecting which parameters are significantly influencing the LCIA results. It guides efforts in good directions by tagging priority action levers within an ecodesign perspective (and on the field as well). The Morris method is supposed to assist the ecodesign process by guiding the strategy and ensuring effective actions.

It is important to notice that the Morris method gives no information about the reason why a parameter is influent on a model result. This mathematical technique only enables one to better understand the behaviour of complex models and to qualitatively evaluate the influence of parameters.

The plant model contains 273 parameters but the parameter set considered in the application of the Morris method is reduced. In this study, a parameter is excluded from the sensitivity analysis when it is not a potential action lever and possible reasons are :

1. The parameter is a technical or legal constraint.
2. The parameter is relative to equipment sizing. In this case study, the plant already exists, so it is considered that it is not possible to modify this kind of parameters.
3. The parameter has no influence at all on the LCIA results so it can be excluded from the sensitivity analysis (e.g. contact time in the coagulation reactor).

The parameter set selected for sensitivity analysis is presented in appendix 5-5. It contains the name and the unit process of each selected parameter and the range of values taken into consideration for applying the Morris method. The default range of values for a parameter is determined by applying +/- 25% on its value defined in the ground modelling scenario. For some parameters, the range of values has been determined after discussion to set a more realistic range of values according to field experience.

There are 4 LCIA results considered for sensitivity analysis: “Climate Change” (Recipe, MidPoint), “Human Toxicity” (Recipe, MidPoint), “Ionising Radiation” (Recipe, MidPoint) and the total score (Recipe, EndPoint). The contribution analysis highlights the importance of “Climate Change” and “Fossil depletion” but other impact categories must be considered as well in the sensitivity analysis. The modified operating conditions (simulated during the Morris method calculations) can make other impact categories contribute to the global environmental impact. Such is the rationale to apply the Morris method on other impact categories than “Climate Change”.

4.2.1 Morris method applied on “Climate Change”impact

According to the Morris graph relative to “Climate Change” (figure 5-6), the result is influenced by the DOC removal objectives of coagulation and PAC addition and by the targeted pH of the neutralisation step. The DOC removal objective of PAC addition (parameter “PAC DOC_R”) is much more influent. The other model parameters do not have a significant influence on the “Climate Change” result.

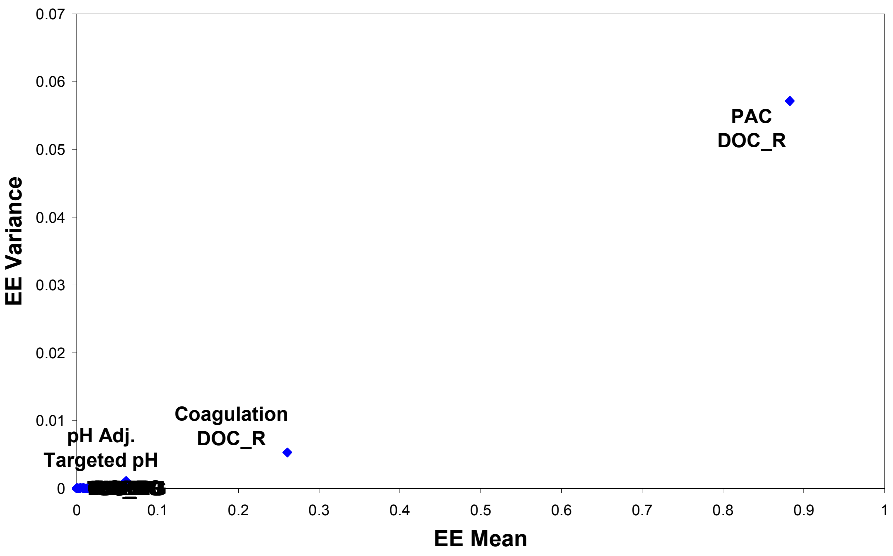


Figure 5-6. Morris graph relative to Climate Change (Recipe, MidPoint).

A probable explanation for the influence of the DOC removal objective of PAC addition is the consumption of PAC which is a direct consequence of this model parameter. PAC is the material whose consumption contributes the most to the “Climate Change” impact category (figure 5-4) hence the influence of the DOC removal objective of PAC addition on this LCIA result.

4.2.2 Morris method applied on "Human Toxicity"impact

The Morris graph about the "Human Toxicity" result (figure 5-7) shows that the same three parameters are influent on this model result. For "Human Toxicity", the DOC removal objective of the coagulation process is the most influent parameter (and not the one of the PAC addition process).

Although the gas transfer efficiency ("GT_NU") in the ozonation reactors of the process lines 1 and 3 seems to be influent, the influence of these two parameters is expected to be negligible compared to the one of DOC removal objectives during coagulation and PAC addition and the targeted pH of the neutralisation step.

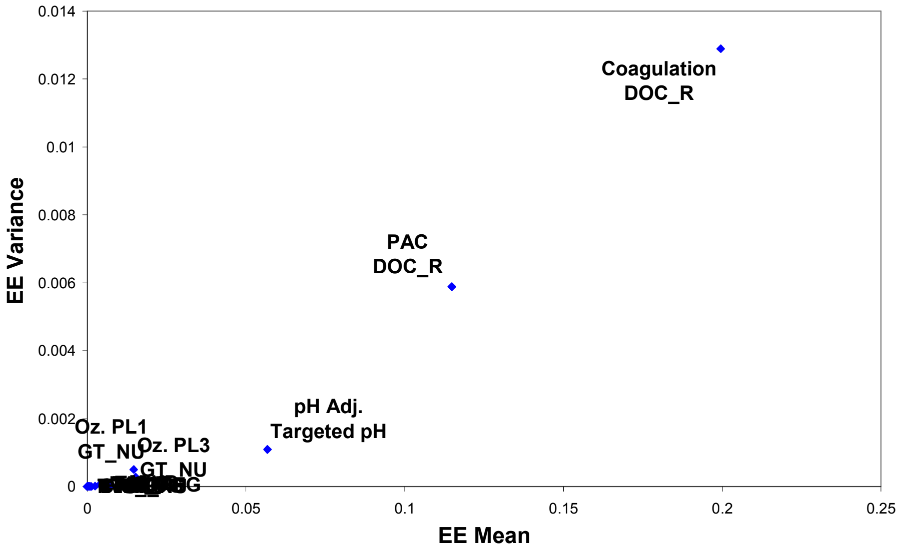


Figure 5-7. Morris graph relative to Human Toxicity (Recipe, MidPoint).

A possible explanation for the major influence of the DOC removal objective of coagulation on "Human Toxicity" impact is the use of aluminium for coagulant production. Indeed, aluminium is often responsible for "Human Toxicity" impact.

4.2.3 Morris method applied on "Ionising Radiation"impact

The Morris graph relative to the "Ionising Radiation" impact (figure 5-8) has a different appearance. There are many more influent parameters on this impact category. The parameters that were influent on the previous studied results ("Climate Change" and "Human Toxicity" results) are also influent on the "Ionising Radiation" result. The mixing duration in the pre-treatment line ("Pre-Treatment MIXD" on the figure 5-8) appears as the most influent whereas it was not detected as influent for the other impact categories previously studied. One will take note that taking action on DOC removal of coagulation and PAC addition and/or the final targeted pH would have an effect on the three LCIA results considered in this sensitivity analysis.

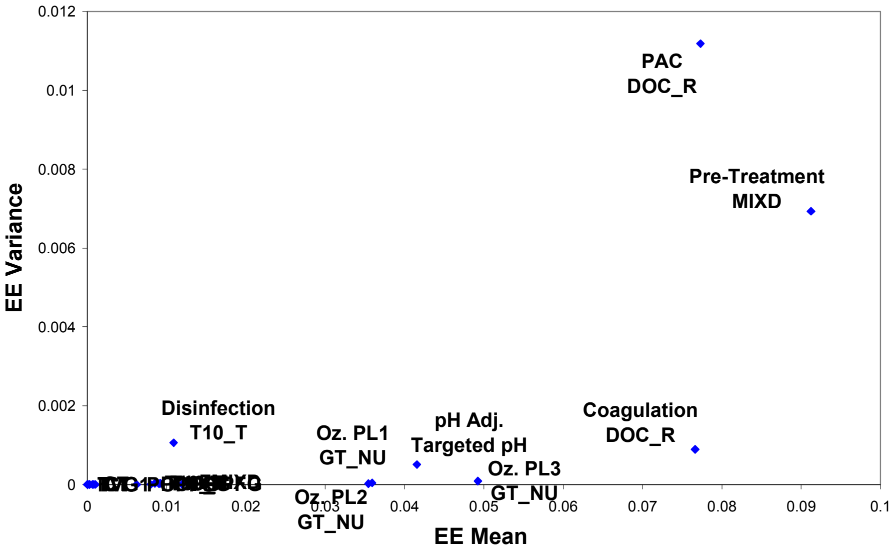


Figure 5-8. Morris graph relative to Ionising Radiation (Recipe, MidPoint).

For this impact category, it is more difficult to find a logical explanation about the parameters' influence. The behaviour of the plant model is complex and less understandable but the Morris method regardless provides qualitative information on the influence of parameters.

4.2.4 Morris method applied on the total EndPoint score

The Morris graph on the total EndPoint score (figure 5-9) allows taking into account different impact categories at the same time. This Morris graph is very similar to the one on "Climate Change" (figure 5-6), which is logical. The impact categories "Climate Change" and "Fossil Depletion" are the most contributing to the EndPoint score (table 5-17) so parameters influencing the "Climate Change" result also influence the EndPoint score.

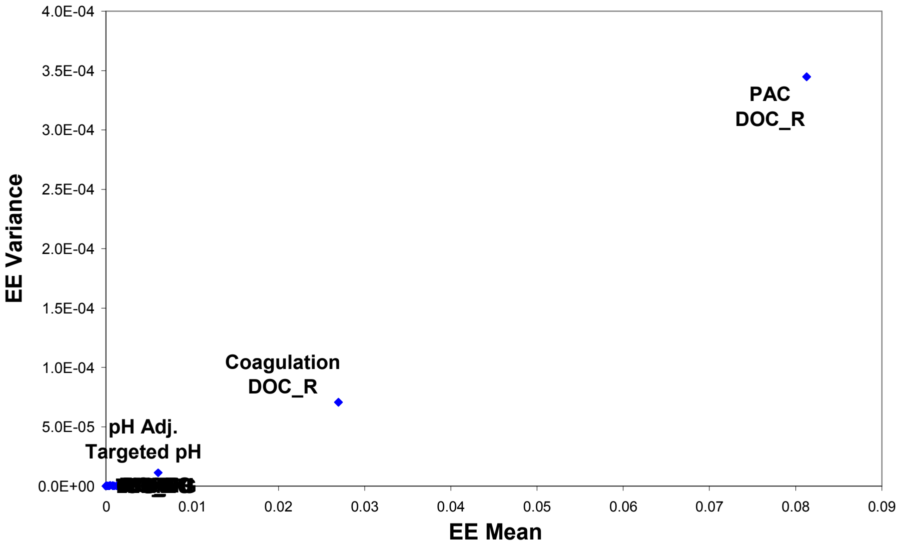


Figure 5-9. Morris graph relative to total EndPoint score (Recipe, EndPoint).

The Morris method applied on the plant model leads to one major conclusion : the two key parameters for the plant model (and thus for the real plant as well) are the DOC removal objectives achieved during the coagulation process and the PAC addition process. They are the most influential parameters on LCIA results, except for "Ionising Radiation" but they are also very influential parameters on this impact category.

4.3 Conclusion

Contribution analysis and sensitivity analysis jointly provide useful information for undertaking effective actions to reduce the environmental impacts provoked by the studied plant. Contribution analysis sheds light on the unit processes and/or material consumptions responsible for the environmental impacts while sensitivity analysis indicates the priority action levers. Both guide the choice of alternative treatment solutions.

The unit processes contributing the most to the environmental impacts generated by drinking water production are :

- PAC addition
- Coagulation
- GAC filtration
- Neutralisation
- Distribution pumping

Nevertheless, the operating conditions of GAC filtration and distribution pumping are already optimised and/or fixed and there is no improvement opportunity related to these processes.

According to the Morris method, actions must be undertaken primarily on PAC addition and coagulation processes (through DOC removal objectives) to effectively reduce the environmental impacts.

5. Alternative treatment solutions - Redesigning the plant within an ecodesign perspective

A predictive model of the studied plant which reproduces the field reality is now established as the ground modelling scenario. Contribution analysis and sensitivity analysis applied to this plant model brought a better understanding of its behaviour, and consequently a better understanding of the actual functioning of the plant. Based on the indications provided by the previous analysis steps, the intention is to simulate alternative treatment solutions aimed at improving the environmental performances of the water treatment plant. Operational costs and technical feasibility of these alternative treatment solutions are discussed for sake of realism.

The redesign trial of the plant must start by optimising coagulant and PAC doses which are calculated according to the user-defined objectives of DOC removal for both processes. The aim is to minimise coagulant and PAC doses and to determine the optimum combination of both. This is a major step as these two process parameters are the most influential on LCIA results according to the sensitivity analysis. Then, several "what-if" scenario trials will be performed in search of potential improvements. The following sections focus on :

1. Optimum combination of coagulant and PAC doses to reduce the environmental impacts while fulfilling the requirements regarding treated water quality.
2. Alternative choices for chemicals at the end of the treatment line (i.e. disinfection and neutralisation steps).
3. Use of different technologies for ozone production.

It may be not completely exhaustive and other "what-if" scenarios could be suggested by water treatment experts.

5.1 Optimum combination of PAC and coagulant doses

The organic matter is the main water quality issue within this plant. UVA and TOC (or DOC) must be correctly removed and closely controlled to ensure that the treated water quality is satisfactory. UVA and TOC are mainly removed by adsorption on PAC and on flocs formed during coagulation. Then, the PAC and coagulant doses must be sufficient to enable the water treatment to remove the required amount of organic matter. At the same time, the less chemicals are used, the less environmental impacts and operational costs are generated.

Considering the actual functioning of the treatment line, 16.5% of the DOC is removed with PAC addition and 41% with coagulation. The treated water obtained in the ground modelling scenario has a TOC of 1.20 g/L and a UVA of 1.16 m^{-1} (table 5-9) while the industrial objectives are a limit TOC of 1.30 g/L and a limit UVA of 1.3 m^{-1} (table 5-8). Lowering the DOC removal during coagulation to 40% leads to a treated water UVA of 1.26 m^{-1}, lowering the DOC removal during coagulation to 39% leads to a treated water UVA of 1.34 m^{-1}.

Thus it is assumed that the coagulant and PAC doses are already minimised and that they could not be lowered without degrading the treated water quality. Besides, it is logical to record this fact in the ground modelling scenario as these chemical doses have already been minimised on the field.

As the PAC and coagulant doses cannot be minimised further, a smart combination of both is sought in order to lower the environmental impacts. The principle is that if one chemical dose is lowered, the other must be increased. Indeed, the treated water quality calculated in alternative scenarios should be approximately equal to the one calculated in the ground modelling scenario, that is to say slightly under the industrial objectives. The idea is to be able to compare different design options leading to similar drinking water quality (i.e. to the same functional unit).

It must be noted that sulphuric acid can be added by plant operators to enhance the coagulation process as mentioned previously. Generally, lowering the operating pH leads to a better adsorption rate of dissolved organic matter on flocs formed during coagulation. A smart combination of the three chemical doses (i.e. PAC, coagulant and sulphuric acid) should be sought for a more rigorous experimentation, but the addition of sulphuric acid is not considered in this set of numerical simulations. The main reason is that the technical audit of the plant (CIRSEE 2002) indicates that sulphuric acid is added only when the pH of the raw water is too high or when the temperature of the raw water is too low. Nevertheless, the EVALEAU library comprises a model for enhanced coagulation so that an optimal combination of PAC, coagulant and sulphuric acid can be sought as well.

Alternative scenarios are studied in what follows. Scenario 0 is the ground modelling scenario representing the actual plant functioning. In scenarios 1 and 2, there is more DOC removed with PAC and less with coagulant compared to scenario 0. Finally, in scenarios 3 and 4, there is less DOC removed with PAC and more during the coagulation step. UVA and TOC in the treated water are checked for validating the alternative scenarios. LCIA results and operational costs are compared in table 5-19 to determine how the plant model reacts to these alternative design options.

Table 5-19. Effects of different PAC and coagulant doses on economical and environmental performances of the plant.

	Scenario 0	Scenario 1	Scenario 2	Scenario 3	Scenario 4
DOC removal with PAC (%)	16.5 %	32.0 %	40.0 %	10.5 %	0.0 %
DOC removal with coagulant (%)	41.0 %	35.0 %	20.0 %	45.0 %	50.7 %
PAC dose (g/m^3)	4.31	12.8	18.6	2.14	0.08
Coagulant dose (g/m^3)	101	55.0	16.3	133.6	204.7
Treated water UVA (m^{-1})	1.16	1.27	1.21	0.89	0.41
Treated water TOC (mg/L)	1.20	1.08	1.17	1.20	1.21
Sludge production (g/m^3)	0.0723	0.0763	0.0795	0.0793	0.1014
Operational costs (€/m^3)	0.0834	0.0728	0.0625	0.0935	0.1167
LCIA results – Climate Change (kgCO$_2$-Eq.)	0.238	0.367	0.453	0.214	0.210
LCIA results – Total Score (Points)	0.0234	0.0354	0.0434	0.0214	0.0212

5.1.1 Water quality

It should be noticed that the UVA and TOC values in the treated water are acceptable in every alternative scenario. The values are not exactly equal to the ones of scenario 0 but they all meet the industrial objectives (UVA < 1.3 m^{-1} and TOC < 1.3 g/L). There is only one significant difference on treated water UVA in scenarios 3 and 4. When adding more coagulant, the pH is lowered and it enhances UVA removal due to coagulation. In scenario 3 and 4, there is less PAC and more coagulant added to the water, then DOC (and consequently TOC) is removed with the same efficiency while UVA is inevitably better removed. This effect cannot be avoided and a perfect comparison is not possible but it only makes the treated water better and it is not considered as a problem for the comparison of alternative scenarios.

5.1.2 LCIA results

The LCIA results are obtained with the Recipe method (Goedkoop et al. 2009). The results considered are the MidPoint impact category “Climate Change” and the total EndPoint score as presented in table 5-19.

Scenarios 1 and 2 show that increasing the PAC dose while reducing the coagulant one strongly influences the LCIA results. The environmental impacts are increased because of the PAC consumption (+54.2% in scenario 1, +90.3% in scenario 2 for “Climate Change” impact). In the ground modelling scenario (i.e. scenario 0), it has been established that the PAC consumption is responsible for 32.6% of the “Climate Change” impact while the coagulant consumption is only responsible for 9.0% (figure 5-4) though the doses are 4.31 g/m^3 for PAC and 101 g/m^3 for coagulant. As PAC is the main chemical contributing to the “Climate Change” impact, increasing its consumption by a factor of 3 or 4 logically leads to significant additional “Climate Change” impact. The same conclusion can be made on the total EndPoint score.

Scenarios 3 and 4 show a decrease of considered environmental impacts (both “Climate Change” impact category and total EndPoint score). Using more coagulant makes the pH of the coagulated water lower and then more soda is required at the end of the treatment to set the pH to the targeted value which is basic. Despite this increase of coagulant and soda consumptions, the effect of reducing PAC consumption benefits to the environmental performances of the plant.

According to the results, use of coagulant instead of PAC should be promoted to reduce the environmental impacts of drinking water production within this plant. Coagulant should be favoured over PAC at least from an environmental point of view.

5.1.3 Operational costs

The calculation of operational costs takes into account the chemical and electricity prices as indicated by the plant operators (appendix 5-6). Unfortunately, the calculation does not consider the cost of sludge disposal (landfilling) which could be problematic and expensive. The results are presented in table 5-19.

The results of scenarios 1 and 2 show that when using more PAC and less coagulant, the operational costs can be significantly reduced (-25.1% for scenario 2). Even if the PAC is more expensive, the quantity that is used is not important compared with the quantity of coagulant. Besides, adding more coagulant implies adding more soda at the end of the treatment line which also increases the total operational costs.

Scenarios 3 and 4 show the opposite tendency. The additional operational costs in both scenarios are significant (+12.1% for scenario 3 and +39.9% for scenario 4). Therefore, scenarios 3 and 4 are not efficient solutions in terms of treatment costs.

Based on the plant model results, PAC addition seems to be more efficient than coagulation to remove DOC from an economic point of view.

5.1.4 Technical feasibility

The four alternative scenarios studied in this section can be put into practice on the field since the required facilities already exist. Nevertheless, sludge production is increased in all alternative scenarios and it is probably an issue.

Sludge disposal is expensive for most drinking water treatment plants. Sludge production is certainly one technical criterion currently retained for plant operation since the ground modelling scenario is the one that minimises it most. In this study, the operational costs do not comprise sludge disposal and the associated cost increase is not taken into account. This economic consideration can prevent these alternative treatment solutions from being implemented on the field and it must be evaluated beforehand.

5.1.5 Conclusion

In this study, different combinations of coagulant and PAC doses have been investigated in four alternative scenarios. The results show that :

- It is not possible to reduce the coagulant dose without increasing the PAC dose and vice versa.
- It is not possible to reduce environmental impacts and operational costs at the same time. In this situation, a suitable trade-off must be difficult to find.
- The alternative solutions generate a higher sludge production which is a potential issue.

5.2 Alternative chemicals for disinfection and neutralisation

The neutralisation step (i.e. pH adjustment) is responsible for 13.2% of the "Climate Change" impact via soda consumption. Even if soda consumption is overestimated by the ground modelling scenario (and thus the "Climate Change" impact due to soda consumption), lowering it could lead to lowering the global environmental impact of the plant.

The targeted pH achieved during this unit process must be in the 7.5-7.8 range mainly for taste reason (CIRSEE 2002). There is no possibility to reduce the targeted pH and the soda dose to adjust it.
Then, one possibility would be to use another basic chemical to set the pH to the targeted value. In drinking water treatment, the chemicals widely used to make the water basic are soda and hydrated lime. Replacing soda by hydrated lime could be a solution to reduce the "Climate Change" impact so it is further investigated in this part of the study.
Another opportunity would be to use another chemical for disinfection. Indeed, chlorine is used for disinfection and its injection makes the water acid while the next step (i.e. pH adjustment) aims at restoring a basic pH. A basic disinfectant like sodium hypochlorite (i.e. bleach) would lower the pH gap to be compensated in the neutralisation step instead of increasing it.

Three "what-if" scenarios are modelled as variants of the ground modelling scenario. Scenario 0 is the ground modelling scenario. Scenario 1 is the one that examines the use of hydrated lime instead of soda. Scenario 2 is the one considering the use of bleach instead of chlorine and soda. Scenario 3 is the one considering joint use of hydrated lime and bleach.

5.2.1 LCIA results

The LCIA results considered are the MidPoint impact category "Climate Change" and the total EndPoint score. The LCIA results presented in table 5-20 are relative to the global water treatment, i.e. these are the environmental impacts of the whole process chain and not only the disinfection and neutralisation processes.

For the three alternative scenarios, it seems that the decrease of the environmental impacts is more important for the EndPoint score than for the "Climate Change" impact. For scenario 1, the improvement of the environmental performances of the plant is significant. Decreasing by

6.72% the Climate Change impact (and by 10.3% the Total Score) of the drinking water production could be a major improvement and it is achievable only by changing the chemical used during neutralisation. This is clearly an improvement opportunity at least in terms of environmental impacts. For scenario 2, the improvement of environmental performances is not significant (less than 1%). Scenario 3 has the same performances as scenario 1 due to the use of lime. The use of bleach has no improving effect.

Therefore, from an environmental point of view, scenario 1 is the most interesting alternative treatment solution and it is better than the ground modelling scenario. Substituting hydrated lime for soda is a realistic opportunity to reduce environmental impacts.

Table 5-20. LCIA results with alternative chemicals for disinfection and/or neutralisation.

	Scenario 0	Scenario 1	Scenario 2	Scenario3
Climate Change (kgCO_2-Eq.)	0.238	0.222	0.236	0.222
Difference on Climate Change	-	- 6.72 %	- 0.84 %	- 6.72 %
Total Score (Points)	0.0234	0.0210	0.0232	0.0210
Difference on Total Score	-	- 10.3 %	- 0.85 %	- 10.3 %

Nevertheless, interpretation of these results is limited because normally, uncertainty analysis must be previously performed to know the accuracy of the model results. It is a prerequisite for drawing definitive conclusions from such “what-if” scenarios. Otherwise, the interpretation must be cautious and only tendencies can be deduced from the previous results.

5.2.2 Operational costs

Operational costs are evaluated for the three scenarios. Indeed, an alternative treatment solution can enhance the environmental performances while increasing operational costs. Appendix 5-6 provides the average costs of electricity and chemicals as purchased by the plant operators.

Table 5-21. Operational costs with alternative chemicals for disinfection and/or neutralisation.

	Scenario 0	Scenario 1	Scenario 2	Scenario3
Operational costs (Euros/m^3)	0.0834	0.1100	0.0828	0.1104
Difference on operational costs	-	31.9 %	- 0.66 %	32.4 %

Scenarios 1 and 3 are inducing a high increase of the operational costs due to the quantity of hydrated lime that must be added to the water (approximately 300 g/m^3 at 10% $Ca(OH)_2$). As the cost increase is more than 30%, it could be a sufficient reason not to implement these treatment solutions on the field. Scenario 2 decreases the operational costs but only by 0.66% which is not significant even more considering the uncertainties of the model.

5.2.3 Technical feasibility

Using hydrated lime instead of soda could eventually cause 2 problems. Firstly, there is a risk of calcium carbonate precipitation (+60.8% of precipitated calcium carbonate in treated water in scenario 1 compared with the scenario 0). It increases the turbidity at the end of the treatment which is potentially prejudicial for treated water quality and distribution network as well.

Finally, the addition of hydrated lime into water increases the calcium concentration, thus it increases the hardness. It can be a problem for the treated water quality if it becomes too hard. The hardness of the treated water when using hydrated lime for neutralisation is 24.2 French degrees (scenario 1) instead of 21.6 French degrees when using soda (scenario 0). The water obtained in scenario 1 is hard but it is still acceptable. However local consumers may complain about the taste of the water and it has to be tested before implementing this alternative treatment solution on the field.

Using bleach for disinfection instead of gaseous chlorine (scenario 2) could be a problem for UVA removal. Indeed, the UVA removal obtained using chlorine is usually better than the one obtained using bleach. As the UVA is a main issue regarding water quality, it could be a technical limitation deterring the plant operators from adopting this solution. Some experimental tests must be carried out before implementing this alternative disinfection process on the field to check if there is any problem regarding UVA in the treated water.

5.2.4 Conclusion

Scenario 3 is not an interesting alternative treatment solution as it is more complex to implement on the field while it does not provide more benefits than scenario 1. Scenario 1 is an interesting improvement opportunity in terms of environmental impacts but the corresponding operational costs are significantly increased which is not a good point. Scenario 2 apparently improves the environmental performances and the operational costs of the water treatment but the benefits are not significant (less than 1%) and model uncertainties do not allow drawing definitive conclusions on this alternative treatment solution. Besides, it may take a lot of time and efforts to implement this solution for insignificant improvement of the plant performances.

For a real enhancement of the plant's environmental performances, more money should be spent on purchasing hydrated lime instead of soda. Therefore, decision-makers must find a suitable trade-off between environmental and economical issues.

However, it is interesting to observe that the neutralisation process is not really involved in making the water potable. In fact, it is only making the water taste better (CIRSEE 2002). The pH adjustment is sometimes put into work in order to avoid leakage of heavy metals from distribution pipes. It is a potential issue but it is not mentioned in the technical audit of the plant unlike the taste issue which is the main source of consumers' complaints.

The legal recommendations on drinking water pH are to set it between 6.5 and 8.5 (French drinking water standard). The pH of the water exiting the disinfection step is 6.8 and thus it complies with the legal recommendation. It means that neutralisation is not mandatory for health issues. There is no health risk in drinking the water exiting the disinfection step and it is only a matter of social acceptance. Soda consumption and its related environmental impacts could be completely avoided and environmental impacts of drinking water production within this plant could be significantly reduced.

5.3 Alternative technology for ozone production

Ozonated gas for ozonation processes can be produced from air or from pure oxygen O_2. Producing ozone from pure oxygen allows consuming less electricity on the one hand but it consumes pure oxygen on the other hand. In the studied plant, the ozonated gas is produced from air and one wonders if the environmental impacts of the plant could be reduced by producing it from pure oxygen. This alternative technology for ozone production is further investigated in this case study. Scenario 0 is the ground modelling scenario and scenario 1 is the one where alternative technology for ozone production is considered. A hypothetical transportation distance of 100 km is considered for pure oxygen delivery.

5.3.1 LCIA results

Although the electricity consumption of the whole process chain is decreased by 6.5% (0.563 kWh/m^3 instead of 0.602 kWh/m^3), the consumption of pure oxygen (60.9 g/m^3) is responsible for additional environmental impacts.

Table 5-22. LCIA results with alternative technology for ozone production.

	Scenario 0	Scenario 1
Climate Change (kgCO_2-Eq.)	0.238	0.260
Difference on Climate Change	-	9.2 %
Total Score (Points)	0.0234	0.0254
Difference on total Score	-	8.5 %

Indeed, as shown in table 5-22, the LCIA results are significantly increased by the tested ozone production technology. It is not an improvement opportunity regarding the environmental performances of the plant and therefore it should not be considered for implementation on the field if such is the objective.

5.3.2 Operational costs

The use of pure oxygen O_2 as a feed gas for ozone production slightly reduces the operational costs as presented in table 5-23.

Table 5-23. Operational costs with alternative technology for ozone production.

	Scenario 0	Scenario 1
Operational costs (Euros/m^3)	0.0834	0.0817
Difference on operational costs	-	-2.0 %

Nevertheless, the operational costs are not significantly reduced and no clear interpretation of such a result can be made with regard to the model's uncertainty. Furthermore, the price of pure oxygen varies a lot depending on the size of its packaging, which depends in turns on the size of the plant and its oxygen demand. The price or pure oxygen, as evaluated in appendix 5-6, is very low because the studied plant has a large size and so a hypothetically high demand for oxygen. It must be noted that the operational costs would have been increased for a small-size plant.

5.3.3 Technical feasibility

Normally, there is no reason why the ozone production technology using pure oxygen could not be used on the field. The feed gas in the ozone production step is different (i.e. air or pure oxygen) but the quantity of ozone injected into water is exactly the same, then the water treatment is not affected at all. Switching from the existing technology to the alternative one is possible with no implementation problem.

One can wonder why pure oxygen is used as a feed gas for ozone production since it generates additional environmental impacts though it is not significantly less expensive. The main reason is that it allows producing an ozonated gas with a higher concentration. Indeed, the concentration of the ozonated gas obtained from pure oxygen is 70 gO_3/Nm^3 on average instead of 18 gO_3/Nm^3 when producing the ozonated from air (Degrémont 2007). The higher concentration of the ozonated gas makes it easier for plant operators to deal with problems such as algal blooms or any temporary pollution requiring strengthened oxidation.

5.3.4 Conclusion

The use of pure oxygen O_2 for ozone production does not improve significantly the operational costs and the environmental performances of the plant are worsened. From the technical point of view, there could be various reasons for implementing this kind of ozone production technologies in drinking water treatment plants but this is not the case for the plant under consideration. This alternative scenario is consequently not worth retaining within an ecodesign perspective.

5.4 Conclusion

One major limitation of the previous "what-if" scenarios is that the uncertainty of the model results is only roughly estimated. Indeed, model uncertainty has been evaluated by comparing the energy and chemical consumptions measured on site with the ones predicted by the plant model in the ground scenario, but no formal uncertainty analysis has been performed. The comparison between two modelling scenarios is consequently affected by this lack of knowledge on model uncertainty. Therefore, no definitive conclusions can be drawn from such modelling study and only tendencies can be trusted.

The proposed alternative treatment solutions are not very different from the present treatment solution because 1/ the plant already exists and 2/ it has been optimised for years. Indeed, the drinking water treatment plant has been studied in detail by the industrial partner and its functioning is already optimised (with technical and economic criteria). Nevertheless, opportunities for reducing the environmental impacts of drinking water production caused by this plant have been investigated providing interesting insights :

- Use of coagulant should be promoted over use of PAC for removing the organic matter from the treated water.
- Replacing soda by hydrated lime in the neutralisation step can reduce the environmental impacts.
- Use of air for producing the ozonated gas is a better solution than use of pure oxygen to reduce the ozonation environmental impacts.

Attention must be paid to the fact that in most cases, reducing environmental impacts implies increasing operational costs and potential technical issues can emerge when implementing these alternative treatment solutions. A suitable trade-off between technical, environmental and economic performances of the plant is likely to be difficult to find as these considerations are most often conflicting.

6. Deterioration of the raw water quality - Facing a rain event

Within the EVALEAU tool, a modelling scenario is a steady-state simulation of a drinking water treatment plant. In this context, raw water quality has been considered constant. Most of the time, this assumption is realistic. However, significant changes in raw water quality can occur and have repercussions on water treatment.

In this section of the study, the aim is to evaluate how a change of the raw water quality can influence the model results. The rationale is to understand if it is necessary to undertake actions to cope with it and which kind of actions.

There can be several reasons for a modification of the raw water quality : rain events, seasonal variations depending on the plant's location and its climate, disturbance in the upstream rivers because of human activities, etc. Climate change can also engender modifications of rivers' water quality in the long run. Some plants around the world are already facing this kind of problem. In the context of the case study, deterioration of the water quality is most often due to rain events so that phenomenon is selected as an example for further investigation. It has to be noticed that the same study principle can be applied by analogy to answer other questions relative to changes of the raw water quality.

6.1 Consequences on treated water quality

Each rain event has a different intensity and duration. In order to build a consistent modelling scenario, discussions have been held with the industrial partner to determine the order of magnitude of these water quality changes.

In the case study, rain events modify organic matter concentration and suspended matter concentration. Suspended and organic matters are drained by the rain which is typical of storm waters. Organic matter concentration is considered to be approximately multiplied twice so the concentration of all corresponding water compounds (UVA, DOC, TOC, BOD, etc) are multiplied twice in the raw water quality of the modelling scenario. Suspended matter concentration is multiplied fivefold as well as turbidity which is proportional to suspended matter concentration.

The table 5-24 shows the treated water quality of different modelling scenarios. Scenario 0 is the ground modelling scenario. Scenario 1 is a modelling scenario considering deteriorated raw water quality and the same operating conditions as the ground modelling scenario (i.e. a modelling scenario where the plant is facing a rain event but no actions have been undertaken). Scenario 2 is a modelling scenario considering deteriorated raw water quality and different operating conditions (i.e. a modelling scenario where the plant is facing a rain event and a number of actions have consequently been undertaken).

Operating conditions are considered to be action levers in this situation (e.g. targeted process performance and relative chemical dose) as opposed to plant design (processes' configuration, equipment sizing, etc).

Table 5-24. Raw and treated water quality in both modelling scenario considering a deteriorated raw water quality and in the ground modelling scenario.

	Raw water quality		Treated water quality		
	Regular situation (scenario 0)	Rain event situation (scenarios 1 & 2)	Scenario 0	Scenario 1	Scenario 2
Turbidity (NTU)	15.0	75.0	0.070	0.283	0.349
UVA (m^{-1})	5.66	11.3	1.16	2.43	0.816
TOC (mg/L)	3.0	6.0	1.20	2.41	1.56
pH	8.0	8.0	7.70	7.70	7.70
Al residual (mg/L)	0.0	0.0	0.0109	0.0176	0.0210
Bromate (µg/L)	0.0	0.0	1.87	1.62	2.33
TTHM (µg/L)	0.0	0.0	8.91	27.0	17.4

The results of scenario 0 have already been discussed since it is the ground modelling scenario. Scenario 1 corresponds to the same plant model except that the water to be treated has a worse quality due to the rain event. Results on treated water quality of scenario 1 are then representative of what would happen if no actions were undertaken during the rain event. Al Residual, Bromate and TTHM are still not an issue in this situation. The turbidity in treated water is significantly increased and its value is above the industrial objective which is 0.1 NTU, but it is below the legal recommended value (0.5 NTU) and the legal limit (1.0 NTU) (table 5-8). It can be considered that turbidity and suspended matter concentration in treated water are not a problem as this is not the regular situation. On the other hand, UVA and TOC values in treated water are far above the industrial objectives and the legal recommended value for TOC (table 5-8). In fact, when the UVA in raw water is above 6 m^{-1}, the industrial objectives are 1.6 g/L for TOC and 1.6 m^{-1} for UVA. Despite these less restrictive industrial objectives, UVA and TOC values in scenario 1 are not satisfactory. It can be concluded that organic matter is an issue for this water treatment plant during a rain event.

The operating conditions must be modified accordingly to cope with this water quality issue. The most adapted process parameters to act effectively on organic matter removal are the DOC removal objectives of both PAC addition and coagulation processes, as confirmed by the technical audit of the plant (CIRSEE 2002). The other process parameters are not modified in the scenario 2.

In scenario 2, DOC removal by PAC addition is changed from 16.5% to 42% and DOC removal by coagulation is changed from 41% to 45%. Theoretically, the maximum DOC removal during the coagulation process is approximately 50% (which is the sum of the humic acids fraction f_{ha} and the non-polar fraction $f_{nonpolar}$ of organic matter). In addition, it has been established that the use of coagulant should be favoured over the use of PAC in order to reduce the environmental impacts related to drinking water production. So one can wonder why the DOC removal objective has not been raised to its maximum.
The last sorbable compounds require much more coagulant to be adsorbed than the first ones because of the adsorption equilibrium. Thus, the DOC removal objective of the coagulation process is not set to its maximum because the previous findings are reversed in this particular situation. Unrealistic coagulant doses would be required and huge amount of sludge would be produced as a consequence.

The resulting treated water quality shown in table 5-24 is satisfactory since the legal limits and industrial objectives are respected (1.6 g/L for TOC and 1.6 m^{-1} for UVA when raw water UVA > 6 m^{-1}).

6.2 Consequences on chemical and electricity consumptions

Chemical and electricity consumptions are necessarily increased. Table 5-25 presents the list of chemical and electricity consumptions in scenarios 0 and 2 (scenario 1 was left aside as it does not provide drinking water).

Table 5-25. Additional chemical and electricity consumptions in the context of a rain event.

	Scenario 0	Scenario 2	Additional consumptions
Soda (g/m^3)	52.6	69.2	31.6 %
Chlorine (g/m^3)	1.21	1.40	15.7 %
PAC (g/m^3)	4.31	20.2	367 %
Aluminium sulphate (g/m^3)	101	155	53.4 %
Flocculant (g/m^3)	0.167	0.235	40.5 %
Hydrated lime (g/m^3)	7.02	26.8	282 %
New GAC (g/m^3)	1.27	1.27	0.0 %
Regenerated GAC (g/m^3)	2.20	2.20	0.0 %
Electricity (kWh/m^3)	0.602	0.607	0.855 %

The functioning of the plant as a consequence of the deterioration of raw water quality generates an increase of all chemical and electricity consumptions. Some of them are strongly increased (e.g. PAC and hydrated lime) so it could be expected that the LCIA results and operational costs will be increased as well.

6.3 Consequences on LCIA results

Additional environmental impacts due to the disturbance caused by the rain event are presented in table 5-26. By comparing the ground modelling scenario and the rain event scenario, it appears clearly that the environmental impacts are highly increased because of the deterioration of the raw water quality.

Table 5-26. Additional environmental impacts in the context of a rain event.

	Scenario 0	Scenario 2	Additional environmental impact
Climate Change (kgCO_2-Eq.)	0.238	0.563	137 %
Total Score (Points)	0.0234	0.0539	131 %

All the chemical consumptions are significantly increased (table 5-25), therefore it is logical to observe the same tendency on LCIA results. Besides, the chemical contributing most to the LCIA results (i.e. PAC) is also the one for which the consumption has most increased. The LCIA results are strongly affected and the environmental impacts of drinking water production are more than doubled in this specific context.

6.4 Consequences on operational costs

The same comparison is made between the two scenarios on operational costs in table 5-27. Operational costs are increased by approximately 40%, which is less than the increase of environmental impacts but still significant.

Table 5-27. Additional operational costs in the context of a rain event.

	Scenario 0	Scenario 2	Additional operational costs
Operational costs (€/m^3)	0.0834	0.116	38.9 %

6.5 Conclusion

As was shown previously, a different raw water quality can lead to different model results and thus to different functioning and performances for the plant. Modifications of the raw water quality can have significant repercussions on the water treatment and they must be anticipated as much as possible. Moreover, when treated water quality does not comply with the regulatory standard, it is mandatory to undertake actions to cope with the deterioration of the raw water quality.

When facing a rain event (as modelled in this case study), the drinking water production within the studied plant requires more energy and chemicals. The environmental impacts and operational costs are highly increased (+137% on ‘Climate Change” impact and +38.9% on operational costs) as a consequence of this natural phenomenon.

At the design stage, several steady-state simulations must be performed representing the set of raw water quality that may be encountered over the plant’s life. A deteriorated raw water quality and its corresponding modelling scenario results can influence the average operating conditions to be planned depending on its frequency of occurrence.

7. Conclusion

In this chapter, the EVALEAU tool has been applied in a pilot study. The studied plant was composed of three process lines in parallel and intersecting recirculation loops, thus making the process network quite complex. The functioning of the plant was very well-known and field data was available because it has been studied for many years by CIRSEE scientists. It was an explicit requirement for this first application of the tool.

The results of the retrofit approach on treated water quality are not accurate except for UVA and TOC thanks to site-specific equations. Nevertheless, the results show that pollutant removals due to water treatment are well assessed and the order of magnitude of the results is acceptable. Water quality modelling is satisfactory for the purpose of the study.

Electricity and chemical consumptions are well forecasted by the predictive plant model except for soda consumption. As a consequence, the LCIA results are well predicted. The “Climate Change” and “Fossil Depletion” impact categories are the ones that contribute most to the total EndPoint score (respectively 46.6% and 36.7%). The “Climate Change” impact is 0.238 kgCO_2-Eq and the “Fossil Depletion” impact is 0.0816 kgOil-Eq in the predictive LCA (instead of 0.212 kgCO_2-Eq and 0.0713 kgOil-Eq in the conventional LCA based on site inventory). The predictive modelling scenario reproduces the regular functioning of the plant and it is established as the ground modelling scenario and used as a basis for further investigations.

Contribution analysis and sensitivity analysis help to detect the main sources of environmental impacts and tagging priority action levers. In the case study, coagulation and PAC addition are the main unit processes to focus on in order to effectively reduce the environmental impacts.

In light of these indications, alternative treatment solutions have been simulated as variants of the ground modelling scenario looking for improvement opportunities. Unfortunately, model uncertainty is roughly evaluated and only tendencies can be deduced from such simulations. No alternative treatment solution clearly stands out because environmental and economic issues are conflicting objectives in all modelling scenarios.

The repercussions of a rain event on the water treatment line and its performances have been assessed. In this context, the environmental impacts are highly increased (+137% on “Climate Change” impact) and operational costs are increased as well (+38.9%).

The retrofit approach can be useful for validating water quality modelling in a case study. In the application case presented in this chapter, site-specific equations have been used for water quality modelling and they strongly improve the accuracy of the results. The EVALEAU tool can efficiently support engineers within an ecodesign perspective but the whole ecodesign process relies on water quality modelling which must be as reliable as possible.

This major issue must be worked out with the scientific community related to water treatment. As already mentioned in chapters 1 and 3, engineering design of water treatment processes is too often based on rules of thumb, engineers' experience and basic experimentation. Therefore, there is a lack of generic descriptions through mechanistic models of physico-chemical phenomena occurring in water treatment. Nevertheless, the models of the EVALEAU library can easily be modified and updated with newly developed and more accurate models.

Considering that water quality modelling is valid, the predictive approach is of particular interest to engineers in charge of designing drinking water treatment plants. Energy and chemical consumptions, operational costs and environmental impacts are well predicted based on technical facts and legal constraints. All these aspects are fully integrated in the EVALEAU tool. As the LCIA results are obtained together with the technical and economic ones, the tool can support a genuine ecodesign process. Moreover, contribution analysis and sensitivity analysis make the behaviour of the plant model more understandable and they consequently tag priority action levers and bring out guidelines for the ecodesign process.

Alternative treatment solutions can be investigated in the quest for better plant performances. Technical feasibility must be taken into consideration so that the proposed alternative scenarios are realistic.

The technical procedure for process ecodesign, proposed in this research work, has been put into practice in this case study. Unfortunately, it did not reveal any unquestionable ecodesign opportunities for the studied plant. Indeed, environmental and economic objectives were found to be conflicting in all the alternative scenarios that were investigated. It must be noted that this is logical since the functioning of the plant has been studied and optimised for many years by engineers and researchers of Suez Environnement.

Nevertheless, this procedure is relevant and well-adapted for the design of drinking water treatment plants, and more generally for the design of process plants. It could provide a means of introducing ecodesign practices in the process industry with minimum effort and reluctance from engineers in charge of plant design since it is close to conventional design practices.

Consequences of the deterioration of raw water quality on the plant's performances have been demonstrated to be very significant at least in the context of the case study. Both environmental and economic performances are normally worsened because of a disturbance like a rain event. A rain event has been simulated as an example of raw water quality deterioration but the same study principle can be applied to anticipate other modifications of raw water quality. Dynamic LCA study can also be performed analogously : varying raw water quality leading to varying LCIA results and operational costs.

Conclusion and prospects

Conclusion et perspectives [FR]

Les objectifs du travail de recherche présentés dans cette thèse étaient le développement d'un outil intégré pour la modélisation des procédés et l'analyse de cycle de vie, ainsi que la formulation d'une approche méthodologique affiliée pour l'écoconception des procédés. L'outil logiciel et l'approche méthodologique sont appliqués à la production d'eau potable.

La revue de la littérature scientifique, présentée au chapitre 1, révéla un besoin flagrant d'efforts de recherche concernant d'une part, l'application de la méthodologie d'analyse de cycle de vie dans l'industrie des procédés, et d'autre part, la modélisation des procédés physico-chimiques dans l'industrie de l'eau. De fait, le manque de modèles génériques et flexibles dans l'industrie des procédés empêche les praticiens de l'analyse de cycle de vie d'étudier l'influence du dimensionnement et des conditions opératoires des procédés unitaires. L'empirisme des approches de modélisation dans le traitement de l'eau pose également problème. La communauté scientifique devrait s'attaquer à ces problèmes. C'est un prérequis incontournable à l'introduction de pratiques d'écoconception dans l'industrie de l'eau. Les principales lignes directrices pour le projet de recherche furent donc clairement établies en fonction de la revue de la littérature scientifique.

Un outil intégré pour la modélisation des procédés et l'analyse de cycle de vie (nommé EVALEAU) fut élaboré pour la première fois dans l'industrie des procédés, consacré au traitement de l'eau. Le chapitre 2 introduisit l'outil EVALEAU, ses caractéristiques spécifiques et les approches de modélisation associées. La bibliothèque logicielle est sans aucun doute le socle de cet outil, mais la boite à outils pour l'analyse de sensibilité est de loin son composant le plus innovant. L'utilisation originale qui est faite de l'analyse de sensibilité apparaît comme très novatrice dans le domaine de l'analyse de cycle de vie et de l'écoconception des procédés. En effet, la méthode de Morris fournit des informations significatives sur le fonctionnement d'un système de procédés, et ce de façon très simple, facilitant ainsi grandement la tâche d'écoconception.

Les approches rétrospective et prédictive sont toutes deux disponibles pour la plupart des modèles de procédés unitaires. La première est plus descriptive et la deuxième plus prospective, et par conséquent plus instructive. Le fort paramétrage et la généricité des modèles de procédés unitaires renforcent considérablement leur flexibilité et permettent de coller à la réalité industrielle d'un projet en tenant compte des contraintes techniques et des choix de conception et de dimensionnement.

Une procédure technique pour l'écoconception des procédés fut formulée à la fin du chapitre afin de définir explicitement l'approche méthodologique proposée pour mettre en œuvre l'écoconception dans l'industrie des procédés.

Le chapitre 3 décrivit tout d'abord la modélisation mathématique des procédés unitaires du point de vue de l'ingénierie logicielle. Le langage de programmation Python^{TM} fut introduit en présentant ses caractéristiques les plus pertinentes pour la recherche scientifique. Les différents fichiers impliqués dans la modélisation d'un procédé unitaire et leur relation furent ensuite expliquées.

Puis, les fonctions génériques, largement utilisées par les modèles de procédés unitaires, furent présentées en détail du point de vue mathématique. La modélisation du procédé de coagulation fut abordée avec une attention toute particulière, comme cela est recommandé dans la littérature scientifique (chapitre 1), par l'adoption d'un modèle mécanistique récemment développé. Un astucieux complément à ce modèle de coagulation fut même proposé pour l'améliorer. L'intégralité du travail de modélisation est présentée dans une annexe dédiée, visant à garantir la transparence.

Le chapitre 4 présenta dans un premier temps une synthèse des concepts fondamentaux et des caractéristiques spécifiques de l'outil EVALEAU. La première étude pilote réalisée grâce à l'outil fut ensuite présentée et les résultats commentés. Cette étude de cas se concentrait davantage sur la validation des résultats de la modélisation que sur leur interprétation, de sorte que la pertinence et la crédibilité de l'approche s'en trouvèrent corroborées.

La comparaison des résultats de modélisation avec les données de terrain permirent d'évaluer l'incertitude du modèle de l'usine étudiée, qui s'avéra acceptable. En effet, la modélisation de la qualité de l'eau fut satisfaisante par rapport aux objectifs d'une telle étude. Les bilans matière et énergie furent aussi calculés avec une précision acceptable (les erreurs de prédiction étaient inférieures à 10% pour toutes les consommations de réactifs et d'énergie).

Le chapitre 5 présenta une étude bien plus approfondie d'une usine de production d'eau potable située dans la région parisienne. Cette usine était composée de plusieurs chaines de procédés en parallèle ainsi que de nombreuses boucles de recirculation, rendant ainsi ce réseau de procédés très complexe. La procédure technique pour l'écoconception des procédés, suggérée au chapitre 2, fut mise en pratique dans cette étude cas.

Tout d'abord, l'approche rétrospective fut utilisée pour valider la modélisation de la qualité l'eau, sur la base de données de site concernant la qualité moyenne de l'eau et les doses moyennes de doses de réactifs utilisées au cours de l'année de référence. Puis, un modèle d'usine, reproduisant la réalité du terrain, fut établi à l'aide de l'approche prédictive. Ce modèle prédictif fut considéré comme le scénario de base et servit à des analyses ultérieures.

Les analyses de contribution et de sensibilité furent mises en œuvre sur ce scénario de base pour identifier les leviers d'action prioritaires pour l'amélioration des performances environnementales de l'usine. On s'aperçut que la consommation de PAC était la principale source d'impact environnemental. Néanmoins, la démonstration fut faite avec la méthode de Morris que les objectifs d'abattement de DOC des procédés de coagulation et d'ajout de PAC étaient les principaux leviers d'action pour réduire les impacts environnementaux générés par la production d'eau potable dans l'usine étudiée, quelle que soit la catégorie d'impact considérée dans la méthode d'évaluation Recipe.

A la lumière de ces indications, des solutions alternatives de traitement furent envisagées, à la recherche d'opportunités d'amélioration des points de vue environnemental et/ou économique. Malheureusement, aucune de ces solutions alternatives ne peut améliorer simultanément les performances environnementales et économiques de l'usine. L'outil EVALEAU apporte seulement une aide au processus de prise de décision, et il est certainement difficile de trouver un compromis satisfaisant dans de tels cas.

Dans la dernière partie de cette étude, l'influence de la qualité de la ressource fut étudiée à travers la simulation d'un épisode pluvieux provoquant la détérioration de la qualité de l'eau brute. Il fut démontré que, dans le contexte de l'usine étudiée, cela peut accroitre de manière significative aussi bien les impacts environnementaux que les coûts opérationnels. Cela doit être pris en compte lors du dimensionnement d'une usine si cette situation est récurrente.

La fiabilité de l'outil EVALEAU, en matière de modélisation de la qualité de l'eau et de prédiction des consommations de matériaux est sans conteste la clé essentielle pour son acceptation par les ingénieurs qui ont pour mission de concevoir les usines de production d'eau potable. Par conséquent, l'incertitude des modèles doit être soigneusement considérée et une attention minutieuse doit être consacrée à ce problème.

L’incertitude du modèle fut évaluée dans les deux études de cas. Etant donné que les ingénieurs n'auraient pas prédit avec plus de précision les consommations de réactifs et d’énergie, l’incertitude des deux usines modélisées est considérée comme acceptable.
Ceci est une exigence obligatoire en général pour tous les outils d'écoconception de procédés, car si l’incertitude des modèles de procédés unitaires est pire que la connaissance empirique des ingénieurs, ils ne s'appuieront jamais sur de tels outils pour mener à bien leur tâche.

La bibliothèque EVALEAU doit continuellement être complétée par de nouveaux modules, notamment pour des procédés unitaires qui manquent actuellement. Par exemple, les technologies membranaires pour le dessalement (par exemple l'osmose inverse) ont vu leur intérêt grandir ces dernières décennies, du fait qu'elles permettent d'utiliser une ressource alternative et abondante : l'eau de mer. Ces technologies sont de plus en plus utilisées pour la production d'eau potable dans différentes régions du monde. Leurs performances environnementales sont souvent mises en doute et c’est pourquoi ces technologies devraient absolument être prises en compte dans des versions futures de l'outil.

Les modèles de procédés unitaires existants pourraient être améliorés, par exemple

- en remplaçant les modèles empiriques par des modèles mécanistiques (ex. les modèles d'adsorption)
- en incluant une description plus détaillée des phénomènes physico-chimiques, et ainsi en incluant davantage de paramètres opératoires dans l'évaluation environnementale.

Plus généralement, les modèles de procédés unitaires dans la bibliothèque logicielle doivent être représentatifs des technologies réellement utilisées dans l'industrie. Lorsque des avancées technologiques sont accomplies et que des procédés innovants sont développés, la bibliothèque logicielle devrait aussi être enrichie si l'on veut qu'elle reste cohérente et représentative des technologies industrielles utilisées sur le terrain.

EVALEAU est un outil prometteur pour une industrie de l'eau durable. Ce travail n'a pas révélé tout son potentiel. Il pourrait être utilisé à différents niveaux, depuis l’affichage environnemental jusqu'à l’optimisation des paramètres opératoires. Dans le contexte de pénurie grandissante et de dégradation des ressources en eau, et alors que des procédés de traitement de plus en plus complexes sont élaborés, l'utilisation d'un outil de contrôle visant à limiter les impacts environnementaux devient une nécessité. L'outil EVALEAU peut apporter une aide concrète à de tels projets en vue d'un choix technique raisonné.

Conclusion and prospects [EN]

The main objectives of the research work, presented in this Ph.D. dissertation, were the development of an integrated tool for Process Modelling & Life Cycle Assessment as well as the formulation of an affiliated methodological approach for process ecodesign. The software tool and the methodological approach were meant to be applied to drinking water treatment.

The literature review, presented in chapter 1, revealed a blatant need for research efforts concerning the application of LCA methodology in the process industry on the one hand, and the modelling of physico-chemical processes in the water industry on the other hand. Indeed, the lack of generic and flexible models in the process industry prevents LCA practitioners from studying the influence of engineering design and operating conditions of unit processes. The empiricism of modelling approaches in water treatment is problematic as well. These issues should be tackled by the scientific community. This is a prerequisite, which cannot be ignored, for introducing ecodesign practices in the water industry. The main guidelines for the research project were then clearly stated in view of the lessons learned from the literature review.

A fully integrated Process Modelling-LCA tool (named EVALEAU) was developed for the first time in the field of process industry, dedicated to water treatment industry. Chapter 2 introduced the EVALEAU tool, its special features and the related modelling approaches. The computational library is no doubt the bedrock of the tool, but the sensitivity analysis toolbox is by far the most innovative component of the framework. The original use of sensitivity analysis is believed to be groundbreaking for the scientific field of LCA and process ecodesign. Indeed, the Morris method brings meaningful information about the functioning of a process system with great simplicity, and therefore facilitates the ecodesign task considerably.

The retrofit and predictive approaches are both available for most unit process models. The first is more descriptive and the latter is more prospective, and consequently more instructive. The high parameterization and the genericity of the unit process models strongly enhance

their flexibility and make it possible to stick to the industrial reality of a project by taking into account technical constraints and engineering design choices.
A technical procedure for process ecodesign was formulated at the end of the chapter in order to define explicitly the methodological approach proposed for performing ecodesign in the process industry.

Chapter 3 first described the mathematical modelling of unit processes from a software engineering point of view. The Python^{TM} programming language was introduced through a discussion of its relevant features for scientific research. The different files involved in the modelling of one unit process and their relationship were explained.
Then, the generic functions, widely used by the unit process models, were presented in detail from a mathematical point of view. The modelling of the coagulation process was tackled with particular attention, as recommended in the literature (chapter 1), by adopting a recently developed mechanistic model. A smart completion of this coagulation model was even proposed to improve it. The integral modelling work is presented in a dedicated appendix as a guarantee of transparency.

Chapter 4 presented a synthesis of the embedded concepts and special features of the EVALEAU tool as a first step. The first pilot study performed using the tool was then presented and the results were discussed. This short case study focused more on the validation of modelling results rather than on their interpretation, so that the relevance and the credibility of the modelling approach were borne out.
The comparison of modelling results with field data made it possible to evaluate the uncertainty of the plant model, which was shown to be acceptable. Indeed, water quality modelling was satisfactory considering the purpose of such a study. Mass and energy balances were calculated with reasonable accuracy as well (prediction errors were less than 10% for all energy and chemical consumptions).

Chapter 5 presented an in-depth study of a drinking water treatment plant located in the Paris area. The plant was composed of several process lines with intersecting recirculation loops, thus making this process network quite complex. The technical procedure for process ecodesign, suggested in chapter 2, was put into practice in this case study.
First, the retrofit approach was used to validate water quality modelling, based on field data concerning average water quality and average chemical doses over the reference year. Then, a

plant model, reproducing the field reality, was established with the predictive approach. This prospective plant model was considered to be the ground modelling scenario and served as a basis for further investigations.

Contribution and sensitivity analyses were then performed on this ground scenario in order to detect and tag the priority action levers for improving the environmental performances of the plant. PAC consumption was found to be the major source of environmental impacts. Nevertheless, it was demonstrated with the Morris method that DOC removal objectives of PAC addition and coagulation processes were the main action levers for reducing the environmental impact generated by drinking water production within the plant under study, regardless of the impact category considered in the Recipe evaluation method.

In the light of these indications, alternative treatment solutions were envisaged, seeking for improvement opportunities from environmental and/or economic points of view. Unfortunately, none of these alternative treatment solutions can improve simultaneously environmental and economic performances of the plant. The EVALEAU tool only supports the decision-making process and it is certainly difficult to find a suitable trade-off in such cases.

In the last part of this study, the influence of source water quality was investigated through the simulation of a rain event causing the deterioration of raw water quality. It was shown that, in the context of the studied plant, it can significantly increase both the environmental impacts and the operational costs of drinking water production. Such facts should be taken into consideration at early design stage if this is to be a recurrent situation.

The reliability of the EVALEAU tool, in terms of water quality modelling and material consumption forecasting, is certainly the most essential key for its acceptance by water engineers in charge of designing water treatment plants. Therefore, the uncertainty of models should be carefully considered and close attention must be devoted to this issue.

The uncertainty of the plant model was estimated in the two case studies. As water engineers would not have better predicted energy and chemical consumptions, the degree of uncertainty of both plant models is considered acceptable.

This is a compulsory requirement in general for process ecodesign tools because if the uncertainty of the unit process models is worse than the empirical know-how of process engineers, they will never rely on such tools for achieving their task.

The EVALEAU library must be continuously complemented with new modules for currently missing unit processes. For instance, membrane-based technologies for desalination (e.g. reverse osmosis) have gained interest in the last decades, since they allow using an alternative and abundant water resource : sea water. Those technologies are increasingly used for drinking water production in different regions of the world. Their environmental performances are often questioned and they should definitely be considered in future versions of the tool.

The existing unit process models could be improved, as for example by :

- replacing empirical ones by mechanistic models (e.g. the adsorption models).
- including more detailed description of physico-chemical phenomena and thus including more process parameters in environmental assessment.

More generally, the unit process models of the computational library must be representative of the technologies actually used in industry. In case technological breakthroughs are achieved and innovative unit processes are developed, the computational library should be expanded as well if it is to remain consistent and representative of industrial technologies used on the field.

EVALEAU is a promising tool for a sustainable water industry. Its potential was not fully revealed in this work. It could be used at different levels, going from environmental labelling to the tuning of operation parameters. In the context of the growing scarcity and degradation of water resources, when more and more sophisticated treatment processes are designed, the use of a control tool for limiting the potential environmental burdens becomes a necessity. The EVALEAU tool can assist such projects in making a reasoned technical choice.

References

Agile Manifesto website, http://www.agilemanifesto.org. Accessed on September 10th, 2012.

Althaus HJ, Bauer C, Doka G, Dones R, Frischknecht R, Hellweg S, Humbert S, Jungbluth N, Köllner T, Loerincik Y, Margni M, Nemecek T (2010) Implementation of Life Cycle Impact Assessment Methods, Data version 2.2. Ecoinvent report n°3, Swiss Centre for Life Cycle Inventories.

Althaus HJ, Doka G, Dones R, Heck T, Hellweg S, Hischier R, Nemecek T, Rebitzer G, Spielmann M, Wernet G (2007) Overview and Methodology, Data version 2.0. Ecoinvent report n°1, Swiss Centre for Life Cycle Inventories.

Antonini G (2007) Lits fluidisés - Caractéristiques générales et applications. Edition Techniques de l'Ingénieur BE 8255.

Azapagic A, Clift R (1999) The application of life cycle assessment to process optimization. Comput Chem Eng 23(10):1509-1526.

Azapagic A, Millington A, Collett A (2006) A methodology for integrating sustainability considerations into process design. Chem Eng Res Des 84(A6):439-452.

Bakshi BR, Fiksel J (2003) The quest for sustainability : challenges for process systems engineering. AICHE J 49(6):1350-1358.

Ban-Ki Moon (2008) Address by the UN Secretary-General to the session “Time is Running Out on Water” to the Davos World Economic Forum, January 24th, 2008, Switzerland. http://www.un.org/apps/news/infocus/sgspeeches/search_full.asp?statID=177. Accessed on September 10th, 2012

Baratto F, Diwekar UM (2005) Life cycle assessment of fuel cell-based APUs. J Power Sources 139(1-2):188-196.

Bare J (2010) Life cycle impact assessment research developments and needs. Clean Techn Environ Policy 12(4):341-351.

Barrios R, Siebel M, van der Helm A, Bosklopper K, Gijzen H (2006) Environmental and financial life cycle impact assessment of drinking water production at Waternet. J Clean Prod 16(4):471-476.

Baudin I, Cagnard O, Grandguillaume JJ, Do-Quang Z (2007) Algae and associated toxins and metabolites : methodology for risk assessment and risk management. Proceedings of the AWWA Annual Conference, Toronto, Ontario, Canada, IWA Publishing.

Benetto E, Nguyen D, Lohmann T, Schmitt B, Schosseler P (2009) Life cycle assessment of ecological sanitation system for small-scale wastewater treatment. Sci Total Environ 407(5):1506-1516.

Bernier E, Maréchal F, Samson R (2012) Optimal greenhouse gas emissions in NGCC plants integrating life cycle assessment. Energy 37(1):639-648.

Bianchi SR, Miyazawa M, de Oliveira EL, Pavan MA (2008) Relationship between the Mass of Organic Matter and Carbon in Soil. Braz Arch Biol Techn 51(2):263-269.

Bojarski AD, Guillén-Gosálbez G, Jiménez L, Espuna A, Puigjaner, L (2008) Life Cycle Assessment coupled with process simulation under uncertainty for reduced environmental impact : application to phosphoric acid production. Ind Eng Chem Res 47(21):8286-8300.

Boulay AM, Bouchard C, Bulle C, Deschênes L, Margni M (2011a) Categorizing water for LCA inventory. Int J Life Cycle Ass 16(7):639-651.

Boulay AM, Bulle C, Bayart JB, Deschênes L, Margni M (2011b) Regional characterization of freshwater use in LCA : modeling direct impacts on human health. Environ Sci Technol 45(20):8948-8957.

Bratby J (2006) Coagulation and flocculation in water and wastewater treatment. IWA Publishing 2nd edition.

Burgess AA, Brennan DJ (2001) Application of life cycle assessment to chemical processes. Chem Eng Sci 56(8):2589-2604.

Campolongo F, Cariboni J, Saltelli A (2007) An effective screening design for sensitivity analysis of large models. Environ Modell Softw 22(10):1509-1518.

Campos C and Harmant P (2002) Assessing the impact of dissolved organic carbon changes on disinfectant stability in a distribution system. Proceedings of the IWA Conference, World Water Congress on water and health, microbiology, monitoring and disinfection 2(3):251-257.

Cariboni J, Gatelli D, Liska R, Saltelli A (2007) The role of sensitivity analysis in ecological modelling. Ecol Model 203(1-2):167-182.

Carvill J (1993) Mechanical Engineer's Data Handbook. Elsevier Science Ltd, 1st edition.

Chen NH (1979) An explicit equation for friction factor in pipes. Ind Eng Chem Fundam 18(3):296-297.

Chen YN, McRae GJ, Gleason KK (2004) Integrating Life Cycle Analysis (LCA) with Process Modeling. In: 2004 AICHE Annual Meeting, conference proceedings, Austin Texas, November 7-12, http://www.nt.ntnu.no/users/skoge/prost/proceedings/aiche-2004/begin.pdf. Accessed on March 20th 2012.

Chen YN, McRae GJ, Gleason KK (2004) Integrating Life Cycle Analysis (LCA) with Process Modeling. Conference proceeding of the AICHE Annual Meeting, Austin Texas, November 7-12, 2004, http://www.nt.ntnu.no/users/skoge/prost/proceedings/aiche-2004/begin.pdf. Accessed on March 20th, 2012.

CIRSEE (1999) Pratique Recommandée - Clarification. Internal document, CIRSEE, Direction Technique de la Recherche (Lyonnaise des Eaux).

CIRSEE (2002) Audit du fonctionnement de l'usine de xxxxx. Internal document, CIRSEE, Pôle Qualité Eau.

CIRSEE (2007) Guide technique pour la gestion et la prospection de voies de valorisation des résidus d'eau potable. Internal document, CIRSEE, Direction Technique de la Recherche (Lyonnaise des Eaux).

CIRSEE (2009) Pratique Recommandée - Désinfection. Internal document, CIRSEE, Direction Technique de la Recherche (Lyonnaise des Eaux).

Clamond D (2009) Efficient Resolution of the Colebrook Equation. Ind Eng Chem Res 48(7):3665-3671.

Confalonieri R, Bellocchi G, Bregaglioa S, Donatelli M, Acutisa M (2010) Comparison of sensitivity analysis techniques : A case study with the rice model WARM. Ecol Model 221(16):1897-1906.

Degrémont (2007) Water Treatment Handbook. Degrémont, Lavoisier 10th edition.

Dietz A, Azzaro-Pantel C, Pibouleau L, Domenech S (2006) Multiobjective optimization for multiproduct batch plant design under economic and environmental considerations. Comput Chem Eng 30(4):599-613.

Dudley J, Dillon G, Rietveld LC (2008) Water treatment simulators. J Water Supply Res T 57(1):13-21.

Edwards M (1997) Predicting DOC removal during enhanced coagulation. J Am Water Works Ass 89(5):78-89.

Engineering tool box website, http://www.engineeringtoolbox.com/air-solubility-water-d_639.html. Accessed on May 23rd, 2011.

Ernzer M, Lindahl M, Masui K, Sakao T (2003) An international study on utilization of design for environment methods (DfE) - a prestudy. Conference proceeding of the 3rd International Symposium on Environmentally Conscious Design and Inverse Manufacturing, December 8-11, 2003.

Faust SD, Aly OM (1998) Chemistry of Water Treatment. Ann Arbor Press, Inc. 2nd edition.

Finnveden G, Hauschild MZ, Ekvall T, Guinée J, Heijungs R, Hellweg, S, Koehler A, Pennington D, Suh S (2009) Recent developments in life cycle assessment. J Environ Manag 91(1):1-21.

French drinking water standard (2001) Décret n°2001-1220 du 20 Décembre 2001 et code de la santé publique, relatifs aux eaux destinée à la consommation humaine.

French legislation relative to water pumping stations. Article 37 du fascicule 73 (équipement hydraulique, mécanique et électrique des stations de pompage d eau) du Cahier des Clauses Techniques Générales (CCTG) des marchés publiques de travaux.

Friedrich E (2001) Environmental Life Cycle Assessment of potable water production. Ph.D. Dissertation, University of Natal, South Africa.

Friedrich E (2002) Life-cycle assessment as an environmental management tool in the production of potable water. Water Sci Technol 46(9):29-36.

Furuholt E (1995) Life cycle assessment of gasoline and diesel. Resour Conserv Recycl 14(3-4):251-263.

Gagnon C, Grandjean BPA, Thibault J (1997) Modelling of coagulant dosage in a water treatment plant. Artif Intell Eng 11(4):401-404.

Gerber L, Gassner M, Maréchal F (2011) Systematic integration of LCA in process systems design : application to combined fuel and electricity production from lignocellulosic biomass. Comput Chem Eng 35(7):1265-1280.

Goedkoop M, Heijungs R, Huijbregts M, Schryver AD, Struijs J, van Zelm R (2009) ReCiPe 2008 : A life cycle impact assessment method which comprises harmonized category indicators at the midpoint and the endpoint level. First edition, Report I : Characterisation. Ruimte en Milieu.

Grossmann IE, Chen B, Arthur WW (2004) Challenges in the new millennium : product discovery and design, enterprise and supply chain optimization, global life cycle assessment. Comp Chem Eng 29(1):29-39.

Grossmann IE, Guillén-Gosálbez G (2010) Scope for the application of mathematical programming techniques in the synthesis and planning of sustainable processes. Comp Chem Eng 34(9):1365-1376.

Grossmann IE, Westerberg AW (2000) Research challenges in process systems engineering. AICHE J 46(9):1700-1703.

Guibelin E (1999) Lutte contre la pollution des eaux - Traitements des boues d'épuration. Edition Techniques de l'Ingénieur G1450.

Guillén-Gosálbez G, Caballero J, Jiménez L (2008) Application of Life Cycle Assessment to the Structural Optimization of Process Flowsheets. Ind Eng Chem Res 47(3):777-789.

Hamby DM (1994) A review of techniques for parameter sensitivity analysis of environmental models. Environ Monit Assess 32(2):135-154.

Harold MP, Ogunnaike BA (2000) Process engineering in the evolving chemical industry. AICHE J 46(11):2123-2127.

Harrington, GW Chowdhury ZK, Owen DM (1992) Developing a computer model to simulate DBP formation during water treatment. J. Am. Water Works Assoc. 84(11):78-87.

Iglesias Jimenez E, Perez Garcia V (1992) Relationships between Organic Carbon and Total Organic Matter in Municipal Solid Wastes and City Refuse Composts. Bioresource Technol 41(3):265-272.

Igos E, Benetto E, Dalle A, Tiruta-Barna L, Baudin I, Méry Y (2012) Life cycle assessment of water treatment : the role of infrastructure vs. operation at unit process level. Sumitted to Cleaner production.

Igos E, Benetto E, Tiruta-Barna L, Baudin I, Méry Y (2012) Cost-performance indicator for comparative assessment of water treatment plants. Sci Total Env, accepted.

Iosif A-M, Hanrot F, Birat J-P, Ablitzer D (2010) Physicochemical modelling of the classical steelmaking route for life cycle inventory analysis. Int J Life Cycle Ass 15(3):304-310.

ISO Standard 14040 (2006) NF EN ISO 14040:2006 - Environmental management - life cycle assessment - principles and framework. AFNOR.

ISO Standard 14062 (2003) XP ISO/TR 14062:2002 - Environmental management - integrating environmental aspects into product design and development. AFNOR.

Jacquemin L, Pontalier P-Y, Sablayrolles C (2012) Life Cycle Assessment (LCA) applied to the process industry : a review. Int J Life Cycle Assess 17(8):1028-1041.

Jolliet O, Margni M, Charles R, Humbert S, Payet J, Rebitzer G, Rosenbaum R (2003) IMPACT 2002+ : A New Life Cycle Impact Assessment Methodology. Int J Life Cycle Ass 8(6):324-330.

Karassik I, Messina J, Cooper P, Heald C (2010) Pump Handbook. McGraw-Hill Publishing, 4th edition.

Kastl G, Sathasivan A, Fisher I (2008) Modeling DOC removal by enhanced coagulation. Research report n°57, Cooperative Research Centre for Water Quality and Treatment.

Kastl G, Sathasivan A, Fisher I, Van Leeuwen J (2004) Modeling DOC removal by enhanced coagulation. J Am Water Works Assoc 96(2):79-89.

Khan F I, Natrajan B R, Revathi P (2001) GreenPro : a new methodology for cleaner and greener process design. J Loss Prevent 14(4):307-328.

Kikuchi Y, Mayumi K, Hirao M, Ferraris GB (2010) Integration of CAPE and LCA tools in environmentally-conscious process design : a case study on biomass-derived resin. Conference proceeding of the 20th European Symposium on Computer Aided Process Engineering 28:1051-1056.

Kniel GE, Delmarco K, Petrie JG (1996) Life cycle assessment applied to process design : environmental and economic analysis and optimization of a nitric acid plant. Environ Prog 15(4):221–228.

Lundie S, Peters GM, Beavis PC (2004) Life Cycle Assessment for sustainable metropolitan waters systems planning. Environ Sci Technol 38(13):3465-3473.

Lundin M, Bengtsson M, Molander S (2000) Life Cycle Assessment of Wastewater Systems : Influence of System Boundaries and Scale on Calculated Environmental Loads. Environ Sci Technol 34(1):180-186.

Maier HR, Morgan N, Chow CWK (2003) Use of artificial neural networks for predicting optimal alum doses and treated water quality parameters. Environ Modell Softw 19(5):485-494.

Masschelein WJ (1991) Ozone et ozonation des eaux. Lavoisier, 2nd edition.

Masson C (2005) Du bon dimensionnement des canalisations / Proper pipe sizing. L' Eau, l'industrie, les nuisances, 284:45-49.

Meier MA (1997) Eco-efficiency of waste gas purification systems in the chemical industry. Ph.D. Dissertation, Swiss Federal Institute of Technology, Zürich, Switzerland.

Milà i Canals L, Chenoweth J, Chapagain A, Orr S, Antón A, Clift R (2008) Assessing freshwater use impacts in LCA : Part I - inventory modelling and characterisation factors for the main impact pathways. Int J Life Cycle Ass 14(1):28-42.

Morris MD (1991) Factorial sampling plans for preliminary computational experiments. Technometrics 33(2):161-174.

Muñoz I, Milà i Canals L, Fernández-Alba AR (2010) Life Cycle Assessment of water supply plans in Mediterranean Spain. J Ind Ecol 14(6):902-918.

NumPy website, http://numpy.scipy.org/. Accessed on October 15th, 2012.

Oberlin C, Girault A, Le Boulch M, Jaume R, Bourgeois J-F (2005) Fours électriques à résistances - Présentation générale. Edition Techniques de l'Ingénieur D5910.

OECD (2008) OECD Key Environmental Indicators. Environment directorate of the Organisation for Economic Development and Co-operation, Paris, France.

Ouattara A, Pibouleau L, Azzaro-Pantel C, Domenech S, Baudet P, Yao P (2011) Economic and environmental strategies for process design. Comput Chem Eng 36(2012):174-188.

Parkhurst D L, Appelo C A J (1995) User's Guide to PHREEQC - a computer program for speciation, reaction-path, advective-transport and inverse geochemical calculations. U.S. Geological Survey, Water-Resources Investigations Report 95-4227, Lakewood, Colorado.

Pearce D, Atkinson G, Mourato S (2006) Cost-benefit analysis and the environment : recent developments. Organisation for Economic Co-operation and Development, Paris.

Pennington DW, Potting J, Finnveden G, Lindeijer E, Jolliet O, Rydberg T, et al. (2004) Life cycle assessment Part 2 : current impact assessment practice. Environ Int 30(5):721-739.

Perie C, Ouimet R (2008) Organic carbon, organic matter and bulk density relationships in boreal forest soils. Can J Soil Sci 88(3):315-325.

Pfister S, Koehler A, Hellweg S (2009) Assessing the environmental impacts of freshwater consumption in LCA. Env Sci Technol 43(11):4098-4104.

PHREEQC website, http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc. Accessed on October 2nd, 2012.

Portha JF, Jaubert JN, Louret S, Pons MN (2010) Life cycle assessment applied to naphtha catalytic reforming. Oil Gas Sci Technol 65(5):793-805.

Python website, http://www.python.org/. Accessed on October 15th, 2012.

Raluy RG, Serra L, Uche J (2005a) Life Cycle Assessment of water production technologies - Part 1 : LCA of different commercial technologies (MSF, MED, RO). Int J Life Cycle Ass 10(4):285-293.

Raluy RG, Serra L, Uche J, Valero A (2005b) Life Cycle Assessment of Water Production Technologies - Part 2 : Reverse Osmosis Desalination versus the Ebro River Water Transfer. Int J Life Cycle Ass 10(5):346-354.

Rebitzer G, Ekvall T, Frischknecht R, Hunkeler D, Norris G, Schmidt W-P, et al. (2004) Life cycle assessment Part 1 : goal and scope definition, inventory analysis, and applications. Environ Int 30(5):701-720.

Renou S, Thomas J-S, Aoustin E, Pons M-N (2007) Influence of impact assessment methods in wastewater treatment LCA. J Clean Prod 16(10):1098-1105.

Roustan M, Debellefontaine H, Do-Quang Z, Duguet J-P (1998) Development of a method for the determination of ozone demand of a water. Ozone Sci Eng 20(6):513-520.

Sadiq R, Rodriguez MJ (2003) Disinfection by-products (DBPs) in drinking water and predictive models for their occurrence : a review. Sci Total Environ 321(1-3):21-46.

Saltelli A, Ratto M, Andres T, Campolongo F, Cariboni J, Gatelli D, Saisana M, Tarantola S (2008) Global Sensitivity Analysis - The Primer. John Wiley & Sons Ltd, 1st edition.

SciPy website, http://www.scipy.org/. Accessed on October 15th, 2012.

SimLab website, http://simlab.jrc.ec.europa.eu. Accessed on October 2nd, 2012.

Smeets P, Rietveld L, Hijnen W, Medema G, Stenström T-A (2006) Efficacy of water treatment processes - Report of the Microrisk project. European Union project on microbiological risk assessment (http://www.microrisk.com).

Sombekke HDM, Voorhoevea DK, Hiemstrab P (1997) Environmental impact assessment of groundwater treatment with nanofiltration. Desalination 113(2-3):293-296.

Sroufe R, Curkovic S, Montabon F, Melnyk S (2001) The new product design process and design for environment - “crossing the chasm”. Int J Oper Prod Man 20(2):267-291.

Sugiyama H, Fischer U, Hungerbühler K, Hirao M (2008) Decision Framework for Chemical Process Design Including Different Stages of Environmental, Health, and Safety Assessment. AICHE J 54(4):1037-1053.

Tapia M, Siebel MA, van der Helm AWC, Baars ET, Gijzen HJ (2006) Environmental, financial and quality assessment of drinking water processes at Waternet. J Clean Prod 16(4):401-409.

Telzhensky M, Birnhack L, Lehmann O, Windler E, Lahav O (2011) Selective separation of seawater Mg^{2+} ions for use in downstream water treatment processes. Chem Eng J 175(2011):136-143.

Thermoddem database website, http://thermoddem.brgm.fr. Accessed on September 14th, 2012.

Tseng T, Edwards M (1999) Predicting full-scale TOC removal. J Am Water Works Ass 91(4):159-170.

UNEP (2002) Sustainable Consumption and Cleaner Production. United Nations Environment Programme, Division of Technology, Industry and Economics. United Nations Publishing.

UNESCO (2009) The United Nations World Water Development Report 3 : Water in a changing world. UNESCO Publishing.

United Nations (1987) Report of the World Commission on Environment and Development : Our Common Future. United Nations Publishing.

US Department of Energy (2003) Improving Compressed Air System Performance : a Sourcebook for Industry. Accessed on February 20th, 2011, at the website http://www1.eere.energy.gov/manufacturing/tech_deployment/pdfs/compressed_air_sourcebook.pdf

van Leeuwen J, Holmes M, Kaeding U, Daly R, Bursill D (2009) Development and implementation of the software mEnCo© to predict coagulant doses for DOC removal at full-scale WTPs in South Australia. J Water Supply Res T 58(4):291-298.

Vince F, Aoustin E, Breant P, Maréchal F (2008a) LCA tool for the environmental evaluation of potable water production. Desalination 220(1-3):37-56

Vince F, Maréchal F, Aoustin E, Breant P (2008b) Multi-objective optimization of RO desalination plants. Desalination 222(1-3): 96-118

Vlasopoulos N, Memon FA, Butler D, Murphy R (2006) Life cycle assessment of wastewater treatment technologies treating petroleum process waters. Sci Total Environ 367(1):58-70.

Wang LK, Shammas NK, Hung YT (2007) Biosolids treatment processes : Handbook of Environmental Engineering volume 6. Humana Press Inc.

Weidema B, Hischier R, Althaus HJ, Bauer C, Doka G, Dones R, Frischknecht R, Jungbluth N, Nemecek T, Primas A, Wernet G (2009) Ecoinvent - Code of practice, Data v2.1. Ecoinvent report No. 2, Swiss Centre for Life Cycle Inventories.

WHO (2011) Guidelines for Drinking Water Quality - 4th edition. WHO Library Cataloguing-in-Publication Data.

WTP manual (2001) User's manual of the Water Treatment Plant (WTP) model version 2.0. Center for Drinking Water Optimization, University of Colorado at Boulder.

Young P, Byrne G, Cotterell M (1997) Manufacturing and the environment. Int J Adv Manuf Technol 13(7):488-493.

Appendix 2-1. Water quality data set.

In the EVALEAU framework, the quality of every water flow is defined by a set of data which is in fact a mathematical vector representing the water composition. It is composed of 170 water quality data, presented and listed below.

Water Quality Data	**Unit**

General parameters	
Temperature	K
Absolute Pressure	Pa
pH	No unit
pH sign	No unit
TAC (or CAT)	French degree
TAC sign	No unit
TH	French degree
Conductivity	µS/cm-1 at 20°C

Radioactivity	
Total alpha activity	Bq/L
Total beta activity	Bq/L
Total Indicative Dose	Bq/L
Tritium	mg/L

Organic Matter	
UVA (254 nm)	m^{-1}
COD	mgO2/L
BOD	mgO2/L
BOD5	mgO2/L
TOC	mg/L
DOC	mg/L
POC	mg/L

SM	mg/L
Turbidity	NTU
Taste	No unit (threshold)
Odor	No unit (threshold)
Color	mg Pt-Co/L
SM-Turbidity ratio	mg/(L.NTU)
BOD5-BOD ratio	mgBOD5/mgBOD
COD-TOC ratio	mgCOD/mgTOC
COD-BOD5 ratio	mgCOD/mgBOD5
DOC-TOC ratio	mgDOC/mgTOC
UVA-DOC ratio	m^{-1}/mgDOC
UVA-Color ratio	L/(mg Pt-Co.m)

Pathogenic Microorganisms	
E. Coli (total)	nb/L
E. Coli O157-H7 (pathogen)	nb/L
Enterococci	nb/L
Salmonella	nb/L
Campylobacter	nb/L
Giarda	nb/L
Cryptosporidium	nb/L
Norovirus	nb/L
Rotavirus	nb/L
Algae	nb/L

Mineral and salt composition	
Cl	mg/L
SO4	mg/L
Br	mg/L
CN	mg/L
Mg	mg/L
Na	mg/L
K	mg/L
Sr	mg/L
Ni	mg/L
Cr	mg/L
Cd	mg/L
Ba	mg/L

B	mg/L
As	mg/L
Se	mg/L
Sb	mg/L
F	mg/L
Pb	mg/L
Hg	mg/L
Cu	mg/L
Zn	mg/L
Ag	mg/L
Be	mg/L
Al Total	mg/L
Al Dissolved	mg/L
Fe Total	mg/L
Fe Dissolved	mg/L
Mn Total	mg/L
Mn Dissolved	mg/L
Ca Total	mg/L
Ca Dissolved	mg/L
C Total	mg/L
C Dissolved	mg/L
Si Total	mg/L
Si Dissolved	mg/L
H_2S	mg/L
PAC	mg/L

Nitrogen and Phosphorus Compounds	
Ammonium NH4	mg/L
Nitrites NO_2	mg/L
Nitrates NO_3	mg/L
Total Phosphorus	mg/L
Hydrolisis Phosphorus PO_4 [mg/L]	mg/L

Micropollutants	
Total Micropllutants	mg/L
Alachlore	mg/L
Anthracène	mg/L
Atrazine	mg/L

Benzène	mg/L
Diphényléthers Bromés	mg/L
Cadmium Coumpounds	mg/L
C10_C13 Chloroalcanes	mg/L
Chlorfenvinphos	mg/L
Chlorpyrifos	mg/L
1_2_Dichloroéthane	mg/L
Dichlorométhane	mg/L
Di_2_éthylhexylphtalate (DEHP)	mg/L
Diuron	mg/L
Endosulfan	mg/L
Fluoranthène	mg/L
Hexachlorobenzène	mg/L
Hexachlorobutadiène	mg/L
Hexachlorocyclohexane	mg/L
Isoproturon	mg/L
Lead Coumpounds	mg/L
Mercury Coumpounds	mg/L
Naphtalène	mg/L
Nickel Coumpounds	mg/L
Nonylphénols	mg/L
Octylphénols	mg/L
Pentachlorobenzène	mg/L
Pentachlorophénol	mg/L
Polycyclic Aromatic Hydrocarbons (PAH)	mg/L
Simazine	mg/L
Tributylétain Coumpounds	mg/L
Trichlorobenzène	mg/L
Trichlorométhane	mg/L
Trifluraline	mg/L
Aldrine	mg/L
Dieldrine	mg/L
Heptachlore	mg/L
Heptachlorepoxyde	mg/L
Acrylamide	mg/L
Benzopyrene	mg/L
Epichlorhydrin	mg/L
Microcystin	mg/L
Vinyl chloride	mg/L
Tétrachloroéthylène and trichloroéthylène	mg/L

Other Compounds	
Coumpound 1	mg/L
Coumpound 2	mg/L
Coumpound 3	mg/L
Coumpound 4	mg/L
Coumpound 5	mg/L
Coumpound 6	mg/L
Coumpound 7	mg/L
Coumpound 8	mg/L
Coumpound 9	mg/L
Coumpound 10	mg/L

Disinfection By-Products	
Total THM	mg/L
THM1 $CHBr_3$	mg/L
THM2 $CHClBr_2$	mg/L
THM3 $CHCl_2Br$	mg/L
THM4 $CHCl_3$	mg/L
Total 9 HAA	mg/L
Total 5 HAA	mg/L
MCAA	mg/L
MBAA	mg/L
DCAA	mg/L
BCAA	mg/L
DBAA	mg/L
TCAA	mg/L
DBCAA	mg/L
DCBAA	mg/L
TBAA	mg/L
Chloramines	mg/L
Chlorine	mg/L
Chlorine Dioxyde	mg/L
Iodine	mg/L
Bromate	mg/L
Chlorate	mg/L
Chlorite	mg/L

Other Reaction Products	
Reaction Product 1	mg/L
Reaction Product 2	mg/L
Reaction Product 3	mg/L
Reaction Product 4	mg/L
Reaction Product 5	mg/L
Reaction Product 6	mg/L
Reaction Product 7	mg/L
Reaction Product 8	mg/L
Reaction Product 9	mg/L
Reaction Product 10	mg/L

Appendix 3-1. List of Python^{TM} chemical objects.

The Python^{TM} chemical objects that are available at this stage of development of the EVALEAU tool are listed below :

Coagulants

- Iron Chloride - $FeCl_3$ at 41%
- Iron Sulfate - $Fe_2(SO_4)_3$ at 45.47%
- Iron Sulfate - $Fe_2(SO_4)_3$ at 35.80%
- Iron Sulfate - $Fe_2(SO_4)_3$ at 42.96%
- Iron Sulfate - $Fe_2(SO_4)_3$ at 47.50%
- Aluminium Sulfate - $Al_2(SO_4)_3$ at 28.5% (8.5% Al_2O_3)
- Aluminium Sulfate - $Al_2(SO_4)_3$ at 57.0% (17.0% Al_2O_3)

Liquid chemicals

- Sulfuric acid - H_2SO_4 at 96%
- Chlorhydric acid - HCl at 33%
- Phosphoric acid - H_3PO_4 at 75%
- Phosphoric acid - H_3PO_4 at 85%
- Nitric acid - HNO_3 at 53%
- Nitric acid - HNO_3 at 62%
- Nitric acid - HNO_3 at 93%
- Sodium Hypochlorite - NaOCl at 13%
- Sodium Hydroxide - NaOH at 30%
- Sodium Hydroxide - NaOH at 40%
- Sodium Hydroxide - NaOH at 50%
- Sodium Bisulfite - $NaHSO_3$ at 25%
- Calcium Hydroxide - $Ca(OH)_2$ at 5%
- Calcium Hydroxide - $Ca(OH)_2$ at 10%

Solid chemicals

- Calcium Hydroxide - $Ca(OH)_2$ at 94%
- Calcium Carbonate - $CaCO_3$ at 95%
- Sodium Carbonate - Na_2CO_3 at 100%

Gaseous chemicals

- Carbon Dioxide - CO_2 at 100%
- Chlorine - Cl_2 at 100%

These Python™ chemical objects are defined by their attributes, which are listed below :

- Name of the chemical.
- PHREEQC® template file.
- Physical state ("Diluted_Liquid", "Concentrated_Liquid", "Solid" or "Gaseous").
- Concentration of the chemical [mass decimal %].
- Density [kg/m3].
- Viscosity [Pa.s].
- Molar Mass [g/mol].
- Price of the chemical for indicative purpose [€/kg].

The modelling of the coagulation process requires the definition of three additional attributes for coagulant objects :

- Stoichiometry of the salt in the coagulant (Al or Fe) [no unit].
- Salt valence in the coagulant [no unit].
- Salt molar mass in the coagulant [g/mol].

Appendix 3-2. Mathematical models for unit processes involved in drinking water treatment.

This appendix describes in detail the mathematical models for unit processes developed during the EVALEAU project. These models concern only unit processes involved in conventional drinking water treatment, i.e. desalination is excluded at this stage of the project as it has been considered out of the scope.

This appendix can be seen as user manual of the EVALEAU tool since it provides fully detailed explanations about the unit process models made available in the EVALEAU library.

The categories of unit processes, presented in this appendix, are listed below. The unit process models themselves are further listed in the sections corresponding to their process category.

- Water pumping
- PAC addition
- Coagulation
- Flocs separation
- Media filtration
- Disinfection - Oxidation
- Neutralisation – Remineralisation
- Sludge treatment

In the following sections, the variable *Water* refers to the quantity of water to be treated [kgWater] (i.e. the input water), the variable *Water_Flow* refers to the nominal water flow to be treated [kgWater/s] (i.e. the input water flow), and the variable *Max_Water_Flow* refers to the maximum water flow to be treated [kgWater/s] (i.e. the maximum input water flow).

1. Water pumping

1.1 Parameters of the unit process model

The model parameters for the unit process « water pumping » are presented in table 1.

Table 1. Parameters for the unit process model « Water pumping ».

- Engineering design facts and/or operating conditions -			
Parameter	Programming Names	Default Values	Unit
Absolute roughness of the pipe(s)	ABS_K	0.0008[1]	m
Diameter of the pipe(s)	D	0.5*	m
Pump efficiency	NU	0.8[2]	dec. %

- Technical and/or legal constraints -			
Parameter Names	Programming Names	Default Values	Unit
Height to be pumped	H	1*	m
Length to be pumped	L	10*	m

* Arbitrary default value or estimation by water treatment experts.

1. The default value for the absolute roughness of the pipe is the one of worn cast iron pipes which are typically encountered in drinking water systems (Carvill 1993). Other absolute roughness values corresponding to other pipe materials are available in the literature.
2. Typical values range between 0.7 and 0.9. Pump efficiency could be 0.6 in case the pump is badly operated (Degrémont 2007).

1.2 Energy and chemical consumptions

There is no chemical consumed for pumping water. The specific electricity consumption *Spec_Elec_Cons* [kWh/kg of pumped water] is calculated thanks to the *Elec_Consumption* function defined in the EVALEAU functions. It is then multiplied by the quantity of water to be pumped *Water* (kg) to obtain the electricity consumption *Elec_Cons_Func_Unit* required to pump the quantity of water corresponding to the functional unit.

Electricity consumption [kWh]

Rho = Water_Density [kg/m^3] (1)

Mhu = Water_Dynamic_Viscosity (Temperature) [Pa.s] (2)

$$\text{Spec\_Elec\_Cons} = \text{Elec\_Consumption}\ (\text{Water\_Flow, H, L, D, ABS\_K, NU, Rho, Mhu}) \qquad [\text{kWh/kg}] \qquad (3)$$

$$\text{Elec\_Cons\_Func\_Unit} = \text{Water} \times \text{Spec\_Elec\_Cons} \qquad [\text{kWh}] \qquad (4)$$

1.3 Output water quality data

No calculation is made since the water is only pumped and its quality does not change during the process. It is assumed that there is no leakage so the water flow does not change either.

1.4 Engineering design facts

The engineering design facts are calculated thanks to the dedicated Python$^{\text{TM}}$ functions defined in the file « EVALEAU_Functions » where all the functions relative to pumping operations are scripted. Calculations are done twice considering the nominal and maximum water flows. This is important for equipment sizing and design (e.g. number of pipes in use or to be installed).

Pump power required for each pump [W]

$$\text{Single\_Pump\_Power\_Used} = \text{Power}\ (\text{Water\_Flow, H, L, D, ABS\_K, NU, Rho, Mhu}) \qquad [\text{W}] \qquad (5)$$

$$\text{Single\_Pump\_Power\_Installed} = \text{Power}\ (\text{Max\_Water\_Flow, H, L, D, ABS\_K, NU, Rho, Mhu}) \qquad [\text{W}] \qquad (6)$$

Number of pipes [no unit]

$$\text{N\_Pipe\_Used} = \text{Pipe\_Number}\ (\text{Water\_Flow, H, L, D, ABS\_K, NU, Rho, Mhu}) \qquad [\text{no unit}] \qquad (7)$$

$$\text{N\_Pipe\_Installed} = \text{Pipe\_Number}\ (\text{Max\_Water\_Flow, H, L, D, ABS\_K, NU, Rho, Mhu}) \qquad [\text{no unit}] \qquad (8)$$

Water flow in one pipe [kg/s]

$$\text{Single\_Pipe\_Flow} = \text{Pipe\_Flow}\ (\text{Water\_Flow, H, L, D, ABS\_K, NU, Rho, Mhu}) \qquad [\text{kg/s}] \qquad (9)$$

$$\text{Max\_Single\_Pipe\_Flow} = \text{Pipe\_Flow}\ (\text{Max\_Water\_Flow, H, L, D, ABS\_K, NU, Rho, Mhu}) \qquad [\text{kg/s}] \qquad (10)$$

Water velocity in one pipe [m/s]

$$\text{Water\_Velocity} = \text{Pipe\_Velocity}(\text{Water\_Flow}, H, L, D, \text{ABS\_K}, \text{NU}, \text{Rho}, \text{Mhu}) \quad [\text{m/s}] \qquad (11)$$

$$\text{Max\_Water\_Velocity} = \text{Pipe\_Velocity}(\text{Max\_Water\_Flow}, H, L, D, \text{ABS\_K}, \text{NU}, \text{Rho}, \text{Mhu}) \quad [\text{m/s}] \qquad (12)$$

2. PAC addition

Four versions of the « PAC addition » model have been developed in order to take into account different variants of the process and its modelling.

The process can be modelled considering that the addition of PAC is achieved in a tank or directly in a pipe. The difference lies in the calculation of the mixing energy (dynamic mixing in a tank and static mixing in a pipe).

The retrofit and predictive approaches are available for this unit process model. The PAC dose can be user-defined and the DOC removal is then calculated (retrofit approach) or the DOC removal objective can be set by the user and the required PAC dose is then determined by the model (predictive approach).

The four different model versions for the unit process « PAC addition » are listed below :

- Version 1 (V1) : *Tank_PAC_Addition* (retrofit model).
- Version 2 (V2) : *Tank_PAC_for_DOC_Removal* (predictive model).
- Version 3 (V3) : *Pipe_PAC_Addition* (retrofit model).
- Version 4 (V4) : *Pipe_PAC_for_DOC_Removal* (predictive model).

2.1 Parameters of the unit process model

The model parameters for the unit process « PAC addition » are presented in table 2.

Table 2. Parameters for the different versions of the unit process model « PAC addition ».

- Engineering design facts and/or operating conditions -

Parameter	Programming Names	Default Values	Unit
Hydraulic residence time	HRT	5* (V1/V2) 0.1* (V3/V4)	min
Mixing duration	MIXD	0.5* (V1/V2)	min
Stirrer efficiency	ST_NU	0.7* (V1/V2)	dec. %
Tank velocity gradient	TVG	700[1] (V1/V2)	s^{-1}
Static mixer pressure drop	SMPD	20000* (V3/V4)	Pa
PAC dose	PAC_D	10* (V1/V3)	g/m^3
DOC removal objective	DOC_R	0.2* (V2/V4)	dec. %

- Technical and/or legal constraints -

Parameter Names	Programming Names	Default Values	Unit
Intake pumped height	IPH	3* (V1/V2) 1* (V3/V4)	m
Intake pump(s) efficiency	IP_NU	0.8[2]	m

* Arbitrary default value or estimation by water treatment experts.

1. Typical values for chemical mixing in drinking water treatment range between 400 s^{-1} and 1000 s^{-1}. (CIRSEE 1999, Degrémont 2007).
2. Typical values range between 0.7 and 0.9. Pump efficiency could be 0.6 in case the pump is badly operated (Degrémont 2007).

A common second-level script exists for the PAC addition models which is named « PAC_Removal_Capacity_Dictionnary ». This file defines a Python™ dictionary which associates a PAC removal capacity to each water quality data (e.g. 1 gDOC/gPAC). Default values have been established in a default Python™ dictionary in accordance with experts' judgement, but these removal capacities are highly dependent on the type of PAC and should be user-defined as far as possible. Indeed, activated carbon can be obtained from numerous raw materials and by numerous activation/production processes, thus leading to a wide variety of PAC and related properties.

2.2 Energy and chemical consumptions

The only chemical consumed during this process is PAC and the only form of energy consumed is electricity.

PAC consumption

PAC dose [g/m^3] and DOC removal [dec.%]

In the predictive versions of the model (versions 2 and 4), the PAC dose must be calculated based on the user-defined DOC removal objective. Equations 13 and 14 allow calculating the required PAC dose from the user-defined DOC removal objective.

$$\text{DOC\_to\_be\_removed} = \text{DOC\_R} \times \text{Input\_Water\_DOC} \qquad [\text{gDOC/m}^3] \qquad (13)$$

$$\text{PAC\_Dose} = \frac{\text{DOC\_to\_be\_removed}}{\text{PAC\_RC\_DOC}} \qquad [\text{gPAC/m}^3] \qquad (14)$$

- *PAC_RC_DOC* : PAC removal capacity for DOC [gDOC/gPAC]. This value is imported from the dictionary defined the second-level script.

In the retrofit approach (model versions 1 and 3), the calculation is reversed to obtain the DOC removal from the user-defined PAC dose. Then, DOC removal is saved as an engineering design fact in the design report.

PAC consumption

$$\text{PAC\_Treatment\_Ratio} = \frac{\text{PAC\_Dose}}{1000 \times \text{Water\_Density}} \qquad [\text{kgPAC/kgWater}] \qquad (15)$$

$$\text{PAC\_Consumption} = \text{PAC\_Treament\_Ratio} \times \text{Water} \qquad [\text{kgPAC}] \qquad (16)$$

Electricity consumption (V1/V2)

Electricity consumption for intake pumping

$$\text{Specific\_Elec\_Cons} = \text{Elec\_Consumption}\,(\text{Water\_Flow, IPH, IP\_NU}) \qquad [\text{kWh/kg pumped water}] \qquad (17)$$

$$\text{Intake\_Elec\_Cons} = \text{Specific\_Elec\_Cons} \times \text{Water} \qquad [\text{kWh}] \qquad (18)$$

Electricity consumption for PAC injection/dosing

Energy consumed for injection of solid chemicals is neglected at this stage of development. The electrical power used by preparation tanks and dosing pumps is negligible in comparison with other electrical powers involved in this process, so it is a reasonable assumption and it does not affect the calculation of total electricity consumption. Nevertheless, an equation is defined in the main script so that the energy for PAC injection/dosing can be taken into account in the calculation of the total electricity consumption in case these models are later refined.

$$\mathrm{PAC\_Dosing\_Elec\_Cons} = 0.0 \qquad [\mathrm{kWh}] \qquad (19)$$

Electricity consumption for the stirrer

$$\mathrm{Mixed\_Volume} = \mathrm{MIXD} \times \frac{\mathrm{Max\_Water\_Flow}}{\mathrm{Water\_Density}} \qquad [\mathrm{m}^3] \qquad (20)$$

$$\mathrm{K} = (0.3842 \times \mathrm{Temperature}) - 81.214 \qquad [\text{no unit}] \qquad (21)$$

$$\mathrm{Stirring\_Power} = \mathrm{Mixed\_Volume} \times \left(\frac{\mathrm{TVG}}{\mathrm{K}}\right)^2 \qquad [\mathrm{W}] \qquad (22)$$

$$\mathrm{Stirring\_Elec\_Power} = \frac{\mathrm{Stirring\_Power}}{\mathrm{ST\_NU}} \qquad [\mathrm{W}] \qquad (23)$$

$$\mathrm{Spec\_Stirring\_Elec\_Cons} = \frac{\mathrm{Stirring\_Elec\_Power}}{\mathrm{Water\_Flow} \times 3600 \times 1000} \qquad [\mathrm{kWh/kgWater}] \qquad (24)$$

$$\mathrm{Stirring\_Elec\_Cons} = \mathrm{Spec\_Stirring\_Elec\_Cons} \times \mathrm{Water} \qquad [\mathrm{kWh}] \qquad (25)$$

- *Mixed_Volume* : Theoretical volume of water submitted to stirring forces.
- *K* : empirical coefficient (CIRSEE 1999).

The mixing in a tank is most often dynamic (Degrémont 2007). The equations 21 and 22 come from an internal document of the industrial partner Suez Environnement (CIRSEE 1999).

The stirring power *Stirring_Power* is the mechanical power that must be exerted on the water to mix it. The stirring electrical power *Stirring_Elec_Power* is the electrical power that must be fed to the stirrer to make it work correctly.

Total electricity consumption

$$\text{Total\_Elec\_Cons} = \text{Intake\_Elec\_Cons} + \text{PAC\_Dosing\_Elec\_Cons} + \text{Stirring\_Elec\_Cons} \qquad [\text{kWh}] \qquad (26)$$

Electricity consumption (V3/V4)

Electricity consumption for intake pumping and static mixing

The mixing in a pipe is most often achieved with a static mixing device (Degrémont 2007). A static mixer generates a pressure drop (model parameter *SMPD*) that must be compensated by a pump. The static mixer pressure drop *SMPD* is therefore expressed in terms of a water height to be pumped and then added to the intake pumped height *IPH*.

$$\text{SMPD\_Height} = \frac{\text{SMPD}}{\text{Water\_Density} \times 9.81} \qquad [\text{m of water to be pumped}] \qquad (27)$$

$$\text{Height\_to\_be\_pumped} = \text{SMPD\_Height} + \text{IPH} \qquad [\text{m of water to be pumped}] \qquad (28)$$

$$\text{Specific\_Elec\_Cons} = \text{Elec\_Consumption}\,(\text{Water\_Flow}, \text{Height\_to\_be\_pumped}, \text{IP\_NU}) \qquad [\text{kWh/kg pumped water}] \qquad (29)$$

$$\text{Pumping\_Elec\_Cons} = \text{Specific\_Elec\_Cons} \times \text{Water} \qquad [\text{kWh}] \qquad (30)$$

Electricity consumption for PAC injection/dosing

The PAC injection/dosing energy is also neglected in these versions (V1/V2) of the model.

$$\text{PAC\_Dosing\_Elec\_Cons} = 0.0 \qquad [\text{kWh}] \qquad (31)$$

Total electricity consumption

$$\text{Total\_Elec\_Cons} = \text{Pumping\_Elec\_Cons} + \text{PAC\_Dosing\_Elec\_Cons} \qquad [\text{kWh}] \qquad (32)$$

2.3 Output water quality data

Dissolved water compounds

Dissolved water compounds are adsorbed on PAC (unlike particulate compounds). The Python$^{\text{TM}}$ dictionary for PAC removal capacity provides values enabling the calculation of adsorbed quantities of dissolved compounds during the operation. The equations 33 and 34 show the calculation in a generic sense.

$$\text{Removed\_X} = \text{PAC\_Dose} \times \text{PAC\_RC\_X} \qquad [\text{mg/L}] \qquad (33)$$

$$\text{Output\_Water\_X} = \text{Input\_Water\_X} - \text{Removed\_X} \qquad [\text{mg/L}] \qquad (34)$$

- *Removed_X* : Adsorbed concentration of a dissolved compound X [mg/L (or g/m^3)].
- *PAC_RC_X* : PAC removal capacity for a dissolved compound X [gX/gPAC].
- *Input_Water_X, Output_Water_X* : Input and output concentrations of a dissolved compound X.

Other water compounds

POC is not adsorbed (particulate compound), so it does not change in this process. TOC is recalculated as the sum of POC and DOC. Suspended matter concentration SM is increased by the addition of PAC, since PAC itself is a particulate compound (and therefore part of the suspended matter). Turbidity is then recalculated from the concentration of suspended matter in the output water thanks to the (SM:Turbidity) ratio which is assumed to be constant.

$$\text{Output\_Water\_TOC} = \text{Input\_Water\_POC} + \text{Output\_Water\_DOC} \qquad [\text{mg/L}] \qquad (35)$$

$$\text{Output\_Water\_SM} = \text{Input\_Water\_SM} + \text{PAC\_Dose} \qquad [\text{mg/L}] \qquad (36)$$

$$\text{Output\_Water\_Turbidity} = \frac{\text{Output\_Water\_SM}}{\text{SM\_Turbidity\_Ratio}} \qquad [\text{NTU}] \qquad (37)$$

Except from the (SM:Turbidity) ratio, all the organic matter ratios (e.g. UVA:DOC ratio) are likely to change during the process (UVA may be better adsorbed than DOC or vice versa). The value of these ratios in the output water is recalculated from the concentration of the corresponding dissolved water compounds.

The mineral composition of the water is not changed due to the addition of PAC and so are the pH, the complete alkalinity titration TAC and the total hardness TH.

Organic matter fractions relative to the coagulation model

The main script calculates the new values of the three fractions of organic matter (f_{ha}, $f_{nonpolar}$ and $f_{nonsorbable}$) after the operation and writes these updated values in the dedicated file

« OM_Information » (paragraph 3.9 of chapter 3). The calculations are presented in equations 38, 39 and 40, based on the UVA and DOC removals obtained by this adsorption process.

$$\mathrm{UVA\_R} = \frac{\mathrm{Input\_Water\_UVA - Output\_Water\_UVA}}{\mathrm{Input\_Water\_UVA}} \qquad [\mathrm{dec.\%}] \qquad (38)$$

$$\mathrm{f_{ha}} = \mathrm{f_{ha,0}} \times \frac{1 - \mathrm{UVA\_R}}{1 - \mathrm{DOC\_R}} \qquad [\mathrm{dec.\%}] \qquad (39)$$

$$\mathrm{f_{nonpolar}} = (1 - \mathrm{f_{ha}}) \times \frac{\mathrm{f_{nonpolar,0}}}{\mathrm{f_{nonpolar,0}} + \mathrm{f_{nonsorbable,0}}} \qquad [\mathrm{dec.\%}] \qquad (40)$$

- $UVA\_R \,/\, DOC\_R$: UVA and DOC removals obtained by PAC addition.
- $f_{ha,0} \,/\, f_{ha}$: Initial and final values of the humic acids fraction.
- $f_{nonpolar,0} \,/\, f_{nonpolar}$: Initial and final values of the non-polar fraction.
- $f_{nonsorbable,0}$: Initial value of non-sorbable fraction.

The adsorption of humic acids on PAC is assessed based on UVA removal. In other words, the removal of humic acids is assimilated to the removal of UVA due to PAC addition. Non-polar and non-sorbable compounds are assumed to be equally adsorbed on PAC because of lack of knowledge.

2.4 Engineering design facts

Tank (or pipe) volume and real hydraulic residence time

$$\mathrm{Volume} = \frac{\mathrm{HRT \times Max\_Water\_Flow}}{\mathrm{Water\_Density}} \qquad [\mathrm{m^3}] \qquad (41)$$

$$\mathrm{Real\_HRT} = \frac{\mathrm{Volume \times Water\_Density}}{\mathrm{Water\_Flow \times 60}} \qquad [\mathrm{min}] \qquad (42)$$

The tank (or pipe) is designed with regard to the maximum water flow. Considering that the nominal water flow is lower, the real hydraulic residence time is consequently higher than the theoretical one. The theoretical hydraulic residence time *HRT* (user-defined parameter), the real one and the volume of the tank (or pipe) are saved in the engineering design report.

PAC flow demand

$$\mathrm{PAC\_Flow\_Demand} = \mathrm{PAC\_Treament\_Ratio} \times \mathrm{Water\_Flow} \times 3600 \quad [\mathrm{kgPAC/h}] \qquad (43)$$

$$\mathrm{PAC\_Max\_Flow\_Demand} = \mathrm{PAC\_Treament\_Ratio} \times \mathrm{Max\_Water\_Flow} \times 3600 \quad [\mathrm{kgPAC/h}] \qquad (44)$$

The PAC nominal and maximum flow demands are reported in the engineering design report together with the PAC treatment ratio.

Electricity consumptions and electrical powers (V1/V2)

The following design facts relative to electricity consumptions and electrical powers (calculated by the versions 1 and 2 of the PAC addition model) are saved in the design report created by the main script :

- Stirring electricity consumption [kWh]
- Specific stirring electricity consumption [kWh/kgWater]
- Stirring electrical power [kW]
- Electricity consumption for intake pumping [kWh]
- Specific electricity consumption for intake pumping [kWh/kg pumped water]
- Intake pumping electrical power (used) [kW]
- Intake pumping electrical power (installed) [kW]
- Total electricity consumption relative to the functional unit [kWh]
- Total specific electricity consumption [kWh/kgWater]

Electricity consumptions and electrical powers (V3/V4)

The following design facts relative to electricity consumptions and electrical powers (calculated by the versions 3 and 4 of the PAC addition model) are saved in the design report created by the main script :

- Intake height to be pumped [m of water to be pumped]
- Static mixing pressure drop to be compensated [m of water to be pumped]
- Total height to be pumped [m of water to be pumped]
- Electricity consumption for pumping [kWh]
- Specific electricity consumption for pumping [kWh/kg pumped water]
- Pumping electrical power (used) [kW]

- Pumping electrical power (installed) [kW]
- Total electricity consumption relative to the functional unit [kWh]
- Total specific electricity consumption [kWh/kgWater]

3. Coagulation

Six versions of the model « Coagulation » have been developed, representing different variants of this unit process and its modelling. The versions of the model differ on the following points detailed below.

- Coagulation is normally achieved in a contact reactor (i.e. a tank) but it can also be done in a pipe. The calculation of the mixing energy differs accordingly (dynamic mixing in a tank and static mixing in a pipe).
- The coagulant dose can be user-defined and the resulting DOC removal is then calculated (retrofit approach) or the DOC removal objective can be user-defined and the required coagulant dose is then forecasted by the model (predictive approach).
- The coagulation process can be enhanced by acid addition or not. Indeed, lowering the pH at which the process is operated allows removing more DOC from the water. It can also allow removing the same quantity of DOC with less coagulant.

The six different model versions for the unit process « Coagulation » are listed below :

- Version 1 (V1) : *Tank_Data_Based_Coagulation* (retrofit model).
- Version 2 (V2) : *Tank_Standard_Coagulation* (predictive model).
- Version 3 (V3) : *Tank_Enhanced_Coagulation* (predictive model).
- Version 4 (V4) : *Pipe_ Data_Based_Coagulation* (retrofit model).
- Version 5 (V5) : *Pipe_ Standard_Coagulation* (predictive model).
- Version 6 (V6) : *Pipe_ Enhanced_Coagulation* (predictive model).

3.1 Parameters of the unit process model

The model parameters for the unit process « Coagulation » are presented in table 3.

Table 3. Parameters for the different versions of the unit process model « Coagulation ».

- Engineering design facts and/or operating conditions -

Parameter	Programming Names	Default Values	Unit
DOC removal objective	DOC_R	0.33[*] (V2/V3/V5/V6)	dec. %
Coagulant dose	COAGD	80[1] (V1/V4)	g/m^3
Coagulation pH	C_PH	6[*] (V3/V6)	no unit
Coagulant choice index	C_CI	1[2]	no unit
Acid choice index	A_CI	1[2] (V3/V6)	no unit
Base choice index	B_CI	1[2] (V3/V6)	no unit
Coagulation mixing duration	CMIXD	1[3] (V1/V2/V3)	min
Coagulation contact time	COAGT	3[4]	min
Coagulation velocity gradient	CVG	700[5] (V1/ V2/V3)	s^{-1}
Flocculant dose	FLOCD	0.1[6]	g/m^3
Flocculation mixing duration	FMIXD	1[7] (V1/V2/V3)	min
Flocculation contact time	FLOCT	20[8]	min
Flocculation velocity gradient - Part 1	FVG1	550[9] (V1/V2/V3)	s^{-1}
Flocculation velocity gradient - Part 2	FVG2	60[10] (V1/V2/V3)	s^{-1}
Stirrer efficiency	ST_NU	0.7[*] (V1/V2/V3)	dec. %
Static mixer pressure drop for coagulation	SMPDC	50000[*] (V4/V5/V6)	Pa
Static mixer pressure drop for flocculation	SMPDF	20000[*] (V4/V5/V6)	Pa
Coagulation pH	C_PH	6[*] (V3/V6)	no unit

- Technical and/or legal constraints -

Parameter Names	Programming Names	Default Values	Unit
Intake pumped height	IPH	3[*]	m
Intake pump(s) efficiency	IP_NU	0.8[11]	m

* Arbitrary default value or estimation by water treatment experts.

1. Typical values range between 5 and 150 g/m^3 (Degrémont 2007).
2. This index defines the selected coagulant/chemical for the operation. Available coagulants/chemicals are listed in appendix 3-1.
3. Typical values range between few secondes to 2 minutes (CIRSEE 1999).
4. Typical values range between 30 s and 5 min (CIRSEE 1999).
5. Typical values for chemical mixing in drinking water treatment range between 400 s^{-1} and 1000 s^{-1}. (CIRSEE 1999, Degrémont 2007).
6. Typical values range between 0.05 and 0.5 g/m^3 (CIRSEE 1999).
7. Typical values range between few secondes and 2 minutes (CIRSEE 1999).
8. Typical values range between 10 and 30 min (CIRSEE 1999).

9. The first part of the flocculation reactor is dedicated to mixing the water and the flocculant. Typical values for the velocity gradient in this part of the reactor range between 300 and 800 s^{-1} (CIRSEE 1999, Degrémont 2007).
10. The second part of the flocculation reactor is dedicated to the circulation of water. Typical values for the velocity gradient in this part of the reactor range between 40 and 80 s^{-1} (CIRSEE 1999, Degrémont 2007).
11. Typical values range between 0.7 and 0.9. Pump efficiency could be 0.6 in case the pump is badly operated (Degrémont 2007).

The second-level script, common to all versions of the coagulation model, is named « Coagulation_Data ». This file contains four parameters that are in fact arguments of the function *Coagulant_Dose_Calculation* (paragraph 3.9 of chapter 3). The four parameters defined in this second-level script are the maximum sorption capacity and the sorption coefficient as described in the model developed by Kastl et al. (Kastl et al. 2004) for both types of coagulants (Al-based or Fe-based coagulants). These parameters are average values from the 14 US waters studied by Kastl et al. and they are listed below :

- *Al_Max_Sorption_Capacity* [mgDOC/meq metal]. Default value is 4.064, the maximum value being 9.0 and the minimum being 1.6.
- *Al_Sorption_Coefficient* [L/mg]. Default value is 181.8, the maximum value being 300.0 and the minimum being 47.0.
- *Fe_Max_Sorption_Capacity* [mgDOC/meq metal]. Default value is 3.2, the maximum value being 6.0 and the minimum being 1.6.
- *Fe_Sorption_Coefficient* [L/mg]. Default value is 179.9, the maximum value being 300.0 and the minimum being 42.0.

It must be kept in mind that the three other parameters of the coagulation model developed by Kastl et al. are defined in the file « OM_Information » located in the water quality database (paragraph 3.9 of chapter 3).

3.2 Energy and chemical consumptions

The chemicals consumed during this unit process are the flocculant, the coagulant (selected by the user) and eventually an acid or a base (also selected by the user) when the coagulation is enhanced (versions 3 and 6 of the model). The only form of energy consumed is electricity.

Coagulant consumption and DOC removal (V1/V4)

Consumptions of coagulant solution and pure coagulant

In the retrofit versions of the model (versions 1 and 4), the coagulant dose is user-defined. The quantity of coagulant solution that is consumed during the process is therefore easily calculated by the model. The quantity of pure coagulant is also calculated, being the one that must be sent back to Umberto® for background process LCI calculations, since the LCA database (i.e. the Ecoinvent database) provides LCI data relative to pure quantities of chemicals (Weidema et al. 2009).

$$\text{Coag\_Treatment\_Ratio} = \frac{\text{COAGD}}{\text{Water\_Density} \times 1000} \quad [\text{kgCoagSol/kgWater}] \qquad (45)$$

$$\text{Coag\_Solution\_Quantity} = \text{Coag\_Treatment\_Ratio} \times \text{Water} \quad [\text{kgCoagSol}] \qquad (46)$$

$$\text{Pure\_Coag\_Quantity} = \text{Coag\_Solution\_Quantity} \times \text{Coag\_Concentration} \quad [\text{kgPureCoag}] \qquad (47)$$

- *Coag_Concentration* : The concentration of the coagulant (and of any chemical in general) is an attribute of the corresponding Python$^{\text{TM}}$ object (appendix 3-1) and thus it is directly available in the code of the main scripts.

Coagulant solution flow demands

$$\text{Coag\_Solution\_Flow\_Demand} = \text{Coag\_Treatment\_Ratio} \times \text{Water\_Flow} \quad [\text{kgCoagSol/s}] \qquad (48)$$

$$\text{Max\_Coag\_Solution\_Flow\_Demand} = \text{Coag\_Treatment\_Ratio} \times \text{Max\_Water\_Flow} \quad [\text{kgCoagSol/s}] \qquad (49)$$

Calculation of the DOC removal obtained with the user-defined coagulant dose

In the retrofit versions of the model (versions 1 and 4), the DOC removal must be calculated based on the user-defined coagulant dose. This is done in two steps :

1. Determination of the pH resulting from the addition of the coagulant in the water (i.e. the coagulation pH).
2. Determination of the DOC removal obtained with the user-defined coagulant dose when the process is operated at the coagulation pH determined in step 1 (the mathematical method applied is the dichotomy method).

The first step is achieved by using the function *Reactant_Addition*. The Python^{TM} object corresponding to the coagulant selected for the process and its treatment ratio (previously calculated) are sent as arguments to the function *Reactant_Addition* together with the mineral composition and pH of the input water. This allows calculating the mineral composition of the coagulated water, its complete alkalinity titration TAC, its total hardness TH and its pH. Thus the coagulation pH at which the process is operated (i.e. the pH of the coagulated water) is accurately calculated.

At this point, the coagulant dose and the coagulation pH are known and only the corresponding DOC removal is lacking. So, the second step is the application of the dichotomy method on the DOC removal itself. The minimum DOC removal is set to 0 and the maximum DOC removal is calculated as the sum of the non-polar fraction $f_{nonpolar}$ and humic acids fraction f_{ha} as defined in the file « OM_Information ». Then, the function *Coagulant_Dose_Calculation* is used. The arguments sent to the function are the coagulation pH as determined in the first step, DOC and UVA of the input water, and an initial value of DOC removal (average value between minimum and maximum DOC removals). The coagulant dose, calculated by the function *Coagulant_Dose_Calculation*, is compared with the user-defined one. Then, the interval considered for DOC removal is restricted accordingly until the calculated coagulant dose coincides with the user-defined one. Finally, the DOC removal, determined by the dichotomy method, is the one obtained with the user-defined coagulant dose at the coagulation pH, also obtained with the user-defined coagulant dose.

It must be noted that the DOC removal is determined by the function *Coagulant_Dose_Calculation* as well as the UVA removal. The mineral composition, the complete alkalinity titration TAC, the total hardness TH and the pH of the coagulated water have been calculated by the function *Reactant_Addition* in the first step.

Coagulant consumption and DOC removal (V2/V5)

Consumptions of coagulant solution and pure coagulant

In the versions 2 and 5 of the model, the approach is predictive (i.e. DOC removal is user-defined and coagulant dose must be forecasted based on it) and it is not considered that coagulation is enhanced by acid addition.

The coagulation pH is unknown and it depends on the coagulant dose, which is also unknown. Therefore, the calculation is iterated with regard to the coagulation pH. It is initially assumed to be equal to the input water pH and then, each iteration is constituted of two steps :

1. The function *Coagulant_Dose_Calculation* is used to calculate the required coagulant dose corresponding to the user-defined DOC removal and the coagulation pH (the one considered in the iteration step).
2. The function *Reactant_Addition* is used to calculate the pH obtained with the coagulant dose obtained in step 1.

The coagulant dose *Coag_Dose* required for fulfilling the user-defined DOC removal objective *DOC_R* is obtained when the coagulation pH and the coagulant dose coincide.

$$\text{Coag\_Treatment\_Ratio} = \frac{\text{Coag\_Dose}}{\text{Water\_Density} \times 1000} \quad [\text{kgCoagSol/kgWater}] \tag{50}$$

$$\text{Coag\_Solution\_Quantity} = \text{Coag\_Treatment\_Ratio} \times \text{Water} \quad [\text{kgCoagSol}] \tag{51}$$

$$\text{Pure\_Coag\_Quantity} = \text{Coag\_Solution\_Quantity} \times \text{Coag\_Concentration} \quad [\text{kgPureCoag}] \tag{52}$$

Coagulant solution flow demands

$$\text{Coag\_Solution\_Flow\_Demand} = \text{Coag\_Treatment\_Ratio} \times \text{Water\_Flow} \quad [\text{kgCoagSol/s}] \tag{53}$$

$$\text{Max\_Coag\_Solution\_Flow\_Demand} = \text{Coag\_Treatment\_Ratio} \times \text{Max\_Water\_Flow} \quad [\text{kgCoagSol/s}] \tag{54}$$

It must be noted that the UVA removal has been calculated by the function *Coagulant_Dose_Calculation*. The mineral composition, the complete alkalinity titration TAC, the total hardness TH and the pH of the coagulated water have been determined by the function *Reactant_Addition* during the iterated calculations.

Chemical consumptions and DOC removal (V3/V6)

Consumptions of coagulant solution and pure coagulant

In the versions 3 and 6 of the model, the approach is predictive and it is considered that coagulation is enhanced by acid (or base) addition. In other words, the coagulant dose must be predicted based on a user-defined DOC removal objective and a fixed coagulation pH (also user-defined).

The function *Coagulant_Dose_Calculation* is used to calculate the required coagulant dose *Coag_Dose* depending on the user-defined DOC removal *DOC_R* and coagulation pH *C_PH* (as well as input water UVA and DOC). Then, the quantity of coagulant solution, flow demand and treatment ratio are calculated based on the following equations.

$$\text{Coag\_Treatment\_Ratio} = \frac{\text{Coag\_Dose}}{\text{Water\_Density} \times 1000} \quad [\text{kgCoagSol/kgWater}] \tag{55}$$

$$\text{Coag\_Solution\_Quantity} = \text{Coag\_Treatment\_Ratio} \times \text{Water} \quad [\text{kgCoagSol}] \tag{56}$$

$$\text{Pure\_Coag\_Quantity} = \text{Coag\_Solution\_Quantity} \times \text{Coag\_Concentration} \quad [\text{kgPureCoag}] \tag{57}$$

Coagulant solution flow demands

$$\text{Coag\_Solution\_Flow\_Demand} = \text{Coag\_Treatment\_Ratio} \times \text{Water\_Flow} \quad [\text{kgCoagSol/s}] \tag{58}$$

$$\text{Max\_Coag\_Solution\_Flow\_Demand} = \text{Coag\_Treatment\_Ratio} \times \text{Max\_Water\_Flow} \quad [\text{kgCoagSol/s}] \tag{59}$$

Acid and base consumptions

In the versions 3 and 6 of the model, the coagulation pH is adjusted thanks to the addition of the appropriate chemical (acid or base).

The mineral composition and the pH *Inter_PH* of the water after coagulant addition are calculated by the function *Reactant_Addition*. Indeed, the coagulant dose *Coag_Dose* calculated in the previous step allows calculating the pH of the water as it would be without any pH adjustment.

Then, this hypothetical pH *Inter_PH* is used together with the targeted coagulation pH *C_PH* by the function *pH_Adjustment* to calculate the required treatment ratios of acid and base to adjust the pH correctly. The quantity of acid and base solutions, their pure quantities, the nominal and maximum flow demands are then determined based on their treatment ratios.

$$\text{Acid\_Quantity} = \text{Acid\_Treatment\_Ratio} \times \text{Water} \quad [\text{kgAcidSol}] \tag{60}$$

$$\text{Base\_Quantity} = \text{Base\_Treatment\_Ratio} \times \text{Water} \quad [\text{kgBaseSol}] \tag{61}$$

$$\text{Pure\_Acid\_Quantity} = \text{Acid\_Quantity} \times \text{Acid\_Concentration} \quad [\text{kgPureAcid}] \tag{62}$$

$$\text{Pure\_Base\_Quantity} = \text{Base\_Quantity} \times \text{Base\_Concentration} \quad [\text{kgPureBase}] \tag{63}$$

$$\text{Acid\_Flow\_Demand} = \text{Acid\_Treatment\_Ratio} \times \text{Water\_Flow} \quad [\text{kgAcidSol/s}] \quad (64)$$

$$\text{Max\_Acid\_Flow\_Demand} = \text{Acid\_Treatment\_Ratio} \times \text{Max\_Water\_Flow} \quad [\text{kgAcidSol/s}] \quad (65)$$

$$\text{Base\_Flow\_Demand} = \text{Base\_Treatment\_Ratio} \times \text{Water\_Flow} \quad [\text{kgBaseSol/s}] \quad (66)$$

$$\text{Max\_Base\_Flow\_Demand} = \text{Base\_Treatment\_Ratio} \times \text{Max\_Water\_Flow} \quad [\text{kgBaseSol/s}] \quad (67)$$

It must be noted that the UVA removal has been calculated by the function *Coagulant_Dose_Calculation*. The mineral composition, the complete alkalinity titration TAC, the total hardness TH and the pH of the coagulated water have been determined by the function *pH_Adjustment*.

Flocculant consumption and flow demands

Flocculant consumption

The flocculant dose is user-defined in all versions of the model. The consumption of flocculant is therefore directly calculated by the model.

$$\text{Floc\_Treatment\_Ratio} = \frac{\text{FLOCD}}{\text{Water\_Density} \times 1000} \quad [\text{kgFloc/kgWater}] \quad (68)$$

$$\text{Floc\_Quantity} = \text{Floc\_Treatment\_Ratio} \times \text{Water} \quad [\text{kgFloc}] \quad (69)$$

Flocculant flow demands

$$\text{Floc\_Flow\_Demand} = \text{Floc\_Treatment\_Ratio} \times \text{Water\_Flow} \quad [\text{kgFloc/s}] \quad (70)$$

$$\text{Max\_Floc\_Flow\_Demand} = \text{Floc\_Treatment\_Ratio} \times \text{Max\_Water\_Flow} \quad [\text{kgFloc/s}] \quad (71)$$

Electricity consumption

Electricity consumption for intake pumping

$$\text{Specific\_Elec\_Cons} = \text{Elec\_Consumption (Water\_Flow, IPH, IP\_NU)} \quad [\text{kWh/kg pumped water}] \quad (72)$$

$$\text{Intake\_Elec\_Cons} = \text{Specific\_Elec\_Cons} \times \text{Water} \quad [\text{kWh}] \quad (73)$$

Electricity consumptions for coagulant and flocculant injection/dosing

Energy consumptions for injection of coagulant and flocculant (which are supposed to be liquid chemicals) are calculated with the function *Elec_Cons*.

$$\begin{aligned}&\text{Coag\_Dosing\_Elec\_Cons} = \text{Coag\_Solution\_Quantity}\\&\times \text{Elec\_Consumption}\,(\text{Coag\_Solution\_Flow\_Demand}, \text{IPH}, \text{rho} = \text{Coagulant\_Density},\\&\text{mhu} = \text{Coagulant\_Dynamic\_Viscosity})\end{aligned} \quad [\text{kWh}] \quad (74)$$

$$\text{Floc\_Dosing\_Elec\_Cons} = \text{Floc\_Quantity} \times \text{Elec\_Consumption}\,(\text{Floc\_Flow\_Demand}, \text{IPH}) \quad [\text{kWh}] \quad (75)$$

- *Coagulant_Density* and *Coagulant_Dynamic_Viscosity* are attributes of the Python™ object corresponding to the coagulant selected by the user for the operation. Density and dynamic viscosity of the flocculant are unknown, so they are not specified and the default values as defined in paragraph 3.4 of chapter 3 (relative to water) are kept as an approximation.

Electricity consumption for stirring in the different parts of the coagulation tank (V1/V2/V3)

The calculation is repeated three times to calculate each electricity consumption due to stirring in the different parts of the coagulation tank (i.e. the coagulation reactor and both parts of the flocculation reactor). So the calculations are presented in a generic sense with the equations below :

$$\text{Mixed\_Volume} = \text{Mixing\_Duration} \times \frac{\text{Max\_Water\_Flow}}{\text{Water\_Density}} \quad [\text{m}^3] \quad (76)$$

$$\text{K} = (0.3842 \times \text{Temperature}) - 81.214 \quad [\text{no unit}] \quad (77)$$

$$\text{Stirring\_Power} = \text{Mixed\_Volume} \times \left(\frac{\text{Velocity\_Gradient}}{\text{K}}\right)^2 \quad [\text{W}] \quad (78)$$

$$\text{Stirring\_Elec\_Power} = \frac{\text{Stirring\_Power}}{\text{ST\_NU}} \quad [\text{W}] \quad (79)$$

$$\text{Spec\_Stirring\_Elec\_Cons} = \frac{\text{Stirring\_Elec\_Power}}{\text{Water\_Flow} \times 3600 \times 1000} \quad [\text{kWh/kgWater}] \quad (80)$$

$$\text{Stirring\_Elec\_Cons} = \text{Spec\_Stirring\_Elec\_Cons} \times \text{Water} \quad [\text{kWh}] \quad (81)$$

- *Mixed_Volume* : Theoretical volume of water submitted to stirring forces.
- *K* : empirical coefficient (CIRSEE 1999).

Finally, these electricity consumptions due to stirring in the different parts of the tank are added :

$$\begin{aligned}\text{Stirring\_Elec\_Cons} &= \text{Coag\_Stirring\_Elec\_Cons} + \text{Floc1\_Stirring\_Elec\_Cons} \\ &+ \text{Floc2\_Stirring\_Elec\_Cons}\end{aligned} \qquad [\text{kWh}] \qquad (82)$$

Total electricity consumption (V1/V2/V3)

$$\begin{aligned}\text{Total\_Elec\_Cons} &= \text{Intake\_Elec\_Cons} + \text{Coag\_Dosing\_Elec\_Cons} \\ &+ \text{Floc\_Dosing\_Elec\_Cons} + \text{Stirring\_Elec\_Cons}\end{aligned} \qquad [\text{kWh}] \qquad (83)$$

Electricity consumption for static mixing (V4/V5/V6)

The static mixer pressure drops *SMPDC* and *SMPDF* (respectively corresponding to the static mixing of coagulant and flocculant) are expressed in terms of a water height to be pumped. Then, the pumping functions allow calculating the electricity required to compensate these pressure drops, the electrical power needed and the specific electricity consumption.

$$\text{SMPDC\_Height} = \frac{\text{SMPDC}}{\text{Water\_Density} \times 9.81} \qquad [\text{m of water to be pumped}] \qquad (84)$$

$$\text{Coag\_Stat\_Mix\_Spec\_Elec\_Cons} = \text{Elec\_Consumption (Water\_Flow, SMPDC\_Height)} \qquad [\text{kWh/kgWater}] \qquad (85)$$

$$\text{Coag\_Stat\_Mix\_Elec\_Cons} = \text{Water} \times \text{Coag\_Stat\_Mix\_Spec\_Elec\_Cons} \qquad [\text{kWh}] \qquad (86)$$

$$\begin{aligned}\text{Coag\_Stat\_Mix\_Elec\_Cons} &= \text{Power (Water\_Flow, SMPDC\_Height)} \\ &\times \text{Pipe\_Number(Water\_Flow, SMPDC\_Height)}\end{aligned} \qquad [\text{kW}] \qquad (87)$$

$$\text{SMPDF\_Height} = \frac{\text{SMPDF}}{\text{Water\_Density} \times 9.81} \qquad [\text{m of water to be pumped}] \qquad (88)$$

$$\text{Floc\_Stat\_Mix\_Spec\_Elec\_Cons} = \text{Elec\_Consumption (Water\_Flow, SMPDF\_Height)} \qquad [\text{kWh/kgWater}] \qquad (89)$$

$$\text{Floc\_Stat\_Mix\_Elec\_Cons} = \text{Water} \times \text{Floc\_Stat\_Mix\_Spec\_Elec\_Cons} \qquad [\text{kWh}] \qquad (90)$$

$$\text{Floc\_Stat\_Mix\_Elec\_Cons} = \text{Power}\,(\text{Water\_Flow}, \text{SMPDF\_Height}) \times \text{Pipe\_Number}(\text{Water\_Flow}, \text{SMPDF\_Height}) \qquad [\text{kWh}] \qquad (91)$$

Total electricity consumption (V4/V5/V6)

$$\text{Total\_Elec\_Cons} = \text{Intake\_Elec\_Cons} + \text{Coag\_Dosing\_Elec\_Cons} + \text{Floc\_Dosing\_Elec\_Cons} + \text{Coag\_Stat\_Mix\_Elec\_Cons} + \text{Floc\_Stat\_Mix\_Elec\_Cons} \qquad [\text{kWh}] \qquad (92)$$

3.3 Output water quality data

Water dilution factor (V1/V2/V4/V5)

$$\text{Water\_Dilution\_Factor} = (1 + \text{Coag\_Treatment\_Ratio} + \text{Floc\_Treatment\_Ratio})^{-1} \qquad [\text{no unit}] \qquad (93)$$

Water dilution factor (V3/V6)

$$\text{Water\_Dilution\_Factor} = \begin{pmatrix} 1 + \text{Coag\_Treatment\_Ratio} + \text{Floc\_Treatment\_Ratio} \\ + \text{Acid\_Treatment\_Ratio} + \text{Base\_Treatment\_Ratio} \end{pmatrix}^{-1} \qquad [\text{no unit}] \qquad (94)$$

Water quantity - nominal and maximum water flows

$$\text{Output\_Water} = \frac{\text{Water}}{\text{Water\_Dilution\_Factor}} \qquad [\text{kg}] \qquad (95)$$

$$\text{Output\_Water\_Flow} = \frac{\text{Water\_Flow}}{\text{Water\_Dilution\_Factor}} \qquad [\text{kg/s}] \qquad (96)$$

$$\text{Max\_Output\_Water\_Flow} = \frac{\text{Max\_Water\_Flow}}{\text{Water\_Dilution\_Factor}} \qquad [\text{kg/s}] \qquad (97)$$

Disinfection by-products, micropollutants and pathogenic microorganisms

Most of the water compounds are not directly affected by the coagulation process but they are diluted during the operation because of the addition of chemical solutions. It concerns disinfection by-products (and other reaction products), micropollutants and pathogenic microorganisms. Their concentration at the exit of the process is expressed in a generic sense in the following equation.

$$\text{Output\_Concentration} = \text{Input\_Concentration} \times \text{Water\_Dilution\_Factor}$$

[mg/L or nb/L] (98)

Mineral composition, TAC, TH and pH of the coagulated water

The mineral composition, the complete alkalinity titration TAC, the total hardness TH and the pH of the water are modified due to the coagulation process. They are calculated by the function *Reactant_Addition* (or by the function *pH_Adjustment* in the case of versions 3 and 6) when predicting the required coagulant dose or the DOC removal (depending on the considered model version).

Suspended matter

It must be noted that the quantity of salt precipitates ($Fe(OH)_3$, MnO_2, $Al(OH)_3$, SiO_2 and $CaCO_3$), before and after coagulation, are stored in two dedicated variables : *Prec_Salts_Before_Coag, Prec_Salts_After_Coag*. The difference is that the dissolved and total salt concentrations have changed due to the chemical reaction (i.e. coagulation). Indeed, the quantity of salt precipitates is normally increased due to coagulation if the process is functioning correctly and it generates an increase of suspended matter that must be taken into account.

$$\begin{aligned}&\text{Prec\_Salts} = 1.91 \times (\text{Fe\_Total - Fe\_Dissolved}) + 1.58 \times (\text{Mn\_Total - Mn\_Dissolved})\\&+ 2.89 \times (\text{Al\_Total - Al\_Dissolved}) + 2.14 \times (\text{Si\_Total - Si\_Dissolved})\\&+ \min[(2.5 \times (\text{Ca\_Total - Ca\_Dissolved})); (8.33 \times (\text{C\_Total - C\_Dissolved}))]\end{aligned}$$

[mg/L] (99)

Strictly speaking, DOC is not removed from water during coagulation. In fact, it is adsorbed on flocs formed during coagulation, which are later removed during physical separation steps (e.g. settling or filtration steps). Then, it is considered that the quantity of DOC removed is transformed into POC, whose concentration is consequently increased during coagulation according to the following equation.

$$\text{Output\_Water\_POC} = \text{Input\_Water\_POC} + (\text{DOC\_Removal} \times \text{Input\_Water\_DOC})$$

[mg/L] (100)

Then, the suspended matter at the end of the operation is calculated, taking into account the increases of both POC and salt precipitates according to the following equation.

$$\text{Output\_Water\_SM} = \text{Input\_Water\_SM} + (\text{Prec\_Salts\_After\_Coag} - \text{Prec\_Salts\_Before\_Coag}) + ((\text{Output\_Water\_POC} - \text{Input\_Water\_POC}) * \text{Ratio\_OM\_C}) \quad [\text{mg/L}] \quad (101)$$

$$\text{Output\_Water\_Turbidity} = \frac{\text{Output\_Water\_SM}}{\text{SM\_Turbidity\_Ratio}} \quad [\text{NTU}] \quad (102)$$

- Ratio_OM_C : Ratio of organic matter and organic carbon, default value is 2.0 gOM/gC. This value is needed to convert the concentration of POC (Particulate Organic Carbon) into the corresponding concentration of particulate organic matter. The order of magnitude of this value is comprised between 1.5-3.8, but mostly around 2.0 gOM/gC (Bianchi et al. 2008; Iglesias Jimenez and Perez Garcia 1992; Perie and Ouimet 2008).

Organic matter compounds

DOC and UVA are partly removed from the water due to the coagulation process and their value in the output water must be calculated.

$$\text{Output\_Water\_DOC} = (1 - \text{DOC\_Removal}) \times \text{Input\_Water\_DOC} \quad [\text{mg/L}] \quad (103)$$

$$\text{Output\_Water\_UVA} = (1 - \text{UVA\_Removal}) \times \text{Input\_Water\_UVA} \quad [\text{mg/L}] \quad (104)$$

The TOC in the output water stays unchanged since the DOC removed is transformed into POC. The different oxygen demands (i.e. COD, BOD and BOD5) are not affected by the process either. The organic matter ratios where UVA and DOC are involved are calculated with their new value. The ratios (UVA:DOC), (DOC:TOC) and (UVA:Color) are concerned.

Organic matter fractions relative to the coagulation model

In the case of coagulation, the main script also calculates the three fractions of organic matter (f_{ha}, $f_{nonpolar}$ and $f_{nonsorbable}$) after the operation and updates these values in the Python^{TM} file « OM_Information ». The calculations based on the UVA and DOC removals obtained by this process are presented in equations 105 and 106.

$$f_{ha} = f_{ha,0} \times \frac{1 - UVA\_Removal}{1 - DOC\_Removal} \qquad [dec.\%] \qquad (105)$$

$$f_{nonpolar} = 1 - f_{ha} - \frac{f_{nonsorbable,0}}{1 - DOC\_Removal} \qquad [dec.\%] \qquad (106)$$

- *UVA_Removal / DOC_Removal* : UVA and DOC removals obtained by coagulation.
- $f_{ha,0}$ / f_{ha} : Initial and final values of the humic acids fraction.
- $f_{nonpolar}$: Final values of the non-polar fraction.
- $f_{nonsorbable,0}$: Initial value of the non-sorbable fraction.

The adsorption of humic acids is assimilated to the removal of UVA due to coagulation. Non-sorbable compounds are not adsorbed during coagulation according to the model of Kastl et al. (Kastl et al. 2004). The adsorption of non-polar compounds is then calculated from the two other organic matter fractions.

Saving the suspended matter concentration before coagulation in a dedicated file

The suspended matter concentration before and after coagulation (*Input_Water_SM* stored as *SM_Before_Coag* and *Output_Water_SM* stored as *SM_After_Coag*) are stored in a dedicated file named « SM_Information ». This file is located in the water quality database like the file « OM_Information ».

This information is used in the next step of water treatment which normally consists in flocs separation (e.g. settling or flotation). In the corresponding unit process models, the SM removal efficiency is user-defined and it refers to the SM value before coagulation. The reason is that the processes of coagulation and settling (or flotation) are often operated in a common facility and they are seen as one process instead of two distinct unit processes.

Therefore, the file « SM_Information » is created by the main script of the coagulation model and it will be used by the main script of the settling /flotation process. The determination of the increase of SM in the coagulated water will be useful for the calculation of sludge production while the SM concentration before the coagulation will be useful as a reference for the calculation of SM after flocs separation.

3.4 Engineering design facts

Volumes and real contact times for both coagulation and flocculation reactors

$$\text{Coag\_Reactor\_Volume} = \frac{\text{COAGT} \times \text{Max\_Water\_Flow}}{\text{Water\_Density}} \qquad [\mathrm{m}^3] \qquad (107)$$

$$\text{Coag\_Real\_Contact\_Time} = \frac{\text{Coag\_Reactor\_Volume} \times \text{Water\_Density}}{\text{Water\_Flow} \times 60} \qquad [\mathrm{min}] \qquad (108)$$

$$\text{Floc\_Reactor\_Volume} = \frac{\text{FLOCT} \times \text{Max\_Water\_Flow}}{\text{Water\_Density}} \qquad [\mathrm{m}^3] \qquad (109)$$

$$\text{Floc\_Real\_Contact\_Time} = \frac{\text{Floc\_Reactor\_Volume} \times \text{Water\_Density}}{\text{Water\_Flow} \times 60} \qquad [\mathrm{min}] \qquad (110)$$

The coagulation and flocculation reactors (or pipes) are designed on the basis of the maximum water flow. Considering that the nominal water flow is lower, the real contact time is consequently higher than the theoretical one.

Coagulant consumption and flow demands

The following information is stored in the engineering design report of the coagulation process :

- Selected coagulant for the process.
- Concentration of the selected coagulant solution [no unit- decimal percentage].
- Flow demand for coagulant solution [kg/s].
- Maximum flow demand for coagulant solution [kg/s].
- Coagulant treatment ratio [kgCoagSolution/kgWater].

Flocculant consumption and flow demands

The following information is stored in the engineering design report of the coagulation process :

- Flow demand for flocculant [kg/s].
- Maximum flow demand for flocculant [kg/s].
- Flocculant treatment ratio [kgFloc/kgWater].

Acid-Base demand and consumption (V3/V6)

The following information is stored in the engineering design report of the enhanced coagulation process :

- Selected acid for the process
- Concentration of the selected acid solution [no unit- decimal percentage]
- Acid treatment ratio [kgAcidSolution/kgWater]
- Flow demand for acid solution [kgAcidSolution/s]
- Maximum flow demand for acid solution [kgAcidSolution/s]
- Selected base for the process
- Concentration of the selected base solution [no unit- decimal percentage]
- Base treatment ratio [kgBaseSolution/kgWater]
- Flow demand for base solution [kgBaseSolution/s]
- Maximum flow demand for base solution [kgBaseSolution/s]

Performances of the coagulation process in terms of organic matter removal

The following information is stored in the engineering design report of the process :

- DOC removal [no unit - decimal percentage]
- Maximum DOC removal [no unit - decimal percentage]
- UVA removal [no unit - decimal percentage]

Electricity consumptions and electrical powers (V1/V2/V3)

The following design facts relative to electricity consumptions and electrical powers (calculated by the versions 1, 2 and 3 of the model) are saved in the engineering design report.

- Electrical power used for intake pumping [kW]
- Electrical power to be installed for intake pumping [kW]
- Electricity consumed for intake pumping [kWh]
- Specific electricity consumption for intake pumping [kWh/kg]
- Electrical power used for coagulant stirring [kW]
- Electricity consumed for coagulant stirring [kWh]
- Specific electricity consumption for coagulant stirring [kWh/kg]
- Electrical power used for flocculant stirring (part 1 of the flocculation reactor) [kW]
- Electricity consumed for flocculant stirring (part 1 of the flocculation reactor) [kWh]
- Specific electricity consumption for flocculant stirring (part 1 of the flocculation reactor) [kWh/kg]

- Electrical power used for water and flocculant circulation (part 2 of the flocculation reactor) [kW]
- Electricity consumed for water and flocculant circulation (part 2 of the flocculation reactor) [kWh]
- Specific electricity consumption for water and flocculant circulation (part 2 of the flocculation reactor) [kWh/kg]
- Specific electricity consumption for coagulant dosing [kWh/kg of coagulant]
- Electricity consumed for coagulant dosing [kWh]
- Specific electricity consumption for flocculant dosing [kWh/kg of flocculant]
- Electricity consumed for flocculant dosing [kWh]
- Total electricity consumption [kWh]
- Total specific electricity consumption [kWh/kgWater]

Electricity consumptions and electrical powers (V4/V5/V6)

The following design facts relative to electricity consumptions and electrical powers (calculated by the versions 4, 5 and 6 of the model) are saved in the engineering design report created by the main script :

- Electrical power used for intake pumping [kW]
- Electrical power to be installed for intake pumping [kW]
- Electricity consumed for intake pumping [kWh]
- Specific electricity consumption for intake pumping [kWh/kg]
- Electrical power for static mixing of the coagulant [kW]
- Electricity consumed for static mixing of the coagulant [kWh]
- Specific electricity consumption for static mixing of the coagulant [kWh/kg]
- Electrical power for static mixing of the flocculant [kW]
- Electricity consumed for static mixing of the flocculant [kWh]
- Specific electricity consumption for static mixing of the flocculant [kWh/kg]
- Specific electricity consumption for coagulant dosing [kWh/kg of coagulant]
- Electricity consumed for coagulant dosing [kWh]
- Specific electricity consumption for flocculant dosing [kWh/kg of flocculant]
- Electricity consumed for flocculant dosing [kWh]
- Total electricity consumption [kWh]
- Total specific electricity consumption [kWh/kgWater]

4. Flocs separation

The two typical unit processes for flocs separation are settling and flotation. Two models have been developed and implemented in the EVALEAU library in order to represent these unit processes whose principle is similar.

These processes do not generate any chemical consumption. Therefore, the corresponding models cannot be retrofit ones (chapter 2). The only form of energy consumed by these processes is electricity and its consumption is predicted.

The two model versions for the process category « Flocs Separation » are listed below :

- Version 1 (V1) : *Settling* (predictive model).
- Version 2 (V2) : *Flotation* (predictive model).

4.1 Parameters of the unit process model

The model parameters for the unit process « Flocs Separation » are presented in table 4.

Table 4. Parameters for the different versions of the unit process model « Flocs Separation ».

- Engineering design facts and/or operating conditions -				
Parameter	Programming Names	Default Values		Unit
Hydraulic residence time	HRT	60*		min
Suspended matter removal efficiency	SM_NU	0.95*		dec. %
Sludge concentration	SLC	20[1] 28[2]	(V1) (V2)	g/L
Surface hydraulic charge	SHC	10* 6.5[3]	(V1) (V2)	$m^3/(m^2.h)$
Single tank surface	STS	100* 50*	(V1) (V2)	m^2
Dissolved air flotation - operating pressure	DAFOP	5[4]	(V2)	bar
Percentage of pressurized water	PPW	0.2[5]	(V2)	dec. %
Pressurizer efficiency	PR_NU	0.8*	(V2)	dec. %

- Technical and/or legal constraints -			
Parameter Names	Programming Names	Default Values	Unit
Intake pumped height	IPH	4*	m
Intake pump(s) efficiency	IP_NU	0.8[6]	m

* Arbitrary default value or estimation by water treatment experts.

1. Typical values range between a few g/L to 40 g/L for settling processes (technology-dependent) but it can reach 120 g/L with modern technologies (Degrémont 2007).
2. Typical values range between a 25 g/L to 30 g/L for flotation processes (technology-dependent) (Degrémont 2007).
3. Typical values range between 3 and 10 $m^3/(m^2.h)$ (Degrémont 2007).
4. The operating pressure for dissolved air flotation is usually comprised between 4 and 7 bars (Guibelin 1999).
5. Typical values range between 7% and 12% according to the bibliographical source (Degrémont 2007), and between 10% and 50% according to the bibliographical source (CIRSEE 1999). Default value is set to 0.2 (20%).
6. Typical values range between 0.7 and 0.9. Pump efficiency could be 0.6 in case the pump is badly operated (Degrémont 2007).

One second-level script exists for each version of the model « Flocs Separation », i.e. for the settling and flotation unit process models. The name of these files is respectively « Settling_Data » and « Flotation_Data ». It contains functions and constants on which these models rely and some of them are shared. They are listed and further explained below.

The function *Sld_Dens* allows evaluating the density of the sludge produced by the settling/flotation process based on its concentration *SLC*. Sludge density is mainly determined by the high water content that has a density of 1000 kg/m^3. The dry matter of the sludge produced during drinking water treatment is mainly composed of metal hydroxide (Al or Fe) and the density of the dry matter in this kind of mineral sludge can be approximated as 1700 kg/m^3 (CIRSEE 2007). Then, the density of the sludge is evaluated by interpolation.

The sludge viscosity *Sludge_Viscosity* is set to 0.003 Pa.s as a default value in both second-level scripts but it must be noted that it can be redefined by the user in a particular context.

The default value for the specific scraping energy *Specific_Scraping_Energy* (6.786 . 1e^{-4} kWh/(m^3 of scraped sludge)) comes from a book providing one single value for a sludge produced during waste water treatment (Wang et al. 2007). This might not be a perfectly adequate value but it gives an order of magnitude and no value better suited for drinking water treatment was to be found in the literature. Nevertheless, the value of this constant can be modified according to on-site measurements for instance. In addition, the flotation process requires two sludge scrapers (one at the bottom of the tank and one at its surface), so in the file « Flotation_Data », the sludge scraping energy is doubled as an approximation of the additional energy consumption.

Two constants concerning the scheduling of sludge pumping are also defined in these second-level scripts. Indeed, sludge pumping is not a continuous process. Sludge is pumped with a pre-determined frequency and the variable *Sludge_Pumping_Cycle_Duration* (set at 180 min by default) is the duration between two pumping phases. The constant *Sludge_Pumping_Phase_Duration* (set as 20 min by default) is the duration of the phase when the sludge is pumped.

Two functions for calculating the removal of THMs and HAAs are defined in both second-level scripts (*THMs_Removal* and *HAAs_Removal*). These empirical equations come from the WTP model (WTP manual 2001) and they are used for assessing the removal of these disinfection by-products based on the TOC removal obtained during flocs separation.

$$\text{THMs\_removal} = 0.875 \times \text{TOC\_Removal} \quad [\text{dec.\%}] \qquad (111)$$

$$\text{HAAs\_removal} = 0.776 \times \text{TOC\_Removal} \quad [\text{dec.\%}] \qquad (112)$$

It must be noted that the same removal is considered for every THM even if they might not be equally removed from the water. The same approximation is done for HAAs.

One supplementary constant is defined in the file « Flotation_Data » and it concerns the air dissolution ratio. This is the decimal percentage of saturated air concentration that must be reached by the water pressurization for air bubbling during the flotation process. For example, at a fixed temperature, the saturated air concentration in water is about X mg/L. Then, the water pressurization will be operated in order to reach an air concentration in water equal to : (Air_Dissolution_Ratio x X). The constant *Air_Dissolution_Ratio* is set at 0.7 by default (Degrémont 2007).

4.2 Energy and chemical consumptions

There is no chemical consumption generated by flocs separation processes and the only form of energy consumed is electricity.

Electricity consumption

Electricity consumption for intake pumping

$$\text{Int\_Spec\_Elec\_Cons} = \text{Elec\_Consumption}\,(\text{Water\_Flow, IPH, IP\_NU}) \qquad [\text{kWh/kg pumped water}] \qquad (113)$$

$$\text{Intake\_Elec\_Cons} = \text{Int\_Spec\_Elec\_Cons} \times \text{Water} \qquad [\text{kWh}] \qquad (114)$$

Electricity consumption for sludge pumping

Sludge pumping is not a continuous process. Sludge is pumped with a pre-determined frequency. So, the quantity of pumped sludge is known but it must be taken into account that it is pumped with a higher flow in a shorter time.

$$\text{Pumped\_Sludge\_Flow} = \text{Sludge\_Flow} \times \frac{\text{Sludge\_Pumping\_Cycle\_Duration}}{\text{Sludge\_Pumping\_Phase\_Duration}} \qquad [\text{kg pumped sludge /s}] \qquad (115)$$

$$\text{Sld\_Pump\_Spec\_Elec\_Cons} = \text{Elec\_Consumption}\,(\text{Pumped\_Sludge\_Flow, IPH, rho} = \text{Sludge\_Density, mhu} = \text{Sludge\_Viscosity}) \qquad [\text{kWh/kg pumped sludge}] \qquad (116)$$

$$\text{Sld\_Pump\_Elec\_Cons} = \text{Sld\_Pump\_Spec\_Elec\_Cons} \times \text{Sludge} \qquad [\text{kWh}] \qquad (117)$$

- The variables *Sludge_Flow* [kg/s] and *Sludge* [kg] are calculated beforehand in the main scripts but these mass balances are presented only at a later stage in the description of these models.

It must be noted that it is assumed that the pumped height for sludge pumping is equal to the pumped height for intake pumping *IPH*. It might not be true and it can be modified in the scripts if the appropriate value is known. Nevertheless, these two pumped heights are of the same order of magnitude.

Electricity consumption for sludge scraping

$$\text{Sld\_Scraping\_Energy} = \text{Specific\_Scraping\_Energy} \times \frac{\text{Sludge}}{\text{Sludge\_Density}} \qquad [\text{kWh}] \qquad (118)$$

Total electricity consumption (V1)

$$\text{Total\_Elec\_Cons} = \text{Intake\_Elec\_Cons} + \text{Sld\_Pump\_Elec\_Cons} + \text{Sld\_Scraping\_Energy} \qquad [\text{kWh}] \qquad (119)$$

Electricity consumption for pressurizing water and air (blowing air) (V2)

$$\text{Pressurized\_Water\_Flow} = \text{PPW} \times \text{Water\_Flow} \qquad [\text{kg/s}] \qquad (120)$$

$$\text{Saturated\_Air\_Concentration} = 23.0 \times \left(\text{DAFOP} \cdot 10^{-5}\right) \qquad [\text{mgAir/L}] \qquad (121)$$

$$\text{Air\_Concentration} = \text{Air\_Dissolution\_Ratio} \times \text{Saturated\_Air\_Concentration} \qquad [\text{mgAir/L}] \qquad (123)$$

The saturated air concentration in water at a pressure of 1 atm is 23.0 mgAir/L. The assumption of equation 121 consists in considering the variation of the *Saturated_Air_Concentration* to be proportional to the operating pressure *DAF_Operating_Pressure* (Engineering tool box website).

$$\text{Air\_Mass\_Flow} = \text{Air\_Concentration} \times \text{Pressurized\_Water\_Flow} \times 10^{-6} \qquad [\text{kgAir/s}] \qquad (124)$$

$$\text{Air\_Density} = 1.293 \qquad [\text{kg/Nm}^3] \qquad (125)$$

$$\text{Air\_Flow} = \frac{\text{Air\_Mass\_Flow}}{\text{Air\_Density}} \qquad [\text{Nm}^3/\text{s}] \qquad (126)$$

$$\text{Air\_Flow\_Ratio} = \frac{\text{Air\_Flow} \times \text{Water\_Density}}{\text{Water\_Flow}} \qquad [\text{Nm}^3 \text{ of air/m}^3 \text{ of water}] \qquad (127)$$

$$\text{Delta\_Pressure} = \text{DAFOP} - \text{Absolute\_Pressure} \qquad [\text{Pa}] \qquad (128)$$

$$\text{Air\_Pressurizer\_Power} = \frac{\text{Air\_Mass\_Flow} \times \text{Delta\_Pressure}}{\text{Air\_Density} \times \text{PR\_NU}} \qquad [\text{W}] \qquad (129)$$

$$\text{Water\_Pressurizer\_Power} = \frac{\text{Pressurized\_Water\_Flow} \times \text{Delta\_Pressure}}{\text{Water\_Density} \times \text{PR\_NU}} \qquad [\text{W}] \qquad (130)$$

$$\text{Pressurizer\_Power} = \text{Air\_Pressurizer\_Power} + \text{Water\_Pressurizer\_Power} \qquad [\text{W}] \qquad (131)$$

$$\text{Spec\_Pressurizing\_Energy} = \frac{\text{Pressurizer\_Power}}{\text{Water\_Flow} \times 3600} \qquad [\text{kWh/kg of input water}] \qquad (132)$$

$$\text{Pressurizing\_Energy} = \text{Spec\_Pressurizing\_Energy} \times \text{Water} \qquad [\text{kWh}] \qquad (133)$$

Total electricity consumption (V2)

$$\begin{aligned}\text{Total\_Elec\_Cons} &= \text{Intake\_Elec\_Cons} + \text{Sld\_Pump\_Elec\_Cons} \\ &+ \text{Sld\_Scraping\_Energy} + \text{Pressurizing\_Energy}\end{aligned} \qquad [\text{kWh}] \qquad (134)$$

4.3 Output water quality data

Dry matter flows

The value of suspended matter before the coagulation *SM_Before_Coag* is imported from the file « SM_Information ». Indeed, this value is required because the efficiency of SM removal *SM_NU* as defined for the settling/flotation process refers to the SM value before coagulation. Dry matter flows in the input water, clarified water and sludge are then calculated.

$$\text{Water\_Dry\_Matter\_Flow} = \text{Water\_Flow} \times \text{SM} \qquad [\text{mgSM/s}] \qquad (135)$$

$$\text{Clarified\_Water\_Dry\_Matter\_Flow} = \text{Water\_Flow} \times \text{SM\_Befor\_Coag} \times (1 - \text{SM\_NU}) \qquad [\text{mgSM/s}] \qquad (136)$$

$$\text{Sludge\_Dry\_Matter\_Flow} = \text{Water\_Dry\_Matter\_Flow} - \text{Clarified\_Water\_Dry\_Matter\_Flow} \qquad [\text{mgSM/s}] \qquad (137)$$

Conversion rate of the process and water/sludge flows

$$\text{Sludge\_Density} = \text{Sld\_Dens(Sludge\_Concentration)} \qquad [\text{kg/m}^3] \qquad (138)$$

$$\text{Sludge\_Flow} = \frac{\text{Sludge\_Dry\_Matter\_Flow} \times \text{Sludge\_Density}}{\text{SLC} \times 1000} \qquad [\text{kg/s}] \qquad (139)$$

$$\text{Clarified\_Water\_Flow} = \text{Water\_Flow - Sludge\_Flow} \qquad [\text{kg/s}] \qquad (140)$$

$$\text{Conversion\_Rate} = \frac{\text{Clarified\_Water\_Flow}}{\text{Water\_Flow}} \qquad [\text{dec.\%}] \qquad (141)$$

$$\text{Max\_Clarified\_Water\_Flow} = \text{Max\_Water\_Flow} \times \text{Conversion\_Rate} \qquad [\text{kg/s}] \qquad (142)$$

$$\text{Max\_Sludge\_Flow} = \text{Max\_Water\_Flow - Max\_Clarified\_Water\_Flow} \qquad [\text{kg/s}] \qquad (143)$$

$$\text{Clarified\_Water} = \text{Water\_Flow} \times \text{Conversion\_Rate} \qquad [\text{kg}] \qquad (144)$$

$$\text{Sludge} = \text{Water - Clarified\_Water} \qquad [\text{kg}] \qquad (145)$$

Elimination ratio between coagulated water and clarified water

This is the ratio between the suspended matter SM in the clarified water and the suspended matter SM in the water entering the settling (or flotation) process. In other words, the value (1-SM_Elimination ratio) is equal to the SM removal efficiency with regard to the suspended matter SM after coagulation (stored as *SM_After_Coag* in the file « SM_Information »).

$$\text{SM\_Elimination\_Ratio} = (1 - \text{SM\_NU}) \times \frac{1}{\text{Conversion\_Rate}} \times \frac{\text{SM\_Before\_Coag}}{\text{SM}} \qquad [\text{dec.\%}] \qquad (146)$$

Suspended matter and organic matter in the clarified water

The non-dissolved compounds (i.e. particulate compounds) are assumed to be removed by settling (or flotation) in the same proportion as the suspended matter (i.e. *SM_Elimination_Ratio* considering the concentrations in coagulated water). The dissolved compounds of coagulated water are not removed by the flocs separation process.

$$\text{Clarified\_Water\_SM} = \text{SM\_Elimination\_Ratio} \times \text{SM} \qquad [\text{mg/L}] \qquad (147)$$

$$\text{Clarified\_Water\_Turbidity} = \frac{\text{Clarified\_Water\_SM}}{\text{SM\_Turbidity\_Ratio}} \qquad [\text{NTU}] \qquad (148)$$

$$\text{Clarified\_Water\_POC} = \text{SM\_Elimination\_Ratio} \times \text{POC} \qquad [\text{mg/L}] \qquad (149)$$

$$\text{Clarified\_Water\_DOC} = \text{DOC} \qquad [\text{mg/L}] \qquad (150)$$

$$\text{Clarified\_Water\_TOC} = \text{Clarified\_Water\_POC} + \text{Clarified\_Water\_DOC} \qquad [\text{mg/L}] \qquad (151)$$

$$\text{Clarified\_Water\_UVA} = \text{UVA} \qquad [\text{m}^{-1}] \qquad (152)$$

$$\text{Clarified\_Water\_COD} = \text{Clarified\_Water\_TOC} \times \text{COD\_TOC\_Ratio} \qquad [\text{mgO}_2\text{/L}] \qquad (153)$$

$$\text{Clarified\_Water\_BOD5} = \frac{\text{Clarified\_Water\_COD}}{\text{COD\_BOD5\_Ratio}} \qquad [\text{mgCOD/mgBOD5}] \quad (154)$$

$$\text{Clarified\_Water\_BOD} = \frac{\text{Clarified\_Water\_BOD5}}{\text{BOD5\_BOD\_Ratio}} \qquad [\text{mgBOD5/mgBOD}] \quad (155)$$

$$\text{Clarified\_Water\_DOC\_TOC\_Ratio} = \frac{\text{Clarified\_Water\_DOC}}{\text{Clarified\_Water\_TOC}} \qquad [\text{mgDOC/mgTOC}] \quad (156)$$

$$\text{Clarified\_Water\_Color} = \frac{\text{Clarified\_Water\_UVA}}{\text{UVA\_Color\_Ratio}} \qquad [\text{mg Pt-Co/L}] \qquad (157)$$

Concentration of pathogenic micro-organisms in the clarified water

The *mean elimination capacity (MEC)* for every pathogenic micro-organisms is taken from Smeets et al. (Smeets et al. 2006). This research work was part of a European Union project on microbiological risk assessment in drinking water production. It allows assessing the removal of the main pathogenic microorganisms by different water treatment processes.

The *mean elimination capacity (MEC)* is equivalent to the average removal of a pathogenic micro-organism. A MEC value is the ratio of the number of microorganisms between the input and the output of the process, expressed with the log_{10} function.

The calculation of the concentrations of pathogenic micro-organisms is expressed in a generic sense in the following equations.

$$\text{Microorganism\_I/O\_Ratio} = 10^{\text{MEC}} \qquad [\text{dec.\%}] \qquad (158)$$

$$\text{Output\_Microorganism} = \frac{\text{Input\_Microorganism}}{\text{Microorganism\_I/O\_Ratio}} \qquad [\text{nb/L}] \qquad (159)$$

The algae removal *Algae_Removal* is taken from Baudin et al. (Baudin et al. 2006). The value is 80% for the settling process and 90% for the flotation process. Indeed, one advantage of the flotation process is that it removes algae from water more efficiently.

$$\text{Output\_Algae} = \text{Input\_Algae} \times (1 - \text{Algae\_Removal}) \qquad [\text{nb/L}] \qquad (160)$$

Concentration of salt precipitates in the clarified water

The dissolved salts are obviously not removed from the water but on the contrary, the salt precipitates ($Fe(OH)_3$, MnO_2, $Al(OH)_3$, SiO_2, $CaCO_3$) are removed in the same proportion as the suspended matter. So the total concentrations of Fe, Mn, Al, Si, Ca and C in the clarified water are calculated taking into account the removal of salt precipitates. Their dissolved concentration does not change. The calculation is presented below in a generic sense.

$$\begin{aligned}&\text{Clarified\_Water\_X\_Total} = \text{Input\_Water\_X\_Dissolved} \\ &+ \big((\text{Input\_Water\_X\_Total} - \text{Input\_Water\_X\_Dissolved}) \times \text{SM\_Elimination\_Ratio}\big)\end{aligned}$$

$$[\text{mg/L}] \qquad (161)$$

PAC concentration in the clarified water

$$\text{Clarified\_Water\_PAC} = \text{SM\_Elimination\_Ratio} \times \text{Input\_Water\_PAC}$$

$$[\text{mg/L}] \qquad (162)$$

Concentration of disinfection by-products in the clarified water

THMs and HAAs have been adsorbed on flocs formed during the previous coagulation step. Then, the settling (or flotation) step is responsible from their removal.

The WTP model approximates the THMs and HAAs removal due to coagulation and settling (or flotation) as a proportion of the TOC removal (WTP manual 2001). The functions *THMs_Removal* and *HAAs_Removal*, defined in the second-level scripts, are used for this calculation. The calculation is presented in a generic sense for any THM or any HAA.

$$\text{TOC\_Removal} = \frac{\text{Input\_Water\_TOC} - \text{Clarified\_Water\_TOC}}{\text{Input\_Water\_TOC}} \qquad [\text{dec.\%}] \qquad (163)$$

$$\text{Clarified\_Water\_THM\_X} = \text{Input\_Water\_THM\_X} \times \big(1 - \text{THMs\_Removal}(\text{TOC\_Removal})\big)$$

$$[\text{mg/L}] \qquad (164)$$

$$\text{Clarified\_Water\_HAA\_X} = \text{Input\_Water\_HAA\_X} \times \big(1 - \text{HAAs\_Removal}(\text{TOC\_Removal})\big)$$

$$[\text{mg/L}] \qquad (165)$$

Water quality data of the sludge

At this point, the water quality data of the input water (i.e. the coagulated water) and the output water (i.e. the clarified water) are all known. Therefore, the water quality data of the sludge produced during flocs separation is calculated based on conventional mass balances as shown in the following generic equation.

$$\text{Sludge\_X} = \frac{\left(\left(\text{Water\_Flow} \times \text{Input\_Water\_X}\right) - \left(\text{Clarified\_Water\_Flow} \times \text{Clarified\_Water\_X}\right)\right)}{\text{Sludge\_Flow}}$$

[Unit corresponding to the water quality under consideration] (166)

- *Sludge_X* : Value of the water quality data in the sludge.
- *Input_Water_X* : Value of the water quality data in the input water (i.e. the coagulated water).
- *Clarified_Water_X* : Value of the water quality data in the clarified water.

4.4 Engineering design facts

General characteristics of the settling (or flotation) tank(s)

The following technical design facts are calculated and reported by the main script of the unit process model :

- Numbers of tank(s) to be installed [no unit]
- Numbers of tank(s) in use [no unit]
- Tank(s) height [m]
- Total settling/flotation surface [m^2]
- Total settling/flotation surface required with regard to the nominal water flow [m^2]
- User-defined surface hydraulic charge [$m^3/(m^2.h)$]
- Real surface hydraulic charge [kgWater/(m^2.s)]
- Real hydraulic residence time [min]
- Settled/Flotated mass flow of suspended matter [kgSM/(m^2.j)]

The nominal flow that is studied is lower than the maximum one. If some of the settling/flotation tanks are disconnected, the hydraulic residence time and the surface hydraulic charge can be kept approximately constant. If the settling/flotation tanks are not disconnected, the hydraulic residence time is higher and the surface hydraulic charge is lower.

In this case, it is considered that some settling/flotation tanks are disconnected when possible in order to keep the hydraulic residence time and the surface hydraulic charge almost constant (lowering the surface hydraulic charge).

The technical design facts of the settling/flotation process are calculated from the following equations :

$$\text{Total\_Surface} = \frac{\text{Max\_Water\_Flow} \times 3600}{\text{SHC} \times \text{Water\_Density}} \qquad [\text{m}^2] \qquad (167)$$

$$\text{Tanks\_Number} = \text{floor}\left(\frac{\text{Total\_Surface}}{\text{STS}}\right) + 1 \qquad [\text{no unit}] \qquad (168)$$

$$\text{Tank\_Height} = \text{HRT} \times \text{SHC} \times 60 \qquad [\text{m}] \qquad (169)$$

$$\text{Required\_Total\_Surface} = \frac{\text{Water\_Flow} \times 3600}{\text{SHC} \times \text{Water\_Density}} \qquad [\text{m}^2] \qquad (170)$$

$$\text{Tanks\_In\_Use\_Number} = \text{floor}\left(\frac{\text{Required\_Total\_Surface}}{\text{STS}}\right) + 1 \qquad [\text{Tanks in use}] \qquad (171)$$

$$\text{Total\_Surface\_In\_Use} = \text{Tanks\_In\_Use\_Number} \times \text{STS} \qquad [\text{m}^2] \qquad (172)$$

$$\text{Real\_SHC} = \frac{\text{Water\_Flow}}{\text{Total\_Surface\_In\_Use}} \qquad [\text{kgWater}/(\text{m}^2.\text{s})] \qquad (173)$$

$$\text{Real\_HRT} = \frac{\text{STS} \times \text{Tank\_Height} \times \text{Tank\_In\_Use\_Number} \times \text{Water\_Density}}{\text{Water\_Flow} \times 60}$$

$$[\text{min}] \qquad (174)$$

$$\text{SM\_Mass\_Flow} = \frac{\text{Water\_Flow} \times \text{SM} \times \text{SM\_NU} \times 3600 \times 24}{\text{Total\_Surface\_In\_Use} \times 10^6} \qquad [\text{kgSM}/(\text{m}^2.\text{j})] \qquad (175)$$

Nominal and maximum sludge flows

The nominal and maximum sludge flows are reported and this information is interesting at the design stage of a drinking water treatment plant since sludge disposal is often an issue for plant operators.

Design facts on air pressurization

The following design facts relative to air pressurization for dissolved air flotation are reported as well :

- Percentage of pressurized water to be recirculated [no unit - decimal percentage]
- Air flow ratio [Nm^3 of air / m^3 of input water]

Electricity consumptions and electrical powers

The following design facts relative to electricity consumptions and electrical powers are stored in the engineering design report :

- Specific electricity consumption for intake pumping [kWh/kgWater]
- Electricity consumption for intake pumping [kWh]
- Pumping power installed for intake pumping [kW]
- Pumping power used for intake pumping [kW]
- Specific electricity consumption for sludge pumping [kWh/kg of sludge]
- Electricity consumption for sludge pumping [kWh]
- Pumping power installed for sludge pumping [kW]
- Pumping power used for sludge pumping [kW]
- Specific sludge scraping energy [kWh/kg of sludge]
- Electricity consumption for sludge scraping [kWh]
- Total electricity consumption [kWh]

The following design facts are specific of the flotation process and they are reported as well in the corresponding design report :

- Specific pressurizing energy [kWh/kg clarified water]
- Electricity consumption due to air and water pressurizing [kWh]
- Power for air and water pressurizing [kW]

The electricity consumption for air and water pressurizing is obviously taken into account in the total electricity consumption of the flotation process.

5. Media filtration

Four versions of the « Media filtration » model have been developed during the project. Rapid filtration is considered in all the versions of the model because it is much more current than slow filtration. The retrofit approach is not available since media filtration processes do not generate any chemical consumption.

The four different model versions for the process category « Media Filtration» are listed below :

- Version 1 (V1) : *Rapid_Sand_Filtration* (predictive model).
- Version 2 (V2) : *Rapid_Anthracite_Filtration* (predictive model).
- Version 3 (V3) : *Rapid_Biolite_Filtration* (predictive model).
- Version 4 (V4) : *Rapid_GAC_Filtration* (predictive model).

5.1 Parameters of the unit process model

The model parameters for the unit process « Media Filtration » are presented in table 5.

Table 5. Parameters for the different versions of the unit process model « Media Filtration ».

- Engineering design facts and/or operating conditions -			
Parameter	Programming Names	Default Values	Unit
Backwash duration - Phase 1	BDP1	3^* (V1/V2/V3) 5^* (V4)	min
Backwash duration - Phase 2	BDP2	8^* (V1/V2/V3) 3^* (V4)	min
Backwash duration - Phase 3	BDP3	5^* (V1/V2/V3) 10^* (V4)	min
Backwash air flow - Phase 1	BAF1	2400^* (V1/V2/V3) 2200^* (V4)	Nm^3/h
Backwash air flow - Phase 2	BAF2	2400^* (V1/V2/V3) 2200^* (V4)	Nm^3/h
Backwash water flow - Phase 2	BWF2	260^* (V1/V2/V3) 800^* (V4)	m^3/h
Backwash water flow - Phase 3	BWF3	800^* (V1/V2/V3) 800^* (V4)	m^3/h
Air compressor(s) efficiency	AC_NU	0.1[1]	dec.%
Backwash pumps efficiency	BWPNU	0.8[2]	dec.%
Filtration cycle duration	FCD	4^* (V1/V2/V3) 8^* (V4)	days
Maximum filtered water in one cycle	MAXFW	15000^* (V1/V2/V3) 12000^* (V4)	M^3
Theoretical filter capacity	TFC	1000^*	$g/\ m^3$
Filter(s) surface	FS	40^*	m^2
Filtration nominal speed	FNS	3.5^* (V1/V2/V3) 10^* (V4)	m/h
Water height in the filter(s)	WH	0.35^* (V1/V2/V3) 1^* (V4)	m
Maximum water height in the filter(s)	MAXWH	1^* (V1/V2/V3) 1.8^* (V4)	m
Media height in the filter(s)	MH	0.8^* (V1/V2/V3) 1^* (V4)	m
Optimisation of the number of filters [3]	NOFO	0	No unit
Media apparent density	MAD	1460^* (V1) 730^* (V2) 1200^* (V3) 480^* (V4)	kg/m^3
Media density	MD	2600^* (V1)	kg/m^3

		1450* (V2) 2000* (V3) 1200* (V4)	
Media annual replacing rate [4]	MARR	0.005 (V1/V2/V3)	dec.%
Turbidity filtration efficiency	TUEFF	0.833	dec.%
GAC regeneration duration	GACRD	15* (V4)	days
GAC regeneration frequency [5]	GACRF	50* (V4)	Unit [5]
GAC replacing rate after each regeneration [7]	GACRR	0.08 (V4)	dec.%
GAC substitution rate [8]	GACSR	0.25 (V4)	dec.%
Filter working rate [9]	FWR	6 (V4)	Unit [10]

- Technical and/or legal constraints -

Parameter Names	Programming Names	Default Values	Unit
Intake pumped height	IPH	1.15* (V1/V2/V3) 2* (V4)	m
Intake pump(s) efficiency	IP_NU	0.8[2]	m

* Arbitrary default value or estimation by water treatment experts.

1. Typical values for chemical mixing in drinking water treatment range between 400 s^{-1} and 1000 s^{-1}. (CIRSEE 1999, Degrémont 2007).
2. Typical values range between 0.7 and 0.9. Pump efficiency could be 0.6 in case the pump is badly operated (Degrémont 2007).
3. The value of this parameter should be 1 if one considers that the inlets of some filters are closed when the flow is not maximum in order to maintain a nominal water flow in each filter in use. The default value is 0, which means that the number of filters in operation is not optimised.
4. This parameter represents the percentage of filter's media lost per year because of backwashing and its value must be less than 0.02 (2%). Otherwise, it means that too much filter's media is escaping the filter during backwashing, so the filter is not functioning properly.
5. The value given to this parameter must be well adapted and the filters' regeneration schedule must be well planned. It is a crucial issue when operating GAC filtration.
6. Unit = Number of filtration cycles before regenerating the GAC.
7. This is an empirical value (7-10 %), representing the GAC that must be replaced because of GAC losses due to regeneration (Degrémont 2007).
8. This is the rate of the GAC substitution in case the GAC is not regenerated but completely replaced instead.
9. This is a ratio between the treated water flow [m^3/h] and the GAC volume [m^3 of GAC] in the filter bed. It is a very important design parameter.
10. Unit = (m^3 of water) / (m^3 of GAC. h).

There is only one second-level script and it is relative to the rapid GAC filtration model. This file defines a Python^{TM} dictionary, named « GAC_Removal_Rate_Dictionnary », and it contains the removal rates of all water compounds (appendix 2-1) due to adsorption on GAC. Indeed, the GAC filter is responsible for adsorption of dissolved water compounds besides physical separation of particulate compounds. Default values have been established in this Python^{TM} dictionary in accordance with experts' judgement (20% by default) but these removal rates are highly dependent on the water compounds and the type of GAC. So they should be user-defined as much as possible. Indeed, activated carbon can be obtained from numerous raw materials and by numerous activation/production processes, thus leading to a wide variety of GAC and related properties.

5.2 Energy and material consumptions

There is no chemical consumption during media filtration. The only material that can be consumed is the filters' media (sand, anthracite, biolite or GAC). This material is consumed when the filters' backwashing are badly operated and some of the filters' media is lost with backwash waters (Degrémont 2007). The only form of energy consumed is electricity.

Number of filters, water flow treated by each filter in use and duration of the filtration cycle

Number of filters installed and used

The number of filters in use is determined depending on whether one chooses to optimise their number or not (parameter *NOFO*). The water flow treated by each filter in use is then calculated.

$$\text{Nominal\_Filter\_Water\_Flow} = \frac{\text{FNS} \times \text{FS} \times \text{Water\_Density}}{3600} \qquad \text{[kg/(s.filter)]} \quad (176)$$

$$\text{Number\_Of\_Filters\_Installed} = \text{floor}\left(\frac{\text{Max\_Water\_Flow}}{\text{Nominal\_Filter\_Water\_Flow}}\right) + 1 \qquad \text{[no unit]} \quad (177)$$

$$\text{If NOFO} = 1 \quad \text{then} \quad \text{Number\_Of\_Filters\_In\_Use} = \text{floor}\left(\frac{\text{Water\_Flow}}{\text{Nominal\_Filter\_Water\_Flow}}\right) + 1 \qquad \text{[no unit]} \quad (178)$$

$$\text{If NOFO} \neq 1 \quad \text{then} \quad \text{Number\_Of\_Filters\_In\_Use} = \text{Number\_Of\_Filters\_Installed} \qquad \text{[no unit]} \quad (179)$$

Water flow treated by each filter in use

$$\text{Filter\_Water\_Flow} = \frac{\text{Water\_Flow}}{\text{Number\_Of\_Filters\_In\_Use}} \qquad [\text{kg/s}] \qquad (180)$$

Duration of the filtration cycle

The filters' backwashing is launched prematurely (i.e. before the end of the regular filtration cycle) in case :

- The maximum amount of water that could be filtered without backwashing (parameter *MAXFW*) is reached.
- The filter is clogged (parameter TFC) so the filtration is not operated correctly.

The duration of the filtration cycle is consequently reduced, as shown in the following logical equations.

$$\text{FCD\_2} = \frac{\text{MAXFW} \times \text{Water\_Density}}{\text{Filter\_Water\_Flow} \times 3600 \times 24} \qquad [\text{days}] \qquad (181)$$

$$\text{Filter\_Volume} = \text{FS} \times \text{MH} \qquad [\text{m}^3] \qquad (182)$$

$$\text{FCD\_3} = \frac{\text{TFC} \times \text{Filter\_Volume} \times 1000}{\text{Filter\_Water\_Flow} \times \text{SM} \times 3600 \times 24} \qquad [\text{days}] \qquad (183)$$

$$\text{Filtration\_Cycle\_Duration} = \text{FCD} \qquad [\text{days}] \qquad (184)$$

$$\text{If } \text{FCD\_2} \le \text{FCD} \text{ then } \text{Filtration\_Cycle\_Duration} = \text{FCD\_2} \qquad [\text{days}] \qquad (185)$$

$$\text{If } \text{FCD\_3} \le \text{FCD} \text{ then } \text{Filtration\_Cycle\_Duration} = \text{FCD\_3} \qquad [\text{days}] \qquad (186)$$

$$\text{Filtration\_Cycle\_Duration} = \text{Filtration\_Cycle\_Duration} \times 24 \times 3600 \qquad [\text{s}] \qquad (187)$$

Consumption of air and water for the backwash of one filter

Air consumption for the backwash of one filter

$$\text{M\_Air} = (0.2 \times 2 \times 15.999) + (0.8 \times 2 \times 14.007) \qquad [\text{g/mol}] \qquad (188)$$

Assumption : Air is composed of 80% of N2 and 20% of O2.

$$\text{Air\_Density} = \frac{\text{M\_Air} \times \text{Absolute\_Pressure}}{8.3145 \times \text{Temperature} \times 1000} \qquad [\text{kg/m}^3] \qquad (189)$$

Assumption : The air is assimilated to a perfect gas and the air temperature is equal to the water temperature.

$$\text{Air\_Volume\_per\_Filter\_Backwash} = \frac{(\text{BAF1} \times \text{BDP1}) + (\text{BAF2} \times \text{BDP2})}{60}$$

[Nm^3/filter's backwash] (190)

$$\text{Air\_Mass\_per\_Filter\_Backwash} = \frac{\text{Air\_Volume\_per\_Filter\_Backwash} \times 10^5 \times \text{M\_Air}}{8.3145 \times 273.15 \times 10^3}$$

[kg/filter's backwash] (191)

Water consumption the backwash of one filter

$$\text{Water\_Volume\_per\_Filter\_Backwash} = \frac{(\text{BWF2} \times \text{BDP2}) + (\text{BWF3} \times \text{BDP3})}{60}$$

[m^3/filter's backwash] (192)

$$\text{Water\_Mass\_per\_Filter\_Backwash} = \text{Water\_Volume\_per\_Filter\_Backwash} \times \text{Water\_Density}$$

[kg/filter's backwash] (193)

Filtered water, backwash waters and backwash air

Filtered water

$$\text{Filtered\_Water\_per\_Cycle} = (\text{Water\_Flow} \times \text{Filtration\_Cycle\_Duration}) - (\text{Number\_Of\_Filters\_In\_Use} \times \text{Water\_Mass\_per\_Filter\_Backwash})$$

[kg/cycle] (194)

$$\text{Filtered\_Water\_Flow} = \frac{\text{Filtered\_Water\_per\_Cycle}}{\text{Filtration\_Cycle\_Duration}}$$

[kg/s] (195)

$$\text{Filtration\_Conversion\_Rate} = \frac{\text{Filtered\_Water\_Flow}}{\text{Water\_Flow}}$$

[dec.%] (196)

$$\text{Max\_Filtered\_Water\_Flow} = \text{Max\_Water\_Flow} \times \text{Filtration\_Conversion\_Rate}$$

[kg/s] (197)

$$\text{Filtered\_Water} = \text{Water} \times \text{Filtration\_Conversion\_Rate}$$

[kg] (198)

Backwash waters

$$\text{Backwash\_Waters\_Flow} = \frac{\text{Number\_Of\_Filters\_In\_Use} \times \text{Water\_Mass\_per\_Filter\_Backwash}}{\text{Filtration\_Cycle\_Duration}}$$

[kg/s] (199)

$$\text{Max\_Backwash\_Waters\_Flow} = \text{Max\_Water\_Flow} \times (1 - \text{Filtration\_Conversion\_Rate})$$

[kg/s] (200)

$$\text{Spec\_Backwash\_Water} = \frac{\text{Number\_Of\_Filters\_In\_Use} \times \text{Water\_Mass\_per\_Filter\_Backwash}}{\text{Filtered\_Water\_per\_Cycle}}$$

[kg backwash waters/kg filtered water] (201)

$$\text{Backwash\_Water} = \text{Spec\_Backwash\_Water} \times \text{Filtered\_Water}$$

[kg backwash waters] (202)

Backwash air

$$\text{Backwash\_Air\_Flow} = \frac{\text{Number\_Of\_Filters\_In\_Use} \times \text{Air\_Mass\_per\_Filter\_Backwash}}{\text{Filtration\_Cycle\_Duration}}$$

[kg/s] (203)

$$\text{Max\_Backwash\_Air\_Flow} = \text{Backwash\_Air\_Flow} \times \frac{\text{Max\_Backwash\_Waters\_Flow}}{\text{Backwash\_Waters\_Flow}}$$

[kg/s] (204)

$$\text{Spec\_Backwash\_Air} = \frac{\text{Number\_Of\_Filters\_In\_Use} \times \text{Water\_Mass\_per\_Filter\_Backwash}}{\text{Filtered\_Water\_per\_Cycle}}$$

[kg backwash air/kg filtered water] (205)

$$\text{Backwash\_Air} = \text{Spec\_Backwash\_Air} \times \text{Filtered\_Water}$$

[kg backwash air] (206)

Material consumption (V1/V2/V3)

Losses of filter's media

$$\text{Annual\_Media\_Losses} = \text{MARR} \times \text{Filter\_Volume} \times \text{MAD} \times \text{Number\_Filters\_In\_Use}$$

[kg/year] (207)

$$\text{Spec\_Media\_Losses} = \frac{\text{Annual\_Media\_Losses}}{\text{Filtered\_Water\_Flow} \times 3600 \times 24 \times 365}$$

[kg/kg of filtered water] (208)

$$\text{Media\_Losses} = \text{Spec\_Media\_Losses} \times \text{Filtered\_Water}$$ [kg] (209)

GAC consumption (V4)

The following calculations establish the quantity of GAC that must be regenerated and the quantity of GAC that must be produced in relation to the filtered water quantity. The related environmental impacts can then be assessed in a subsequent step.

The production of GAC is required in two cases : 1/ to replace the proportion of GAC that needs to be replaced (parameter *GACSR*) and 2/ to compensate the GAC losses occurring during the GAC regeneration (parameter *GACRR*).

Quantity of GAC to be treated (regeneration or replacement)

It represents the whole annual GAC quantity that must be treated, either regenerated or simply replaced.

$$\text{Annual\_GAC\_To\_Be\_Treated} = \frac{\text{Filter\_Volume} \times \text{MAD} \times \text{Number\_Of\_Filters\_In\_Use}}{\text{GACRF} \times \left(\text{Filtration\_Cycle\_Duration} \big/ (3600 \times 24 \times 365) \right)}$$

[kgGAC/year] (210)

Quantity of GAC to be regenerated

It represents the annual GAC quantity that must be regenerated.

$$\text{Annual\_GAC\_To\_Be\_Regenerated} = \text{Annual\_GAC\_To\_Be\_Treated} \times (1 - \text{GACSR})$$

[kgGAC/year] (211)

Annual GAC losses

The regeneration of the GAC material causes GAC losses due to the regeneration process itself. It must be noted that the regeneration is not operated in the drinking water treatment plant but in a specific plant. In fact, GAC is used in the drinking water treatment plant, but it is produced and regenerated elsewhere.

Nevertheless, these GAC losses are calculated, since the regeneration of GAC generates an environmental impact which must include the production of some additional GAC to replace the losses due to the regeneration of the initial GAC. The rationale is that the mass of GAC returned after regeneration must be the same to correctly fill the filters' bed.

$$\text{Annual\_GAC\_Losses} = \text{Annual\_GAC\_To\_Be\_Regenerated} \times \text{GACRR}$$

[kgGAC/year] (212)

Quantities of GAC that must be regenerated in relation to the quantity of filtered water

$$\text{Spec\_GAC\_To\_Be\_Regenerated} = \frac{\text{Annual\_GAC\_To\_Be\_Regenerated}}{\text{Filtered\_Water\_Flow} \times 3600 \times 24 \times 365}$$

[kgGAC/kg filtered water] (213)

$$\text{GAC\_To\_Be\_Regenerated} = \text{Spec\_GAC\_To\_Be\_Regenerated} \times \text{Filtered\_Water}$$

[kgGAC] (214)

Quantity of GAC to be replaced

It represents the annual GAC quantity that must be replaced.

$$\text{Annual\_GAC\_To\_Be\_Replaced} = \text{Annual\_GAC\_To\_Be\_Treated} \times \text{GACSR}$$

[kgGAC/year] (215)

Quantities of GAC that must be produced relatively to the quantity of filtered water

$$\text{Spec\_GAC\_To\_Be\_Produced} = \frac{\text{Annual\_GAC\_To\_Be\_Replaced} + \text{Annual\_GAC\_Losses}}{\text{Filtered\_Water\_Flow} \times 3600 \times 24 \times 365}$$

[kgGAC/kg filtered water] (216)

$$\text{GAC\_To\_Be\_Produced} = \text{Spec\_GAC\_To\_Be\_Produced} \times \text{Filtered\_Water}$$

[kgGAC] (217)

Electricity consumption

Electricity consumption for intake pumping

$$\text{Specific\_Elec\_Cons} = \text{Elec\_Consumption (Water\_Flow, IPH, IP\_NU)}$$

[kWh/kg pumped water] (218)

$$\text{FW\_Spec\_Elec\_Cons} = \frac{\text{Specific\_Elec\_Cons}}{\text{Filtration\_Conversion\_Rate}}$$

[kWh/kg filtered water] (219)

$$\text{Intake\_Elec\_Cons} = \text{Specific\_Elec\_Cons} \times \text{Water}$$ [kWh] (220)

Electricity consumption for backwash water pumping

The filter's media (e.g. sand) needs to be fluidised to unclog the filter. The filter's bed needs to be fluidised at the minimum level because losses of filter's media can occur if the backwash is operated with an excessive level of fluidisation (e.g. sand would be escaping the filter's bed). This is taken into account through the parameter *MARR*. At the minimum fluidisation level, the head loss is equal to the apparent weight of the filter divided by the surface of the filter.

$$\text{Head\_Loss\_Filter\_Bed} = \frac{\text{MD - Water\_Density}}{\text{MD}} \times \frac{\text{MAD} \times \text{Filter\_Volume} \times 9.81}{\text{FS}} \quad [\text{Pa}] \qquad (221)$$

The water distributor is responsible for a certain head loss. This head loss ranges between 10% and 30% of the head loss due to the solid bed with a minimum value of 3500 Pa (Antonini 2007).

$$\text{Head\_Loss\_Water\_Distributor} = \max\left(\left(0.2 \times \text{Head\_Loss\_Filter\_Bed}\right); 3500\right) \quad [\text{Pa}] \qquad (222)$$

These two head losses are added up to obtain the total head loss to be compensated by the backwash water pumping and then, they are expressed in terms of water height to be pumped. Finally, this is added to the height of the filter (media height *MH* + maximum water height *MAXWH*) since the backwash waters must flow from the bottom to the filters up to their surface.

$$\text{Head\_Loss} = \text{Head\_Loss\_Filter\_Bed} + \text{Head\_Loss\_Water\_Distributor} \quad [\text{Pa}] \qquad (223)$$

$$\text{Head\_Loss\_Height} = \frac{\text{Head\_Loss}}{\text{Water\_Density} \times 9.81} \quad [\text{m}] \qquad (224)$$

$$\text{Total\_Backwash\_Height} = \text{MAXWH} + \text{MH} + \text{Head\_Loss\_Height} \quad [\text{m}] \qquad (225)$$

The electricity consumptions due to backwash water pumping during phases 2 and 3 are then calculated with the following equations.

$$\text{BW\_Flow\_2} = \frac{\text{BWF2} \times \text{Water\_Density}}{3600} \quad [\text{kg backwash water/s}] \qquad (226)$$

$$\text{BW\_Spec\_Elec\_Cons\_2} = \text{Elec\_Consumption(BW\_Flow\_2, Total\_Backwash\_Height, Pump\_Efficiency} = \text{BWPNU)} \quad [\text{kWh/kg backwash water}] \qquad (227)$$

$$\mathrm{BW\_Elec\_Cons\_2} = \frac{\mathrm{Number\_Of\_Filters\_In\_Use} \times \mathrm{BW\_Spec\_Elec\_Cons\_2} \times \mathrm{BW\_Flow\_2} \times \mathrm{BDP2} \times 60}{\mathrm{Filtered\_Water}}$$

[kWh/kg filtered water] (228)

$$\mathrm{BW\_Flow\_3} = \frac{\mathrm{BWF3} \times \mathrm{Water\_Density}}{3600}$$

[kg backwash water/s] (229)

$$\mathrm{BW\_Spec\_Elec\_Cons\_3} = \mathrm{Elec\_Consumption(BW\_Flow\_3, Total\_Backwash\_Height, Pump\_Efficiency = BWPNU)}$$

[kWh/kg backwash water] (230)

$$\mathrm{BW\_Elec\_Cons\_3} = \frac{\mathrm{Number\_Of\_Filters\_In\_Use} \times \mathrm{BW\_Spec\_Elec\_Cons\_3} \times \mathrm{BW\_Flow\_3} \times \mathrm{BDP3} \times 60}{\mathrm{Filtered\_Water}}$$

[kWh/kg filtered water] (231)

Electricity consumption for backwash air compressing

The principle of the calculation is the same as previously presented for electricity consumption for pumping backwash waters except that this time, air is compressed.

$$\mathrm{Head\_Loss\_Filter\_Bed\_Air} = \frac{\mathrm{MD - Air\_Density}}{\mathrm{MD}} \times \frac{\mathrm{MAD} \times \mathrm{Filter\_Volume} \times 9.81}{\mathrm{FS}}$$

[Pa] (232)

$$\mathrm{Head\_Loss\_Air\_Distributor} = \max\left(\left(0.2 \times \mathrm{Head\_Loss\_Filter\_Bed\_Air}\right);3500\right)$$

[Pa] (233)

$$\mathrm{Head\_Loss\_Air} = \mathrm{Head\_Loss\_Filter\_Bed\_Air} + \mathrm{Head\_Loss\_Air\_Distributor}$$

[Pa] (234)

$$\mathrm{BW\_Air\_Flow\_1} = \frac{\mathrm{BAF1} \times \mathrm{Air\_Density}}{3600}$$

[kg backwash air/s] (235)

$$\mathrm{BW\_Air\_Power\_1} = \frac{\mathrm{BW\_Air\_Flow\_1} \times \mathrm{Head\_Loss\_Air}}{\mathrm{Air\_Density} \times \mathrm{AC\_NU}}$$

[W] (236)

$$\mathrm{BW\_Air\_Elec\_Cons\_1} = \frac{\mathrm{BW\_Air\_Power\_1} \times \mathrm{BDP1} \times 60 \times \mathrm{Number\_Of\_Filters\_In\_Use}}{\mathrm{Filtered\_Water} \times 3.6 \cdot 10^6}$$

[kWh/kg filtered water] (237)

$$\mathrm{BW\_Air\_Flow\_2} = \frac{\mathrm{BAF2} \times \mathrm{Air\_Density}}{3600}$$

[kg backwash air/s] (238)

$$\text{BW\_Air\_Power\_2} = \frac{\text{BW\_Air\_Flow\_2} \times \text{Head\_Loss\_Air}}{\text{Air\_Density} \times \text{AC\_NU}} \quad \text{[W]} \quad (239)$$

$$\text{BW\_Air\_Elec\_Cons\_2} = \frac{\text{BW\_Air\_Power\_2} \times \text{BDP2} \times 60 \times \text{Number\_Of\_Filters\_In\_Use}}{\text{Filtered\_Water} \times 3.6 \cdot 10^6}$$

$$\text{[kWh/kg filtered water]} \quad (240)$$

Total electricity consumption

$$\text{Total\_Spec\_Elec\_Cons} = \text{FW\_Spec\_Elec\_Cons} + \text{BW\_Elec\_Cons\_2}$$
$$+ \text{BW\_Elec\_Cons\_3} + \text{BW\_Air\_Elec\_Cons\_1} + \text{BW\_Air\_Elec\_Cons\_2}$$

$$\text{[kWh/kg filtered water]} \quad (241)$$

$$\text{Total\_Elec\_Cons} = \text{Total\_Spec\_Elec\_Cons} \times \text{Filtered\_Water}$$

$$\text{[kWh]} \quad (242)$$

5.3 Output water quality data

Organic matter and suspended matter in the filtered water

Media filtration removes suspended matter SM and all particulate compounds, so part of the organic matter is removed by filtration since POC is removed. It is assumed that all the particulate compounds (SM, POC, etc) are removed with the same efficiency as the turbidity (parameter *TUEFF*).

$$\text{Filtered\_Water\_Turbidity} = \text{Input\_Water\_Turbidity} \times (1 - \text{TUEFF}) \quad \text{[NTU]} \quad (243)$$

$$\text{Filtered\_Water\_SM} = \text{Input\_Water\_SM} \times (1 - \text{TUEFF}) \quad \text{[mg/L]} \quad (244)$$

$$\text{Filtered\_Water\_POC} = \text{Input\_Water\_POC} \times (1 - \text{TUEFF}) \quad \text{[mg/L]} \quad (245)$$

$$\text{Filtered\_Water\_DOC} = \text{DOC} \quad \text{[mg/L]} \quad (246)$$

$$\text{Filtered\_Water\_TOC} = \text{Filtered\_Water\_POC} + \text{Filtered\_Water\_DOC} \quad \text{[mg/L]} \quad (247)$$

$$\text{Filtered\_Water\_UVA} = \text{UVA} \quad [\text{m}^{-1}] \quad (248)$$

$$\text{Filtered\_Water\_COD} = \text{Filtered\_Water\_TOC} \times \text{COD\_TOC\_Ratio} \quad [\text{mgO}_2\text{/L}] \quad (249)$$

$$\text{Filtered\_Water\_BOD5} = \frac{\text{Filtered\_Water\_COD}}{\text{COD\_BOD5\_Ratio}} \quad [\text{mgO}_2\text{/L}] \quad (250)$$

$$\text{Filtered\_Water\_BOD} = \frac{\text{Filtered\_Water\_BOD5}}{\text{BOD5\_BOD\_Ratio}} \quad [\text{mgO}_2\text{/L}] \quad (251)$$

$$\text{Filtered\_Water\_DOC\_TOC\_Ratio} = \frac{\text{Filtered\_Water\_DOC}}{\text{Filtered\_Water\_TOC}} \qquad [\text{mgDOC/mgTOC}] \qquad (252)$$

Concentration of pathogenic micro-organisms in the filtered water (V1/V2/V3)

The calculation performed for evaluating the removal of pathogenic microorganisms thanks to media filtration are similar to the ones done for flocs separation processes (paragraph 4.3) and they are based on the work of Smeets et al. (Smeets et al. 2006). The only difference is that the *mean elimination capacity* (MEC) values are specific of filtration processes for these calculations.

$$\text{Microorganism\_I/O\_Ratio} = 10^{\text{MEC}} \qquad [\text{dec.\%}] \qquad (253)$$

$$\text{Output\_Microorganism} = \frac{\text{Input\_Microorganism}}{\text{Microorganism\_I/O\_Ratio}} \qquad [\text{nb/L}] \qquad (254)$$

The average value for algae removal *Algae_Removal* is 70% for any media filtration process (Baudin et al. 2006).

$$\text{Output\_Algae} = \text{Input\_Algae} \times (1 - \text{Algae\_Removal}) \qquad [\text{nb/L}] \qquad (255)$$

Concentration of pathogenic micro-organisms in the filtered water (V4)

The calculations are the same except that the MEC values from the work of Smeets et al. are different for GAC filters (Smeets et al. 2006). Algae removal *Algae_Removal* is still approximated as 70% (Baudin et al. 2006).

Dissolved water compounds in the filtered water (V1/V2/V3)

Dissolved water compounds (e.g. micropollutants or disinfection by-products) are not removed by media filtration because they are not stopped by the filter's bed which is a physical barrier for particulate compounds only.

Dissolved water compounds in the filtered water (V4)

Dissolved water compounds (i.e. micropollutants, nitrogen and phosphorus compounds, disinfection by-products and some organic matter parameters like DOC or UVA) are removed by GAC filtration (version 4 of the media filtration process model). Indeed, this filter's media is responsible for an adsorption phenomenon.

The Python^{TM} dictionary « GAC_Removal_Rate_Dictionnary » is used to calculate the concentration of dissolved water compounds in the filtered water. The following equation shows the performed calculation in a generic sense.

$$\text{Filtered\_Water\_X} = \text{Input\_Water\_X} \times (1 - \text{GAC\_Removal\_Rate\_X})$$

$$\text{[unit corresponding to the water quality data under consideration]} \qquad (256)$$

- *Filtered_Water_X* : Concentration of the dissolved water compound X in the filtered water.
- *Input_Water_X* : Concentration of the dissolved water compound X in the input water.
- *GAC_Removal_Rate_X* : Removal rate of the dissolved water compound X due to the GAC filtration process (as defined in the Python^{TM} dictionary « GAC_Removal_Rate_Dictionnary »)

It must be noted that the ratios of organic matter parameters (e.g. *UVA_DOC_Ratio*) are recalculated afterwards since the corresponding compounds may not be adsorbed in the same proportion.

Concentration of salt precipitates in the filtered water

The dissolved salts are not removed from the water. The salt precipitates are removed in the same proportion as the turbidity and the total concentrations of Fe, Mn, Al, Si, Ca and C in the filtered water are calculated taking into consideration the removal of these precipitates. The calculation is presented below in a generic sense.

$$\text{Filtered\_Water\_X\_Total} = \text{Input\_Water\_X\_Dissolved} + \left((\text{Input\_Water\_X\_Total} - \text{Input\_Water\_X\_Dissolved}) \times (1 - \text{TUEFF}) \right) \qquad \text{[mg/L]} \qquad (257)$$

PAC concentration in the filtered water

$$\text{Filtered\_Water\_PAC} = \text{Input\_Water\_PAC} \times (1 - \text{TUEFF}) \qquad \text{[mg/L]} \qquad (258)$$

Water quality of the backwash waters

At this point, the water quality data of the input water is known and that of the filtered water has been calculated. The increases of suspended matter and turbidity due to potential losses of filters' media are taken into account (except in the version 4 since there are no GAC losses) as shown in the equation 259a for SM and turbidity of backwash waters. Equation 259b is for version 4 which concerns GAC filtration where no GAC losses occur.

$$\begin{aligned}\text{Backwash\_Waters\_SM} &= \frac{(\text{Input\_Water\_SM} \times \text{Water\_Flow})}{\text{Backwash\_Waters\_Flow}} \\ &- \frac{(\text{Filtered\_Water\_SM} \times \text{Filtered\_Water\_Flow})}{\text{Backwash\_Waters\_Flow}} \\ &+ \frac{\text{Annual\_Media\_Losses} \times 1e^{6}}{\text{Backwash\_Waters\_Flow} \times 3600 \times 24 \times 365}\end{aligned} \qquad [\text{mg/L}] \qquad (259a)$$

$$\begin{aligned}\text{Backwash\_Waters\_SM} &= \frac{(\text{Input\_Water\_SM} \times \text{Water\_Flow})}{\text{Backwash\_Waters\_Flow}} \\ &- \frac{(\text{Filtered\_Water\_SM} \times \text{Filtered\_Water\_Flow})}{\text{Backwash\_Waters\_Flow}}\end{aligned} \qquad [\text{mg/L}] \qquad (259a)$$

$$\text{Backwash\_Waters\_Turbidity} = \frac{\text{Backwash\_Waters\_SM}}{\text{SM\_Turbidity\_Ratio}} \qquad [\text{NTU}] \qquad (260)$$

The water quality data of the backwash waters produced is then calculated based on conventional mass balances as shown in the following generic equation.

$$\begin{aligned}\text{Backwash\_Waters\_X} &= \frac{\text{Water\_Flow} \times \text{Input\_Water\_X}}{\text{Backwash\_Waters\_Flow}} \\ &- \frac{\text{Backwash\_Waters\_Flow} \times \text{Backwash\_Waters\_X}}{\text{Backwash\_Waters\_Flow}}\end{aligned}$$

[Unit corresponding to the water quality under consideration] (261)

- *Backwash_Waters_X* : Value of the water quality data in the backwash waters.
- *Input_Water _X* : Value of the water quality data in the input water.

The ratios concerning organic matter parameters are recalculated when required.

Organic matter fractions relative to the GAC filtration model (V4)

The new values of the three fractions of organic matter (f_{ha}, $f_{nonpolar}$ and $f_{nonsorbable}$) after the operation are calculated and updated in the dedicated file « OM_Information ». The calculations are presented in equations 262 to 265, based on the UVA and DOC removals.

$$\mathrm{DOC\_R} = \frac{\mathrm{Input\_Water\_DOC - Filtered\_Water\_DOC}}{\mathrm{Input\_Water\_DOC}} \qquad [\mathrm{dec.\%}] \qquad (262)$$

$$\mathrm{UVA\_R} = \frac{\mathrm{Input\_Water\_UVA - Filtered\_Water\_UVA}}{\mathrm{Input\_Water\_UVA}} \qquad [\mathrm{dec.\%}] \qquad (263)$$

$$f_{ha} = f_{ha,0} \times \frac{1 - \mathrm{UVA\_R}}{1 - \mathrm{DOC\_R}} \qquad [\mathrm{dec.\%}] \qquad (264)$$

$$f_{nonpolar} = (1 - f_{ha}) \times \frac{f_{nonpolar,0}}{f_{nonpolar,0} + f_{nonsorbable,0}} \qquad [\mathrm{dec.\%}] \qquad (265)$$

- *UVA_R / DOC_R* : UVA and DOC removals obtained by GAC filtration.
- $f_{ha,0}$ / f_{ha} : Initial and final values of the humic acids fraction.
- $f_{nonpolar,0}$ / $f_{nonpolar}$: Initial and final values of the non-polar fraction.
- $f_{nonsorbable,0}$: Initial value of non-sorbable fraction.

The adsorption of humic acids on GAC is assessed based on UVA removal. In other words, the removal of humic acids is assimilated to the removal of UVA due to GAC filtration. Non-polar and non-sorbable compounds are assumed to be equally adsorbed on GAC.

5.4 Engineering design facts

Filter(s) general characteristics

The following general characteristics of the media filtration process are saved in the engineering design report :

- Numbers of filters to be installed [no unit]
- Numbers of filters in use [no unit]
- Filter surface [m^2]
- Filter media height [m]
- Filter water height [m]
- Filter maximum water height [m]
- Media porosity [no unit - decimal percentage]

- Turbidity removal efficiency [no unit - decimal percentage]
- Filtration conversion rate
- Annual media losses [kg/year] (V1/V2/V3)
- Annual GAC to be regenerated [kg/year] (V4)
- Annual GAC losses [kg/year] (V4)
- New GAC replacing old GAC and that must be produced [kg/year] (V4)

Filtration cycle and characteristics of the backwash phases

The following design facts relative to the filtration cycle and the different phases of filters' backwash are saved in the engineering design report :

- Filtration cycle duration [h/cycle]
- Phase 1 : Fouling removal with air
    - Duration [min]
    - Air flow [Nm3/s]
- Phase 2 : Cleaning with air and water
    - Duration [min]
    - Air flow [Nm3/s]
    - Water flow [m3/s]
- Phase 3 : Rinsing with water
    - Duration [min]
    - Water flow [m3/s]

Electricity consumptions and electrical powers (V1/V2/V3)

The following design facts relative to electricity consumptions and electrical powers are saved in the engineering design report :

- Phase 1 : Fouling removal with air
    - Electricity consumed for air compressing [kWh/kg filtered water]
- Phase 2 : Cleaning with air and water
    - Electricity consumed for air compressing [kWh/kg filtered water]
    - Electricity consumed for backwash water pumping [kWh/kg filtered water]
- Phase 3 : Rinsing with water
    - Electricity consumed for backwash water pumping [kWh/kg filtered water]
- Total specific electricity consumption for backwashes [kWh/kg filtered water]

6. Disinfection and oxidation processes

Seven unit process models have been developed for the process category « Disinfection-Oxidation » in order to take into consideration different types of oxidation processes and their modelling.

The processes are modelled considering that the reactant addition is achieved in a tank with several contact chambers and with an appropriate system of baffles. It is the most current situation for disinfection-oxidation processes since the water and the oxidant have to be in contact for a prolonged time due to the kinetics of oxidation reactions.

The mixing in this kind of process is most often a static one. It can be induced by the injection of the oxidant itself when it is a gaseous chemical for instance. The bubbles themselves trigger a good mixing and mass transfer of the gas into the water and then, the circulation of the water through the contact chambers ensures that the oxidation reaction is correctly achieved (CIRSEE 2009; Degrémont 2007). If the oxidant is a liquid chemical, the water circulation and the point of injection of the oxidant are more crucial for the good quality of mixing. In such a case, the reactor must comprise a sufficient number of contact chambers and the system of baffles must be adequately positioned (CIRSEE 2009; Degrémont 2007).

The retrofit and predictive approaches are available for these unit process models. The oxidant dose can be user-defined and the resulting water quality is then calculated (retrofit approach).

The CT (Concentration x Time) is a specific concept concerning disinfection processes. It combines the disinfectant residual at the exit of the reactor (C) and the effective contact time (T). It enables one to assess the inactivation of pathogenic microorganisms. So the CT is a treatment objective which can be user-defined for some model versions. The required disinfectant dose is then determined based on it (predictive approach).

One version of the model also exists where a UVA removal objective can set by the user and the required ozone dose is then forecasted based on this process objective (predictive approach). It was not possible to develop the same model version for other oxidants for lack of knowledge (i.e. the WTP model provides an empirical equation for estimating the UVA removal due to ozonation but it gives no information on UVA removal due to other oxidation processes).

The seven model versions for the process category « Disinfection-Oxidation » are listed below :

- Version 1 (V1) : *Bleach_Addition* (retrofit model).
- Version 2 (V2) : *Bleach_Disinfection* (predictive model).
- Version 3 (V3) : *Chlorine_Addition* (retrofit model).
- Version 4 (V4) : *Chlorine_Disinfection* (predictive model).
- Version 5 (V5) : *Ozone_Addition* (retrofit model).
- Version 6 (V6) : *Ozone _Disinfection* (predictive model).
- Version 7 (V7) : *Ozone_UVA_Removal* (predictive model).

6.1 Parameters of the unit process model

The parameters for the unit process models from the category « Disinfection-Oxidation » are presented in table 6.

Table 6. Parameters for the different versions of the unit process model « Disinfection-Oxidation ».

- Engineering design facts and/or operating conditions -				
Parameter	Programming Names	Default Values		Unit
Reactant dose	REACD	20^* 2^*	(V1) (V3/V5)	g/m^3
CT (i.e. Oxidant residual x T10)	CT	15[1] 1.6^*	(V2/V4) (V6)	mg/(L.min)
UVA removal objective	UVA_R	0.2^*	(V7)	dec.%
Pre-treatment index	PTI	1[2]		no unit
Static mixer pressure drop	SMPD	20000^*		Pa
Theoretical contact time in the tank	T	60^*		min
T10/T Ratio[3]	T10_T	0.5^*		no unit
Gas (ozone) transfer efficiency	GT_NU	0.85[4]	(V5/V6/V7)	dec.%
Percentage of pure oxygen in the feed gas[5]	POPFG	0	(V5/V6/V7)	dec.%

- Technical and/or legal constraints -				
Parameter Names	Programming Names	Default Values		Unit
Intake pumped height	IPH	3^* 5^*	(V1/V2/V3/V4) (V5/V6/V7)	m
Intake pump(s) efficiency	IP_NU	0.8[6]		m

* Arbitrary default value or estimation by water treatment experts.

1. This default values is the CT value recommended by the World Health Organisation (WHO) to inactivate E.Coli in general conditions (pH < 8 and turbidity < 1 NTU) (WHO 2011). The requirements for microorganism inactivation are very case-dependent and the CT values must be considered carefully.
2. The Pre-treatment index (PTI) defines the type of water to be oxidised for the calculation of DBPs formation. This index can be set at 1, 2, 3 or 4. (PTI = 1) means that raw water is oxidised, (PTI = 2) means that coagulated/softened water is oxidised, (PTI = 3) means that refined water is oxidised (by GAC or membrane filtration), (PTI = 4) is for cases with site-specific equations. The reason is that the calculation of DBPs formation is based on the WTP model equations (WTP manual) and they are different depending on the type of water to be oxidised.
3. T is the theoretical contact time in the tank and T10 is the real the time it takes to get 10% of a tracer out of the tank. This ratio T10/T represents somehow the quality of the hydrodynamics in the contact tank. (T10/T = 1) is for an ideal plug flow reactor. Typical values for the ratio T10/T are 0.3 for a contact tank without any wall/partition, 0.5 for a tank with 1 or 2 wall(s) / partition(s), 0.7 for a tank with more wall(s) / partition(s) and 0.8 for a piston reactor (CIRSEE 2009).
4. The ozonation process can be operated in different types of reactor. The most current is a reactor with several contact chambers where the mixing is done by an appropriate ozone injection. Another current

ozonation reactor is the “U” tube that performs a very good transfer of ozone into the water. Other technical solutions like a regular mixing tank can work as well but there will not be considered here because they are exceptional in the case of ozonation. The gas transfer efficiency is comprised between 75% and 95% for ozonation reactors with contact chambers, and between 90% and 99% for “U” tube reactors (Degrémont 2007; Masschelein 1991).

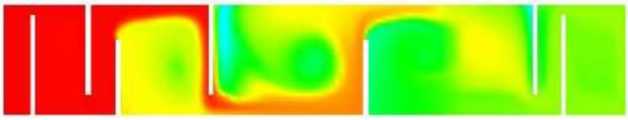
5. The feed gas for ozone production is made up of air and/or pure oxygen. This parameter represents the percentage of pure oxygen in the feed gas.
6. Typical values range between 0.7 and 0.9. Pump efficiency could be 0.6 in case the pump is badly operated (Degrémont 2007).

Three chemicals are considered in the modelling of disinfection-oxidation processes : sodium hypochlorite NaOCl (i.e. bleach), chlorine Cl_2 and ozone O_3. Therefore, three second-level scripts, one for each chemical, have been created and their names are « NaOCl_Chlorination_Data », « Cl2_Chlorination_Data » and « Ozonation_Data ».

In each second-level script, a Python^{TM} dictionary defines the values of immediate oxidant demand (chlorine or ozone demand) due to the presence of different water compounds which react instantaneously with the oxidant. These compounds responsible for an oxidant demand are Fe, Mn, CN, Br (only responsible for chlorine demand), NO_2, H_2S, NH_4 and also some organic matter compounds. They are expressed in “mgOxidant/mgCompound”. The chlorine demand due to organic matter is expressed as a function of DOC (Campos and Harmant) and the ozone demand due to organic matter is proportional to TOC ($mgO_3/mgTOC$) (CIRSEE 2009). The values of oxidant demand (for each disinfectant and for each water compounds) are defined in Python^{TM} dictionaries. They are not listed here, as they can be found in the literature (Campos and Harmant 2002; CIRSEE 2009; Degrémont 2007).

In each second-level script, a function named *Pathogen_MEC* allows calculating the mean elimination capacity (i.e. the $\log_{10}$ value of the ratio (number of micro-organisms at input / number of micro-organisms at output)) due to the disinfection process under consideration. It is mainly based on the research work of Smeets et al. (Smeets et al. 2006). The equations 266 and 267 show the initial equations as formulated by the authors. The variables are the oxidant residual C, the hydraulic residence time t_h in the contact tank, the hydraulic quality index j in the contact tank (theoretical number of Continuously Stirred Tank Reactors (CSTR) in series), the absolute temperature T, the activation energy Ea and the frequency factor A.

Therefore, two Python™ dictionaries per second-level script define the activation energies and frequency factors for each pathogen under study.



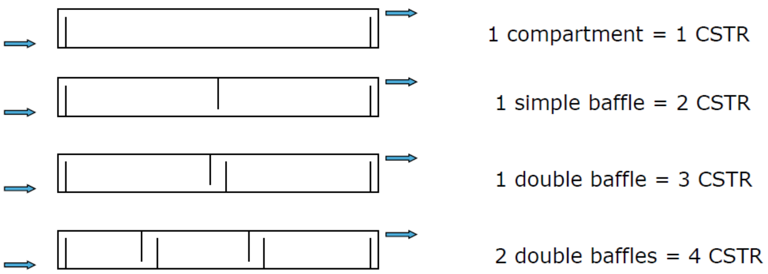
$$\frac{N}{N_0} = \frac{1}{\left(1 + \frac{Ke \times C \times t_h}{j}\right)^j} \qquad \text{[no unit]} \qquad (266)$$

$$Ke = A \times \exp\left(\frac{-Ea}{RT}\right) \qquad [\text{L.mg}^{-1}\text{min}^{-1}] \qquad (267)$$

$$MEC = \log_{10}\left(\frac{N_0}{N}\right) \qquad \text{[no unit]} \qquad (268)$$

- N / N_0 : number of micro-organisms at output / number of micro-organisms at input [nb/L].
- Ke : inactivation rate constant [L.mg^{-1}min^{-1}].
- C : disinfectant concentration at CSTR outlet [mg.L^{-1}].
- t_h : hydraulic residence time in the CSTR [min^{-1}].
- j : number of theoretical CSTR in series (1 to 6 at maximum) [no unit].
- A : frequency factor [L.mg^{-1}min^{-1}].
- Ea : activation energy [J.mol^{-1}].
- R : ideal gas constant [8.314 J. mol^{-1}.K^{-1}].
- T : absolute temperature [K].
- MEC : Mean Elimination Capacity [no unit].

It must be noted that there is a parallel between the hydraulic quality index j of the previous equation and the ratio *T10_T*, which is a model parameter. They both depend on the number and the positioning of the baffles in the contact tank. The variable j goes from 1 to 6 while the ratio T10_T goes from 0.3 to 0.8. An interpolation is therefore made to associate a value of j to any user-defined value of the ratio *T10_T*. It avoids defining inter-dependent model parameters.



Three Python^{TM} dictionaries have been created in order to define the removal rate of micropollutants due to the oxidation processes (*NaOCl_Removal_Rate*, *Cl2_Removal_Rate*, *O3_Removal_Rate*). The default value is 0.5 (i.e. 50%) for all micropollutants and for all oxidants but they should be user-defined as far as possible if the results about micropollutant concentrations in treated water are crucial in the context of one study.

For the chlorination processes (i.e. addition of sodium hypochlorite NaOCl or addition of chlorine Cl_2), different functions with the corresponding empirical coefficients are defined based on the WTP modelling approach in order to evaluate the formation of DBPs during disinfection-oxidation (WTP manual 2001). The different functions are used depending on the type of water to be chlorinated (parameter *PTI*).

For the ozonation process, the WTP modelling approach is also adopted to calculate the DBPs formation, except that there is only one DBP that is formed which is bromate BrO_3. The Br removal is calculated as a consequence. It must be noted that the WTP model also provides an empirical equation to evaluate the UVA removal due to ozonation, which has enabled us to develop version 7 of this process model.

The ozonation process requires to produce ozone and to destroy its residual in the gas exiting the process. Both production and destruction of ozone are performed on-site with specific technologies. So, in the second level-script « Ozonation_Data », several constants are defined to describe the functioning of these crucial steps of ozonation. Indeed, a significant amount of the energy consumed by the ozonation process is due to these steps which do not concern water treatment strictly speaking. These constant of the ozonation models (model versions 5, 6 and7) are listed below :

Energy for air desiccation

Desiccation_Specific_Energy = 0.06 [kWh/Nm^3]

Note : The pre-treatment for air (desiccation) could be done at high pressure (relative pressure of 5-7 bars) or low pressure (relative pressure = 0.8 bars), but the low pressure involves a following step which is refrigeration and adsorption, involving an adsorbant consumption that is not taken into account. Except for the adsorbant consumption, only electricity is consumed in both pre-treatment processes. Typical values are 0.1 kWh/Nm^3 for high pressure desiccation and 0.06 kWh/Nm^3 for low pressure desiccation (Masschelein 1991). High pressure is not very common and is used on small plants for maintenance reasons. The low pressure system is more often used. So, the default value is the one of the low pressure treatment.

Specific energy for injection of the ozonated gas

Ozonated_Gas_Inj_Spec_Energy = 0.01 [kWh/gO_3]

Note : Default value is set at 0.01 kWh/gO_3, a typical value for contact chamber reactors, which are the most commonly found. Typical values are comprised between 0.002 to 0.02 kWh/gO_3 for contact chamber reactors. They are unknown for "U" tube reactors and the velocity gradient (when using a regular tank with dynamic mixing) would be 150 s^{-1} (Degrémont 2007; Masschelein 1991).

Specific energy for the production of the ozonated gas from air or pure oxygen O_2

Air_O3_Prod_Spec_Energy = 15.5 [kWh/gO_3]

O2_O3_Prod_Spec_Energy = 6.0 [kWh/gO_3]

O_3 concentration of the ozonated gas produced from air or O_2

Air_O3_Concentration = 18.0 [gO_3/Nm^3 of ozonated gas]

O2_O3_Concentration = 70.0 [gO_3/Nm^3 of ozonated gas]

Note : The mean value for O_3 concentration in an ozonated gas produced from air is 18 gO_3/Nm^3. The energy consumed for its production is comprised between 13 and 18 kWh/gO_3. The mean value for O_3 concentration in an ozonated gas produced from pure oxygen O_2 is 70 gO_3/Nm^3. The energy consumed for its production is approximately 6 kWh/kgO_3 (Degrémont 2007).

Data concerning the destruction of the ozonated gas

The destruction of the ozonated gas exiting the ozonation tank can be done mainly in one of two ways : thermal destruction or catalytic destruction. Catalytic destruction is much less often used because of some technical problems (catalyst poisoning, maintenance, etc). 0.25-0.4 kg of catalyst is necessary for 1 Nm^3/h of treated gas. Better performances are obtained with Cu/MnO_2 and a temperature of 50-70°C. The global electricity consumption is nearly equal to that resulting from thermal destruction. Thermal destruction is the one that is considered in these versions of the ozonation process because it is much more commonly used. The gas is heated by electrical resistances in an industrial furnace.

Specific heat of the ozonated gas (Masschelein 1991)

Gas_Specific_Heat = 368.0 . 10^{-6} [kWh/(K.Nm^3)]

Furnace efficiency

Furnace_Efficiency = 0.65 [dec.%]

Note : It is the ratio between the electrical energy consumed by the furnace and the thermal energy actually received by the treated gas. The difference comes from the electrical efficiency (always very high, more than 95%) and the heat transfer efficiency (much lower). Typical efficiency for industrial furnaces is comprised between 50-75%. Default value is set at 65% (Oberlin et al. 2005).

Heating temperature and duration

Heating_Temperature = 325.0 [°C]

Heating_Duration = 3.0 [s]

Note : For a good achievement of ozone thermal destruction, the treated gas needs to be heated at a temperature of 300-350°C during 2-4 s. It results in a specific energy for ozone destruction of 27-35 Wh/Nm^3 (Degrémont 2007; Masschelein 1991).

Heat recovery

Heating_Recovery_Efficiency = 0.8 [dec.%]

Note : Heat recovery is usually done when the flow exceeds 200 Nm^3/h of treated gas (or 4 kgO_3/h). The typical value is 80%. If there is no heat recovery, the constant *Heating_Recovery_Efficiency* must be set at 0 by the user (Degrémont 2007; Masschelein 1991).

6.2 Energy and chemical consumptions

There is only one chemical consumed for each of the processes considered in this section. This chemical is inevitably an oxidant and depending on the model version, it can be bleach (V1/V2), chlorine (V3/V4) or ozone (V5/V6/V7). It must be noted that ozone consumption is calculated but ozone is produced on-site from air or pure oxygen O_2. So these are the materials appearing in the mass balances at plant level. The only form of energy consumed is electricity.

Oxidant demand and oxidant consumption (V1/V3/V5)

Pure oxidant concentration introduced into the water

$$\text{Pure\_Ox\_Conc\_Introduced} = \text{REACD} \times \text{Oxidant\_Concentration} \qquad [\text{g/m}^3 \text{ or mg/L}] \qquad (269)$$

- *Oxidant_Concentration* : Concentration of the oxidant (attribute of the corresponding Python^{TM} object) [dec.%].

Calculation of the oxidant demand

$$\text{Oxidant\_Demand} = \sum \left(\text{Input\_Water\_X} \times \text{Spec\_Oxidant\_Demand\_X}\right) \qquad [\text{mg/L}] \qquad (270)$$

- *Input_water_X* : concentration of the water compound X (responsible for an oxidant demand) in the input water [mgX/L].
- *Spec_Oxidant_Demand_X* : Specific oxidant demand of the water compound X [mgOx/mgX].

Minimum residual oxidant concentration

$$\text{Oxidant\_Residual} = \max\left(0; \left(\text{Pure\_Ox\_Conc\_Introduced - Oxidant\_Demand}\right)\right) \qquad [\text{mg/L}] \qquad (271)$$

Disinfection CT

$$\text{CT} = \text{Oxidant\_Residual} \times \left(\text{T} \times \text{T10\_T}\right) \qquad [\text{mg.min/L}] \qquad (272)$$

Oxidant flow demand

$$\text{Oxidant\_Flow\_Demand} = \frac{\text{Pure\_Ox\_Conc\_Introduced} \times \text{Water\_Flow}}{\text{Oxidant\_Concentration}}$$

[kg/s] (273)

$$\text{Max\_Oxidant\_Flow\_Demand} = \frac{\text{Pure\_Ox\_Conc\_Introduced} \times \text{Max\_Water\_Flow}}{\text{Oxidant\_Concentration}}$$

[kg/s] (274)

Oxidant treatment ratio

$$\text{Oxidant\_Treatment\_Ratio} = \frac{\text{Oxidant\_Flow\_Demand}}{\text{Water\_Flow}} \qquad \text{[kgOx/kgWater]} \qquad (275)$$

$$\text{Water\_Dilution\_Factor} = \frac{1}{1 + \text{Oxidant\_Treatment\_Ratio}} \qquad \text{[no unit]} \qquad (276)$$

Oxidant consumption

$$\text{Oxidant\_Quantity} = \text{Oxidant\_Treatment\_Ratio} \times \text{Water}$$

[kg of oxidant solution or gas] (278)

$$\text{Ouput\_Water} = \text{Water} + \text{Oxidant\_Quantity} \qquad \text{[kg]} \qquad (279)$$

$$\text{Ouput\_Water\_Flow} = \text{Water\_Flow} + \text{Oxidant\_Flow\_Demand} \qquad \text{[kg]} \qquad (280)$$

These are the generic equations for calculating the disinfection CT, the oxidant demand and the corresponding consumption. It must be noted that the concentration of the bleach is expressed in mgCl_2-Eq/L, which makes the calculation in versions 1 and 3 very similar.

Concerning the ozonation model (version 5), the concentration of the ozonated gas is calculated by interpolating the ozone concentrations *Air_O3_Concentration* and *Air_O3_Concentration* (as defined in the corresponding level script) thanks to the parameter *POPFG* which defines the proportion of air and pure oxygen used for producing the ozonated gas. The ozone transfer efficiency (parameter *GT_NU*) is taken into account for the calculation of the required ozonated gas (quantity and flow). So, the air and oxygen consumptions are calculated and they are used later for the calculation of energy consumptions.

Oxidant demand and oxidant consumption (V2/V4/V6)

These versions of the model are predictive. There is no oxidant dose defined but a process objective, the disinfection *CT*, is user-defined instead. The calculations previously presented for the versions 1, 3 and 5 are reversed by calculating the required oxidant residual based on the *CT* value. Therefore, the oxidant dose is the sum of the required oxidant residual and the oxidant demand to be compensated.

Oxidant demand and oxidant consumption (V7)

This version of the model is also predictive. The required ozone dose is calculated based on the user-defined UVA removal. The function for calculating the UVA removal due to ozonation is defined in the second-level script and is taken from the WTP modelling approach (WTP model 2001).

The dichotomy method is then used to find the pure ozone dose which allows removing the UVA removal as defined by the parameter *UVA_R*. Then, the rest of the calculations are the same as those of the model version 5.

Electricity consumption

Electricity consumption for intake pumping and static mixing

A static mixer generates a pressure drop (model parameter *SMPD*) that must be compensated by a pump. The static mixer pressure drop *SMPD* is expressed in terms of a water height to be pumped and then added to the intake pumped height *IPH*.

$$\text{SMPD\_Height} = \frac{\text{SMPD}}{\text{Water\_Density} \times 9.81} \qquad \text{[m of water to be pumped]} \qquad (281)$$

$$\text{Height\_to\_be\_pumped} = \text{SMPD\_Height} + \text{IPH} \qquad \text{[m of water to be pumped]} \qquad (282)$$

$$\text{Specific\_Elec\_Cons} = \text{Elec\_Consumption (Water\_Flow, Height\_to\_be\_pumped, IP\_NU)} \qquad \text{[kWh/kg pumped water]} \qquad (283)$$

$$\text{Pumping\_Elec\_Cons} = \text{Specific\_Elec\_Cons} \times \text{Water} \qquad \text{[kWh]} \qquad (284)$$

Electricity consumption for injection/dosing of the oxidant (V1/V2/V3/V4)

The injection/dosing energy is neglected in versions 3 and 4 of the model as chlorine is a gaseous chemical and the energy for the injection of this kind of chemical was not evaluated during this project.

$$\text{Spec\_Elec\_Cons} = 0.0 \qquad \text{[kWh/kg dosed chlorine]} \qquad (285)$$

For bleach injection/dosing, the pumping functions are used. The material used for pipes when pumping bleach should be a plastic material, the most commonly used being PVC. The absolute roughness is therefore set as *Pipe_Absolute_Roughness*=0.000001 for PVC and plastic pipes, needed for bleach piping.

$$\begin{aligned}&\text{Spec\_Elec\_Cons} = \text{Elec\_Consumption (Bleach\_Flow\_Demand, IPH,}\\&\text{Pipe\_Absolute\_Roughness} = 0.000001, \text{rho} = \text{Rho\_Bleach, mhu} = \text{Mhu\_Bleach)}\end{aligned} \qquad \text{[kWh/kg pumped bleach]} \qquad (286)$$

$$\text{Dosing\_Elec\_Cons} = \text{Spec\_Elec\_Cons} \times \text{Oxidant\_Quantity} \qquad \text{[kWh]} \qquad (287)$$

Total electricity consumption (V1/V2/V3/V4)

$$\text{Total\_Elec\_Cons} = \text{Pumping\_Elec\_Cons} + \text{Dosing\_Elec\_Cons} \qquad \text{[kWh]} \qquad (288)$$

Electricity consumption for feed air treatment (V5/V6/V7)

$$\text{Feed\_Air\_Treatment\_Energy} = \text{Air\_Volume\_Quantity} \times \text{Desiccation\_Specific\_Energy} \qquad \text{[kWh]} \qquad (289)$$

Electricity consumption for injection of the ozonated gas (V5/V6/V7)

$$\text{Ozonated\_Gas\_Injection\_Energy} = \text{Pure\_O3\_Quantity} \times \text{Ozonated\_Gas\_Inj\_Spec\_Energy} \qquad \text{[kWh]} \qquad (290)$$

Electricity consumption for ozone production (V5/V6/V7)

$$\begin{aligned}\text{Ozone\_Prod\_Spec\_Energy} &= \left((1 - \text{POPFG}) \times \text{Air\_O3\_Prod\_Spec\_Energy}\right)\\&+ \left(\text{POPFG} \times \text{O2\_O3\_Prod\_Spec\_Energy}\right)\end{aligned} \qquad [\text{kWh/kgO}^3] \qquad (291)$$

$$\text{Ozone\_Production\_Energy} = \text{Pure\_O3\_Quantity} \times \text{Ozone\_Prod\_Spec\_Energy} \qquad \text{[kWh]} \qquad (292)$$

Electricity consumption for destruction of the ozonated gas (V5/V6/V7)

$$\text{Gas\_Volume\_Reduction} = \text{O3\_Concentration} \times \text{GT\_NU} \times \frac{8.3145 \times 273.15}{3.0 \times 15.99 \times 101325}$$

$$[\text{Nm}^3 \text{ of } O_3 \,/\, \text{Nm}^3 \text{ of ozonated gas}] \qquad (293)$$

$$\text{Transferred\_Heat} = \text{Gas\_Specific\_Heat} \times (\text{Heating\_Temperature} - \text{Temperature})$$

$$[\text{kWh/Nm}^3] \qquad (294)$$

$$\text{Recovered\_Heat} = \text{Heating\_Recovery\_Efficiency} \times \text{Transferred\_Heat}$$

$$[\text{kWh/Nm}^3] \qquad (295)$$

$$\text{Heating\_Spec\_Electricity} = \frac{\text{Transferred\_Heat} - \text{Recovered\_Heat}}{\text{Furnace\_Efficiency}}$$

$$[\text{kWh/Nm}^3] \qquad (296)$$

$$\text{Destruction\_Energy} = \text{Heating\_Spec\_Electricity} \times \text{Output\_Ozonated\_Gas\_Quantity}$$

$$[\text{kWh}] \qquad (297)$$

Total electricity consumption (V5/V6/V7)

$$\text{Total\_Elec\_Cons} = \text{Pumping\_Elec\_Cons} + \text{Feed\_Air\_Treatment\_Energy} + \text{Ozonated\_Gas\_Injection\_Energy} + \text{Ozone\_Production\_Energy} + \text{Destruction\_Energy}$$

$$[\text{kWh}] \qquad (298)$$

6.3 Output water quality data

Mineral composition, TAC, TH and pH

At this point, the oxidant dose to be added to the water is known regardless of the model version. Then, the function *Reactant_Addition* is used to calculate the mineral composition, the complete alkalinity titration TAC, the total hardness TH and the pH of the water after disinfection.

Disinfection by-products

The WTP model developed by the US EPA allows calculating the formation of disinfection by-products during disinfection-oxidation with empirical equations. Although calibration of these equations with on-site measurements is preferred (*PTI* = 4), the equations as presented in the WTP user manual are used by default (WTP manual 2001). It must be noted that the model parameter *PTI* enables the user to distinguish the types of water to be oxidised (raw water, coagulated water or refined water). Indeed, the formation of disinfection by-products is a function of some characteristics of the water, determined by its nature.

Suspended matter and organic matter

The suspended matter is not removed by disinfection-oxidation processes. So, the suspended matter concentration and the turbidity of the water are not affected by these unit processes.
The organic matter is not removed strictly speaking but it is oxidised and the nature of its compounds is changed. The consequence is that some UVA is removed from the oxidised water but neither DOC nor TOC are removed.

Unfortunately, the UVA removal has not been evaluated in chlorination models (version 1, 2, 3 and 4) for lack of knowledge. A variable exists in the main script to take it into account when possible. The UVA and the (UVA:DOC) ratio are calculated based on this UVA removal value which is 0 by default since it is generally unknown.
The UVA removal due to ozonation (model versions 5, 6 and 7) is assessed based on the empirical equation provided by the WTP model (WTP manual 2001). The UVA of the ozonated water and its (UVA:DOC) ratio are then calculated.

Concentration of pathogenic microorganisms

The concentration of pathogenic microorganisms is calculated with the function *Pathogen_MEC*. The form of the equations is the same for all versions of the model but the parameters (activation energy Ea, frequency factor A) are specific for each pathogenic microorganism. More information can be found in the original work of Smeets et al. (Smeets et al. 2006).

Micropollutants

The Python dictionaries *NaOCl_Removal_Rate*, *Cl2_Removal_Rate*, *O3_Removal_Rate*, defined in the second-level script, are used to calculate the concentration of micropollutants in the oxidised water thanks to the removal rate specifically defined for each considered micropollutant. It must be noted that these removal rates should be preferably user-defined. The generic equation is presented below.

$$\text{Output\_Water\_X} = \text{Input\_Water\_X} \times (1 - \text{Oxidant\_Removal\_Rate\_X}) \qquad [\text{mg/L}] \qquad (299)$$

- $Output\_Water\_X$: Concentration of the micropollutant X in the oxidised water.
- $Input\_Water\_X$: Concentration of the micropollutant X in the input water.
- $Oxidant\_Removal\_Rate\_X$: Removal rate of the micropollutant X due to the oxidation-disinfection process (as defined in one of the Python^{TM} dictionaries *NaOCl_Removal_Rate*, *Cl2_Removal_Rate*, *O3_Removal_Rate*)

Organic matter fractions relative to the coagulation model

In the case of disinfection/oxidation processes, the main script calculates the three fractions of organic matter (f_{ha}, $f_{nonpolar}$ and $f_{nonsorbable}$) after the operation and writes these new values in the dedicated file « OM_Information ». The calculations are presented in equations 300 and 301, based on the UVA removal obtained by these processes.

$$f_{ha} = (1 - \text{UVA\_Removal}) \times f_{ha,0} \qquad [\text{no unit}] \qquad (300)$$

$$f_{nonpolar} = f_{nonpolar,0} + (\text{UVA\_Removal} \times f_{ha,0}) \qquad [\text{no unit}] \qquad (301)$$

- $UVA\_Removal$: UVA removal obtained by the process.
- $f_{ha,0} / f_{ha}$: Initial and final values of the humic acids fraction.
- $f_{nonpolar,0} / f_{nonpolar}$: Initial and final values of the non-polar fraction.

The humic acids which are oxidised during the process are assumed to become non-polar compounds. Therefore, it results in a decrease of the humic acids fraction and a proportional increase of the non-polar fraction.

6.4 Engineering design facts

General characteristics of the tank

- Volume of the contact tank [m^3]
- Theoretical contact time T [min]
- Real contact time [min]
- Effective contact time T_10 [min]

Inactivation of pathogenic micro-organisms (Log values)

- Inactivation of E. Coli
- Inactivation of Campylobacter
- Inactivation of Giarda
- Inactivation of Cryptosporidium
- Inactivation of Norovirus
- Inactivation of Rotavirus

Oxidant demand, consumption and flow demand (V1/V2/V3/V4)

- Residual oxidant concentration [mgCl_2-Eq/L]
- Water oxidant demand [mgCl_2-Eq/L]
- Total oxidant added to the water [mgCl_2-Eq/L]
- Oxidant quantity relative to the functional unit [kgOxidant]
- Pure oxidant quantity relative to the functional unit [kgCl_2-Eq]
- Oxidant treatment ratio [kgOxidant/kgWater]
- Disinfection CT of the chlorination process [mg.min/L]
- Oxidant flow demand [kgOxidant/s]
- Maximum oxidant flow demand [kgOxidant/s]

Electricity consumptions and electrical powers (V1/V2/V3/V4)

- Electrical power used for intake pumping [kW]
- Electrical power to be installed for intake pumping [kW]
- Electricity consumed for intake pumping [kWh]
- Electricity consumed for oxidant dosing [kWh]

Ozone demand - Air and O_2 consumption (V5/V6/V7)

- Minimum residual ozone concentration [mgO_3/L]
- Water ozone demand [mg O_3/L]
- Ozone concentration in the ozonated gas [gO_3/Nm^3 of oz. gas]
- Ozone flow demand [kgO_3/s]
- Ozonated gas flow demand [Nm^3 of oz. gas/s]
- Feed gas flow demand [Nm^3 of feed gas/s]
- Pure O_2 flow demand [Nm^3 of pure O_2/s]
- Air flow demand [Nm^3 of air/s]

- Ozonated gas treatment ratio [Nm^3 of oz. gas/kgWater]
- Feed gas treatment ratio [Nm^3 of feed gas/kgWater]
- Pure O_2 treatment ratio [Nm^3 of pure O_2 gas/kgWater]
- Air treatment ratio [Nm^3 of air/kgWater]
- Disinfection CT of the ozonation process [mg.min/L]

<u>Organic matter removal (V5/V6/V7)</u>

- UVA removal [dec/%]

<u>Electricity consumptions and electrical powers (V5/V6/V7)</u>

- Electrical power used for intake pumping [W]
- Electrical power to be installed for intake pumping [W]
- Electricity consumed for intake pumping [kWh]
- Electricity consumption for feed air treatment [kWh]
- Electricity consumption for injection of the ozonated gas [kWh]
- Specific electricity consumption for ozone production [kWh/kgO_3]
- Electricity consumption for ozone production [kWh]
- Transferred heat for destruction of the ozonated gas [kWh/Nm^3]
- Recovered heat for injection of the ozonated gas [kWh/Nm^3]
- Specific electricity consumption for ozone destruction by heating [kWh/Nm^3]
- Electricity consumption for ozone destruction [kWh]
- Total electricity consumption [kWh]

7. Neutralisation and remineralisation processes

Twelve versions of the model « Neutralisation-Remineralisation » have been developed in order to represent different variants of this unit process and their respective modelling. Such processes aim at adjusting the pH and/or the complete alkalinity titration TAC of the water to more appropriate values. Possible motives can be for instance to get a better water taste, to avoid leakage of lead Pb in old pipes during water distribution or to protect those distribution pipes against corrosion.

Neutralisation is the action to get the pH of the water closer to approximate neutrality. Remineralisation is the action of adding salts and/or carbonate ions to the water in order to increase its alkalinity (i.e. its TAC). Remineralisation is also called recarbonatation. The opposite process (i.e. lowering the TAC) is called softening.

The twelve model versions of this process category differ on the following points as detailed below :

- The neutralisation and the remineralisation/softening processes can be achieved in a chemical reactor (i.e. a tank) but they can also be carried out in a pipe. The calculation of the mixing energy differs accordingly (dynamic mixing in a tank and static mixing in a pipe), as was already shown for other process categories (e.g. coagulation).
- The chemical dose can be user-defined and the resulting pH and TAC are then calculated (retrofit approach). A targeted value, concerning pH or TAC, can be user-defined and the required chemical dose is then forecasted by the unit process model (predictive approaches).
- All the chemicals that can be used for these processes are liquid chemicals except for carbon dioxide which is gaseous (at least in the EVALEAU framework). Therefore, the modelling is slightly different when considering the use of carbon dioxide because of some technical considerations (gas transfer efficiency into water or on-site CO_2 emissions released into air).

The twelve different model versions developed for the unit process category called « Neutralisation-Remineralisation » are listed below :

- Version 1 (V1) : *Pipe_Chemical_Addition* (retrofit model).
- Version 2 (V2) : *Pipe_CO2_Addition* (retrofit model).

- Version 3 (V3) : *Pipe_pH_Adjustment* (predictive model).
- Version 4 (V4) : *Pipe_pH_Adjustment_with_CO2* (predictive model).
- Version 5 (V5) : *Pipe_ TAC_Adjustment* (predictive model).
- Version 6 (V6) : *Pipe_ TAC_Adjustment_with_CO2* (predictive model).
- Version 7 (V7) : *Tank_Chemical_Addition* (retrofit model).
- Version 8 (V8) : *Tank_CO2_Addition* (retrofit model).
- Version 9 (V9) : *Tank_ pH_Adjustment* (predictive model).
- Version 10 (V10) : *Tank_ pH_Adjustment_with_CO2* (predictive model).
- Version 11 (V11) : *Tank_ TAC_Adjustment* (predictive model).
- Version 12 (V12) : *Tank_ TAC_Adjustment_with_CO2* (predictive model).

7.1 Parameters of the unit process model

The model parameters for the unit process « Neutralisation-Remineralisation » are presented in table 7.

Table 7. Parameters for the different versions of the unit process model « Neutralisation-Remineralisation ».

- Engineering design facts and/or operating conditions -			
Parameter	Programming Names	Default Values	Unit
Chemical dose	CH_D	100[1] (V1/V7)	g/m^3
Carbon dioxide CO_2 dose	CO2_D	100[1] (V2/V8)	g/m^3
Targeted pH	T_PH	7[2] (V3/V4/V9/V10)	no unit
Targeted TAC	T_TAC	16* (V5/V6/V11/V12)	°f
Chemical choice index	CH_CI	1[3] (V1/V7)	no unit
Acid choice index	A_CI	1[3] (V3/V9)	no unit
Base choice index	B_CI	1[3] (V3/V9)	no unit
Mineraliser choice index	M_CI	1[3] (V5/V11)	no unit
Softener choice index	S_CI	1[3] (V5/V11)	no unit
Static mixer pressure drop	SMPD	20000* (V1/V2/V3/V4/V5/V6)	Pa
Hydraulic residence time	HRT	0.1* (V1/V2/V3/V4/V5/V6) 5* (V7/V8/V9/V10/V11/V12)	min
Tank velocity gradient	TVG	700[4] (V7/V8/V9/V10/V11/V12)	s^{-1}
Mixing duration	MIXD	1[5] (V7/V8/V9/V10/V11/V12)	min
Stirrer efficiency	ST_NU	0.7* (V7/V8/V9/V10/V11/V12)	dec. %
Gas (CO_2) transfer efficiency	GT_NU	0.9[6] (V2/V4/V6) 0.8[6] (V8/V10/V12)	dec. %

- Technical and/or legal constraints -			
Parameter Names	Programming Names	Default Values	Unit
Intake pumped height	IPH	1* (V1/V2/V3/V4/V5/V6) 3* (V7/V8/V9/V10/V11/V12)	m
Intake pump(s) efficiency	IP_NU	0.8[7]	m

* Arbitrary default value or estimation by water treatment experts.

1. Typical values range between 5 and 200 g/m^3 (Degrémont 2007).
2. The neutral pH is supposed to be acceptable as a default value.

3. These indexes define the selected chemicals for the operation. Available chemicals are listed in appendix 3-1.
4. Typical values for chemical mixing in drinking water treatment range between 400 s^{-1} and 1000 s^{-1}. (CIRSEE 1999, Degrémont 2007).
5. Typical values range between few secondes and 2 minutes (CIRSEE 1999).
6. The most current technical solution for injecting carbon dioxide in water is a chemical reactor with porous diffuser and several contact chambers where the mixing is done by an appropriate injection of CO2 bubbles. Nevertheless, the best technical solution is static mixing within a pipe (better gas transfer efficiency). Other solutions like a regular mixing tank can work too but they are not satisfactory in many cases. Typical values for CO_2 transfer efficiency are 80% for porous diffuser (in a tank), 90% for a static mixer (in a pipe) and around 60% with a regular mixing tank (Degrémont 2007).
7. Typical values range between 0.7 and 0.9. Pump efficiency could be 0.6 in case where the pump is badly operated (Degrémont 2007).

There is no second-level script for any of the model versions.

7.2 Energy and chemical consumptions

The chemicals consumed during this type of unit process can be acids, bases, mineralisers or softeners (selected by the user) as well as carbon dioxide for some versions of the model. The only form of energy consumed is electricity.

Chemical consumption

Consumption of chemical solution, pure quantity of chemical and treatment ratio (V2/V8)

In the retrofit versions of the model where a liquid chemical is selected for the operation (versions 2 and 8), the chemical dose is user-defined (parameter *CH_D*). The quantity of chemical solution consumed during the process, is therefore easily calculated by the main script. The quantity of pure chemical is calculated, as it is the one that must be sent back to Umberto® for background process LCI calculations, since the LCA database (i.e. the Ecoinvent database) provides LCI data relative to pure quantities of chemicals (Weidema et al. 2009).

$$\text{Chem\_Treatment\_Ratio} = \frac{\text{CH\_D}}{\text{Water\_Density} \times 1000} \quad [\text{kgChemSol/kgWater}] \qquad (302)$$

$$\text{Chem\_Solution\_Quantity} = \text{Chem\_Treatment\_Ratio} \times \text{Water} \quad [\text{kgChemSol}] \qquad (303)$$

$$\text{Pure\_Chem\_Quantity} = \text{Chem\_Solution\_Quantity} \times \text{Chem\_Concentration}$$

[kgPureChem] (304)

- *Chem_Concentration* : The concentration of the chemical is an attribute of the corresponding Python$^{\text{TM}}$ object (appendix 3-1), directly available in the main script.

Consumption of carbon dioxide - Transferred into water and released quantities, treatment ratios (V1/V7)

In the retrofit versions of the model where carbone dioxide is used for the operation (versions 1 and 7), the CO_2 dose is user-defined (parameter *CO2_D*). The quantity of CO_2 transferred into water and the one released into the atmosphere are then calculated based on this user-defined dose.

$$\text{Injected\_CO}_2 = \text{CO2\_D} \times 10^{-3} \times \frac{\text{Water}}{\text{Water\_Density}} \qquad [\text{kgCO}_2] \qquad (305)$$

$$\text{Released\_CO}_2 = \text{CO2\_D} \times 10^{-3} \times (1 - \text{GT\_NU}) \times \frac{\text{Water}}{\text{Water\_Density}} \qquad [\text{kgCO}_2] \qquad (306)$$

$$\text{Transferred\_CO}_2 = \text{CO2\_D} \times 10^{-3} \times \text{GT\_NU} \times \frac{\text{Water}}{\text{Water\_Density}} \qquad [\text{kgCO}_2] \qquad (307)$$

$$\text{Injected\_CO}_2\text{\_Treatment\_Ratio} = \frac{\text{CO2\_D} \times 10^{-3}}{\text{Water\_Density}} \qquad [\text{kgCO}_2/\text{kgWater}] \qquad (308)$$

$$\text{Released\_CO}_2\text{\_Treatment\_Ratio} = \frac{\text{CO2\_D} \times 10^{-3} \times (1 - \text{GT\_NU})}{\text{Water\_Density}}$$

[kgCO$_2$/kgWater] (309)

$$\text{Transferred\_CO}_2\text{\_Treatment\_Ratio} = \frac{\text{CO2\_D} \times 10^{-3} \times \text{GT\_NU}}{\text{Water\_Density}}$$

[kgCO$_2$/kgWater] (310)

The quantity of CO_2 that is consumed is the result *Injected_CO$_2$* (multiplied by the CO_2 concentration in the gas which is 100%) and the on-site CO_2 emissions to air are represented by the result *Released_CO$_2$*.

Consumption of chemical solution, pure quantity of chemical and treatment ratio (V3/V4/V9/V10)

In the predictive versions of the model where the pH is adjusted based on a user-defined targeted value (parameter *T_PH*), the required chemical dose is calculated by the function *pH_Adjustment* (introduced in chapter 3). It concerns model versions 3, 4, 9 and 10.

Depending on the pH of the input water, the function *pH_Adjustment* determines whether the pH needs to be increased or lowered in view of the targeted pH (parameter *T_PH*). Then, it calculates the required dose of the adequate chemical (i.e. the acid or the base pre-selected by the user with the parameters *A_CI* and *B_CI*).

It must be noted that in the model versions where CO_2 is used, it is supposed that the pH needs to be lowered since CO_2 is an acid but soda (sodium hydroxide NaOH 50%) is defined as a default base chemical in case the pH needs in fact to be increased. A warning is then printed in a dedicated window of the Umberto® graphical user interface.

Once the required chemical dose is calculated by the function *pH_Adjustment*, the same calculations presented previously are performed to obtain the pure quantity of chemical and the treatment ratio.

Consumption of chemical solution, pure quantity of chemical and treatment ratio (V5/V6/V11/V12)

In the predictive versions of the model where the TAC is adjusted based on a user-defined targeted value (parameter *T_TAC*), the required chemical dose is calculated by the function *TAC_Adjustment* (introduced in chapter 3). It concerns model versions 5, 6, 11 and 12.

The principle is the same as when adjusting the pH with the corresponding function. Once the chemical dose required for adjusting the TAC of the water is calculated by the function *TAC_Adjustment*, the calculations presented previously are performed to determine the pure quantity of chemical and the treatment ratio.

Chemical solution flow demands

$$\text{Chem\_Solution\_Flow\_Demand} = \text{Chem\_Treatment\_Ratio} \times \text{Water\_Flow} \qquad [\text{kgChemSol/s}] \qquad (311)$$

$$\text{Max\_Chem\_Solution\_Flow\_Demand} = \text{Chem\_Treatment\_Ratio} \times \text{Max\_Water\_Flow}$$

[kgChemSol/s] (312)

Electricity consumption

Electricity consumption for intake pumping and static mixing (V1/V2/V3/V4/V5/V6)

A static mixer generates a pressure drop (model parameter *SMPD*) that must be compensated by a pump. The static mixer pressure drop *SMPD* is expressed in terms of a water height to be pumped and then added to the intake pumped height *IPH*.

$$\text{SMPD\_Height} = \frac{\text{SMPD}}{\text{Water\_Density} \times 9.81}$$

[m of water to be pumped] (313)

$$\text{Height\_to\_be\_pumped} = \text{SMPD\_Height} + \text{IPH}$$

[m of water to be pumped] (314)

$$\text{Spec\_Elec\_Cons} = \text{Elec\_Consumption}\,(\text{Water\_Flow}, \text{Height\_to\_be\_pumped}, \text{IP\_NU})$$

[kWh/kg pumped water] (315)

$$\text{Pumping\_Elec\_Cons} = \text{Spec\_Elec\_Cons} \times \text{Water}$$

[kWh] (316)

Electricity consumption for intake pumping (V7/V8/V9/V10/V11/V12)

$$\text{Spec\_Elec\_Cons} = \text{Elec\_Consumption}\,(\text{Water\_Flow}, \text{IPH}, \text{IP\_NU})$$

[kWh/kg pumped water] (317)

$$\text{Intake\_Elec\_Cons} = \text{Spec\_Elec\_Cons} \times \text{Water}$$

[kWh] (318)

Electricity consumption for stirring (dynamic mixing) in the tank (V7/V8/V9/V10/V11/V12)

$$\text{Mixed\_Volume} = \text{MIXD} \times \frac{\text{Max\_Water\_Flow}}{\text{Water\_Density}}$$

[m^3] (319)

$$\text{K} = (0.3842 \times \text{Temperature}) - 81.214$$

[no unit] (320)

$$\text{Stirring\_Power} = \text{Mixed\_Volume} \times \left(\frac{\text{TVG}}{\text{K}}\right)^2$$

[W] (321)

$$\text{Stirring\_Elec\_Power} = \frac{\text{Stirring\_Power}}{\text{ST\_NU}}$$

[W] (322)

$$\text{Spec\_Stirring\_Elec\_Cons} = \frac{\text{Stirring\_Elec\_Power}}{\text{Water\_Flow} \times 3600 \times 1000}$$

[kWh/kgWater] (323)

$$\text{Stirring\_Elec\_Cons} = \text{Spec\_Stirring\_Elec\_Cons} \times \text{Water}$$

[kWh] (324)

- $Mixed\_Volume$: Theoretical volume of water submitted to stirring forces.
- K : empirical coefficient (CIRSEE 1999).

Electricity consumption for chemical injection/dosing

The energy consumption for the injection of the chemical is calculated with the function $Elec\_Cons$ taking into account the density and the dynamic viscosity of the chemical under consideration as well as the absolute roughness of the pipe. Indeed, PVC and plastic pipes are required for chemical pumping (their absolute roughness is about 10^{-6} m).

$$\text{Chem\_Dosing\_Spec\_Elec\_Cons} = \text{Elec\_Consumption (Chem\_Solution\_Flow\_Demand, IPH, Pipe\_Absolute\_Roughness} = 10^{-6}, \text{rho} = \text{Chem\_Density, mhu} = \text{Chem\_Dynamic\_Viscosity)} \quad \text{[kWh/kg of pumped chemical]} \qquad (325)$$

$$\text{Chem\_Dosing\_Elec\_Cons} = \text{Chem\_Solution\_Quantity} \times \text{Chem\_Dosing\_Spec\_Elec\_Cons} \quad \text{[kWh]} \qquad (326)$$

- $Chem\_Density$ and $Chem\_Dynamic\_Viscosity$ are attributes of the Python^{TM} object corresponding to the chemical used for the operation.

It must be noted that the injection of carbon dioxide CO_2 is neglected (in case it is used) for lack of knowledge.

Total electricity consumption (V1/V2/V3/V4/V5/V6)

$$\text{Total\_Elec\_Cons} = \text{Pumping\_Elec\_Cons} + \text{Chem\_Dosing\_Elec\_Cons} \quad \text{[kWh]} \qquad (327)$$

Total electricity consumption (V7/V8/V9/V10/V11/V12)

$$\text{Total\_Elec\_Cons} = \text{Intake\_Elec\_Cons} + \text{Chem\_Dosing\_Elec\_Cons} + \text{Stirring\_Elec\_Cons} \quad \text{[kWh]} \qquad (328)$$

7.3 Output water quality data

Water dilution factor

$$\text{Water\_Dilution\_Factor} = \frac{1}{1 + \text{Chem\_Treatment\_Ratio}} \quad \text{[no unit]} \qquad (329)$$

Water quantity - nominal and maximum water flows

$$\text{Output\_Water} = \frac{\text{Water}}{\text{Water\_Dilution\_Factor}} \qquad \text{[no unit]} \qquad (330)$$

$$\text{Output\_Water\_Flow} = \frac{\text{Water\_Flow}}{\text{Water\_Dilution\_Factor}} \qquad \text{[no unit]} \qquad (331)$$

$$\text{Max\_Output\_Water\_Flow} = \frac{\text{Max\_Water\_Flow}}{\text{Water\_Dilution\_Factor}} \qquad \text{[no unit]} \qquad (332)$$

Mineral composition, TAC, TH and pH of the treated water

The mineral composition, the complete alkalinity titration TAC, the total hardness TH and the pH of the water are modified due to the neutralisation or remineralisation/softening process. Based on the user-defined chemical dose *CH_D* that is added to the water, these water quality data are calculated by the function *Reactant_Addition* in the retrofit versions of the model (versions 1, 2, 7 and 8).

Based on the user-defined targeted pH *T_PH* for the treated water, these water quality data are calculated together with the required chemical dose by the function *pH_Adjustment* in the predictive versions of the model (versions 3, 4, 9 and 10).

Based on the user-defined targeted TAC *T_TAC* that is sought in the treated water, these water quality data are calculated together with the required chemical dose by the function *TAC_Adjustment* in the predictive versions of the model (versions 5, 6, 11 and 12).

Other water quality data

The other water quality data are not affected by the neutralisation, remineralisation or softening processes. They are only diluted and this is taken into account thanks to the water dilution factor *Water_Dilution_Factor* previously calculated.

7.4 Engineering design facts

General characteristics of the pipe/tank

- Volume of the pipe/tank [m^3]
- Theoretical contact time T [min]
- Real contact time T [min]

Alkalinity and pH of the treated water

- Alkalinity [French Degree]
- pH [no unit]

Selected chemical for the operation : consumption, treatment ratio and flow demand (V1/V3/V5/V7/V9/V11)

- Name of the chemical selected for the process [no unit]
- Concentration of the selected chemical [dec.%]
- Quantity of chemical solution introduced in the water [kgChemSolution]
- Quantity of pure chemical introduced in the water [kgPureChem]
- Chemical treatment ratio [kgChemSolution/kgWater]
- Chemical flow demand [kgChemSolution/h]
- Maximum chemical flow demand [kgChemSolution/h]

Quantities of carbon dioxide CO_2 injected, transferred and released (V2/V4/V6/V8/V10/V12)

Quantity of CO_2 injected [kgCO_2]
Quantity of CO_2 transferred into the water [kgCO_2]
Quantity of CO_2 released into the atmosphere [kgCO_2]
Injected CO_2 treatment ratio [kgCO_2/kgWater]
Transferred CO_2 treatment ratio [kgCO_2/kgWater]
Released CO_2 treatment ratio [kgCO_2/kgWater]
CO_2 flow demand [kgCO_2/h]
Maximum CO_2 flow demand [kgCO_2/h]

Head losses, electricity consumptions and electrical powers (V1/V2/V3/V4/V5/V6)

- Heights to be pumped
    - Intake height [m]
    - Static mixing pressure drop [m of water to be pumped]
    - Total height to be pumped [m]
- Electricity consumptions and electrical powers
    - Electrical power used for pumping [kW]
    - Electrical power installed for pumping [kW]
    - Specific electricity consumption for pumping [kWh/kg pumped water]

    - Electricity consumption for pumping [kWh]
    - Electricity consumption for chemical dosing [kWh] (Warning if CO_2 injection as the injection energy is neglected in this case)
    - Total specific electricity consumption [kWh/kgWater]
    - Total electricity consumption [kWh]

<u>Electricity consumptions and electrical powers (V7/V8/V9/V10/V11/V12)</u>

- Electricity consumption and electrical power for dynamic mixing
    - Stirring electricity consumption [kWh]
    - Specific stirring electricity consumption [kWh/kgWater]
    - Stirring electricity power [kW]
- Electricity consumption and electrical power for intake pumping and chemical dosing
    - Electrical power used for intake pumping [kW]
    - Electrical power installed for intake pumping [kW]
    - Specific electricity consumption for intake pumping [kWh/kg pumped water]
    - Electricity consumption for intake pumping [kWh]
    - Electricity consumption for chemical dosing [kWh] (Warning if CO_2 injection as the injection energy is neglected in this case)
- Total electricity consumption
    - Total specific electricity consumption [kWh/kgWater]
    - Total electricity consumption [kWh]

8. Sludge treatment

The sludge produced during drinking water treatment is most often a mineral sludge mainly composed of metal hydroxide formed during the coagulation process. Therefore, it does not have a real agricultural value unless it has been limed during sludge treatment. The sludge can then be used as a liming material but in most cases, it is not an interesting by-product. Sludge disposal (e.g. incineration) becomes an issue for plant operators, as it is expensive.

The aim of sludge treatment, in the context of drinking water production, is to reduce as much as possible the quantity of sludge that must be sent to incineration or landfilling for instance. Sludge overflow is returned in the process line (usually at the entrance of the coagulation process) or sent to sewer if it is too concentrated.

The processes for sludge thickening (settling and flotation) are adapted for sludges which are not concentrated (i.e. a few g/L). These two processes allow concentrating the treated sludge somewhere between 20 g/L or 40 g/L (120 g/L at most) (Degrémont 2007). It must be noted that modern settling technologies often comprise a compartment in the settlers for performing a pre-settling of the sludge, thus enabling plant operators to skip this step in sludge treatment.
The processes for sludge dehydration (centrifuging, filter press, belt filter and vacuum filter) make it possible to obtain much more concentrated sludge (from 150 g/L to 500 g/L) but they require an initial sludge concentration above 20 g/L (5 g/L for belt filters) to function correctly (Degrémont 2007).
The processes for sludge drying (e.g. thermal drying) are rarely put into practice. They generate high energy consumptions (when using heat from a furnace) or require large surface areas during a long period for natural drying (Degrémont 2007). The main reasons for treating the sludge by thermal drying is the lack of technical options for sludge disposal and/or the high cost of the disposal technical solution.

It must be noted that all the unit process models presented here are retrofit models. It was not possible to predict the chemical consumptions (hydrated lime and flocculant) so the chemical doses are user-defined and the modelling approach is the retrofit one. In fact, the energy consumptions are calculated based on ratios defined in the second-level scripts. It is due to the fact that the functioning of these processes has not been studied in detail and there were no satisfactory models found in the literature. In conclusion, the unit process models for sludge treatment, in the context of drinking water production, are very descriptive and not predictive because of the state-of-the-art.

The seven model versions for the process category « Sludge treatment » are listed below :

- Version 1 (V1) : *Sld_Thick_Settling* (retrofit model).
- Version 2 (V2) : *Sld_Thick_Flotation* (retrofit model).
- Version 3 (V3) : *Sld_Dehyd_Belt_Filter* (retrofit model).
- Version 4 (V4) : *Sld_Dehyd_Centrifuging* (retrofit model).
- Version 5 (V5) : *Sld_Dehyd_Filter_Press* (retrofit model).
- Version 6 (V6) : *Sld_Dehyd_Vacuum_Filter* (retrofit model).
- Version 7 (V7) : *Sld_Thermal_Drying* (retrofit model).

8.1 Parameters of the unit process model

The model parameters for the unit process « Flocs Separation » are presented in table 4.

Table 8. Parameters for the different versions of the unit process model « Sludge treatment ».

- Engineering design facts and/or operating conditions -			
Parameter	Programming Names	Default Values	Unit
Hydrated lime dose	HLD	300[1] (V1/V3/V4/V5/V6) 0[2] (V7)	kgCa(OH)$_2$/tSM
Polymer flocculant dose	PFD	2[3] (V1/V2) 5[4] (V3/V4/V5/V6) 0[2] (V7)	kg/tSM
Recovery rate efficiency [5]	RR_NU	0.9[6] (V1/V2/V3/V4/V5/V6)	dec. %
Sludge concentration (after treatment)	SLC	30[7] (V1) 40[8] (V2) 220[9] (V3) 280[10] (V4) 350[11] (V5/V6)	g/L
Hydraulic residence time	HRT	24* (V1/V2)	h
Single tank surface	STS	25* (V1/V2)	m^2
Surface suspended matter charge	SSMC	50[12] (V1) 100[13] (V2) 60[14] (V5) 40[15] (V6)	kg/(m^2.day)
Length suspended matter charge	LSMC	3000[16] (V3)	kg/(m.day)
Single filter belt length	SFBL	1* (V3)	m
Single filter surface	SFS	50* (V5/V6)	m^2
Output dry solid content	ODSC	0.8 (V7)	dec. %

* Arbitrary default value or estimation by water treatment experts.

1. The hydrated lime dose is expressed as a mass of pure $Ca(OH)_2$ divided by the mass of solid matter (SM) of the sludge. The addition of lime for sludge settling is not indispensable, so the value of this parameter can be set to 0. When it is needed, typical values for the hydrated lime dose range between 5% and 50% (i.e.50-500 $kgCa(OH)_2/tSM$) depending on sludge characteristics. Default value for this dose is set at 300 $kgCa(OH)_2/tSM$ (CIRSEE 2007; Degrémont 2007).
2. The addition of hydrated lime and/or flocculant for sludge drying (V7) is not common at all, so the default value of these parameters is set to 0. The reason is that normally, previous sludge treatment steps already occurred and hydrated lime and/or flocculant have already been added (Degrémont 2007).
3. Typical values range between 1 and 3 kg/tSM so the default value is set to 2 kg/tSM. The mass of flocculant is given in term of commercial product (CIRSEE 2007; Degrémont 2007).
4. Typical values range between 1 and 10 kg/tSM, so the default value is set at 5 kg/tSM. The mass of flocculant is given in term of commercial product (CIRSEE 2007; Degrémont 2007).
5. The parameter RR_NU somehow represents the process separation efficiency. This is the proportion of solid matter (i.e. dry matter / suspended matter) retained in the concentrated sludge while the rest stays in the sludge overflow.
6. A typical value is 0.9 (90%), but it can be higher using flocculant (about 95%) (CIRSEE 2007).
7. The concentration of the sludge obtained after settling depends on the technology used for the process, the use of polymer, etc. The default value for this parameter is 30 g/L but here are other values for specific cases. For static thickening : range is 10-100 g/L, typical value is 30 g/L. For lamellar thickening : range is 50-200 g/L, typical value is 120 g/L (CIRSEE 2007; Degrémont 2007). Those values are much higher in the case of decarbonatation sludge (around 100 and 800 g/L).
8. Typical values range between 25 and 50 g/L. Default value is set at 40 g/L (CIRSEE 2007; Degrémont 2007).
9. The concentration of the sludge obtained after filtering depends on the technology used for the process, the use of polymer, etc. Typical values range between 200 and 250 g/L (CIRSEE 2007; Degrémont 2007). Those values are much higher in the case of decarbonatation sludge.
10. The concentration of the sludge obtained after centrifuging depends on the technology used for the process, the use of polymer, etc. Typical values range between 150 and 400 g/L (CIRSEE 2007; Degrémont 2007). Those values are much higher in the case of decarbonatation sludge.
11. The concentration of the sludge obtained after filtering depends on the technology used for the process, the use of polymer, etc. Typical values range between 300 and 400 g/L for filter press (V5) and between 200 and 500 g/L for vacuum filter (V6) (CIRSEE 2007; Degrémont 2007). Those values are much higher in the case of decarbonatation sludge.
12. Default value is 50 $kg/(m^2.day)$ but it depends a lot on the type of sludge that is treated (e.g. decarbonatation, pure hydroxide sludge, organic sludge, etc) (CIRSEE 2007; Degrémont 2007).
13. A typical value is 100 $kg/(m^2.day)$ (Degrémont 2007).
14. Typical values range from 24 to 120 $kg/(m^2.day)$ so the default value is set to60 $kg/(m^2.day)$ but it depends on the type of sludge that is treated (e.g. decarbonatation, pure hydroxyde sludge, organic sludge, etc) (CIRSEE 2007; Degrémont 2007; Guibelin 1999).
15. Typical values range from 20 to 60 $kg/(m^2.day)$ (CIRSEE 2007; Degrémont 2007).

16. Typical values range from 2000 to 4000 kg/(m.day) so the default value is set to 3000 kg/(m.day) but it is very variable and depends on the commercial model of belt filter used for the process, the type of sludge that is treated (e.g. decarbonatation, pure hydroxyde sludge, organic sludge, etc) (CIRSEE 2007).
17. The dry solid content of the sludge at the output of the thermal drying process (V7) could be regulated. Typical values range between 65% and 95%, so the default value is set to 80%.

One second-level script exists for each model version of the process category « Sludge treatment ». These Python^{TM} scripts define the functions and constants on which these models rely and they are described in what follows.

The function *Sld_Dens*, as defined in the second-level scripts of settling and flotation (i.e. the files named « Settling_Data » and « Flotation_Data »), are also part of the second-level scripts introduced here. Indeed, sludge density also needs to be evaluated from its concentration.

Second-level script corresponding to sludge settling (V1) - « ST_Settling_Data »

Electricity consumption in relation to the treated mass of solid matter (i.e. suspended matter)

Energy_Consumption_Ratio = 7.5 [kWh/tSM]

Note : Typical values range between 5 and 10 kWh/tSM, so the default value is set at 7.5 kWH/tSM (CIRSEE 2007; Degrémont 2007).

Minimum height of the settling tank

Min_Height = 3.5 [m]

Note: This is an arbitrary default value estimated in accordance with water treatment experts.

Second-level script corresponding to sludge flotation (V2)- « ST_Flotation_Data »

Electricity consumption in relation to the treated mass of solid matter (i.e. suspended matter)

Energy_Consumption_Ratio = 200.0 [kWh/tSM]

Note : This ratio for electricity consumption due to sludge flotation is variable and the user must pay attention to this value (Degrémont 2007; Guibelin 1999).

Minimum height

Min_Height = 3.5 [m]

Note: This is an arbitrary default value estimated in accordance with water treatment experts.

Second-level script corresponding to belt filtration (V3) - « ST_Belt_Filter_Data »

Electricity consumption in relation to the treated mass of solid matter (i.e. suspended matter)

Energy_Consumption_Ratio = 17.5 [kWh/tSM]

Note : Typical values range between 10 and 25 kWh/tSM, so the default value is set at 17.5 kWh/tSM (CIRSEE 2007; Degrémont 2007).

Water consumption for belt filter cleaning

Water_Consumption_Ratio = 25.0 [kgH_2O/kgSM]

Note : This ratio is variable and should be refined when necessary (Degrémont 2007; Guibelin 1999).

Second-level script corresponding to sludge centrifuging (V4) - « ST_Centrifuging_Data »

Electricity consumption in relation to the treated mass of solid matter (i.e. suspended matter)

Energy_Consumption_Ratio = 45.0 [kWh/tSM]

Note : Typical values range between 30 and 60 kWh/tSM, so the default value is set at 45 kWH/tSM (Degrémont 2007).

Second-level script corresponding to press filtration (V5) - « ST_Filter_Press_Data »

Electricity consumption in relation to the treated mass of solid matter (i.e. suspended matter)

Energy_Consumption_Ratio = 30.0 [kWh/tSM]

Note : Typical values range between 20 and 40 kWh/tSM, so the default value is set at 30 kWh/tSM (CIRSEE 2007; Degrémont 2007).

Second-level script corresponding to vacuum filtration (V6) - « ST_Vaccum_Filter_Data »

Electricity consumption in relation to the treated mass of solid matter (i.e. suspended matter)

Energy_Consumption_Ratio = 100.0 [kWh/tSM]

Note : Typical values range between 50 and 150 kWh/tSM, so the default value is set at 100 kWh/tSM (Degrémont 2007).

Water consumption for vacuum filter cleaning

Water_Consumption_Ratio = 25.0 [kgH_2O/kgSM]

Note : This ratio is variable and should be refined when necessary (Degrémont 2007; Guibelin 1999).

Second-level script corresponding to thermal drying (V7) - « ST_Thermal_Drying_Data »

Thermal energy consumption ratio

Therm_Energy_Consumption_Ratio = 0.989 [kWh-th/kg of vaporized water]

Note : Typical values range between 700 and 1000 kJ/kg of vaporized water, so the default value is set at 850 kJ/kg of vaporized water, which is equivalent to 0.989 kWh/kg of vaporized water (Degrémont 2007; Guibelin 1999).

Electrical energy consumption ratio

Elec_Energy_Consumption_Ratio = 0.05 [kWh-el/kg of vaporized water]

Note : Typical values range between 0.03 and 0.07 kWh/kg of vaporized water, so the default value is set to 0.05 kWh/kg of vaporized water (Guibelin 1999).

Contactor drying capacity for heat transfer

Contactor_Drying_Capacity = 13.0 [kg of vaporized water/(m^2.h)]

Note : Typical values range between 12 and 14 kg of vaporized water/(m2.h), so the default value is set to 13 kg of vaporized water/(m^2.h) (Degrémont 2007).

8.2 Energy and chemical consumptions

Hydrated lime and flocculant are the two typical chemicals consumed during sludge treatment. Hydrated lime is added for sludge stabilization and flocculant for sludge conditioning.

The only form of energy consumed by sludge treatment processes is electricity, except that the thermal drying process also consumes heat in different forms regarding their availability.

Chemical consumptions

Flocculant consumption and flow demand

$$\text{Spec\_Floc\_Cons} = \frac{\text{PFD} \times \text{Input\_Sludge\_SM}}{\text{Input\_Sludge\_Density} \times 10^3} \quad \text{[kg/kg of input sludge]} \qquad (333)$$

$$\text{Floc\_Flow} = \text{Spec\_Floc\_Cons} \times \text{Input\_Sludge\_Flow} \quad \text{[kg/s]} \qquad (334)$$

$$\text{Floc\_Quantity} = \text{Spec\_Floc\_Cons} \times \text{Input\_Sludge} \quad \text{[kg]} \qquad (335)$$

Hydrated lime consumption and flow demand (V1/V3/V4/V5/V6/V7)

$$\mathrm{Spec\_Hyd\_Lime\_Cons} = \frac{\mathrm{HLD} \times \mathrm{Input\_Sludge\_SM}}{\mathrm{Input\_Sludge\_Density} \times 10^3}$$

[kgCa(OH)$_2$/kg of input sludge] (336)

$$\mathrm{Hyd\_Lime\_Flow} = \mathrm{Spec\_Hyd\_Lime\_Cons} \times \mathrm{Input\_Sludge\_Flow}$$

[kgCa(OH)$_2$/s] (337)

$$\mathrm{Hyd\_Lime\_Quantity} = \mathrm{Spec\_Hyd\_Lime\_Cons} \times \mathrm{Input\_Sludge}$$

[kgCa(OH)$_2$] (338)

It must be noted that these quantities of hydrated lime refer to pure hydrated lime (i.e. Ca(OH)$_2$).

Electricity consumption (V1/V2/V3/V4/V5/V6)

Electricity consumption for intake pumping, reactant(s) injection, harrowing and scraping

$$\mathrm{Spec\_Elec\_Cons} = \frac{\mathrm{Energy\_Consumption\_Ratio} \times \mathrm{Input\_Sludge\_SM}}{\mathrm{Input\_Sludge\_Density} \times 10^6}$$

[kWh/kg of input sludge] (339)

Total electricity consumption

$$\mathrm{Total\_Elec\_Consumption} = \mathrm{Spec\_Elec\_Cons} \times \mathrm{Input\_Sludge}$$

[kWh] (340)

Electrical powers

$$\mathrm{Electrical\_Power\_Used} = \mathrm{Spec\_Elec\_Cons} \times \mathrm{Input\_Sludge\_Flow} \times 3600$$

[kW] (341)

$$\mathrm{Electrical\_Power\_To\_Be\_Installed} = \mathrm{Spec\_Elec\_Cons} \times \mathrm{Max\_Input\_Sludge\_Flow} \times 3600$$

[kW] (342)

Electricity consumption (V7)

Electricity consumption for intake pumping, reactant(s) injection, and other purposes

$$\mathrm{Spec\_Elec\_Cons} = \mathrm{Elec\_Energy\_Consumption\_Ratio} \times \mathrm{Spec\_Vaporized\_Water\_Ratio}$$

[kWh-el/kg of input sludge] (343)

Total electricity consumption

$$\text{Total\_Elec\_Consumption} = \text{Spec\_Elec\_Cons} \times \text{Input\_Sludge}$$

[kWh-el] (344)

Electrical powers

$$\text{Electrical\_Power\_Used} = \text{Spec\_Elec\_Cons} \times \text{Input\_Sludge\_Flow} \times 3600$$

[kW] (345)

$$\text{Electrical\_Power\_To\_Be\_Installed} = \text{Spec\_Elec\_Cons} \times \text{Max\_Input\_Sludge\_Flow} \times 3600$$

[kW] (346)

Thermal energy consumption for heating and drying

$$\text{Spec\_Therm\_En\_Cons} = \text{Therm\_Energy\_Consumption\_Ratio} \times \text{Spec\_Vaporized\_Water\_Ratio}$$

[kWh-th/kg of input sludge] (347)

Total thermal energy consumption

$$\text{Total\_Therm\_En\_Consumption} = \text{Spec\_Therm\_En\_Cons} \times \text{Input\_Sludge}$$

[kWh-th] (348)

Electrical powers

$$\text{Thermal\_Power\_Used} = \text{Spec\_Therm\_En\_Cons} \times \text{Input\_Sludge\_Flow} \times 3600$$

[kW-th] (349)

$$\text{Thermal\_Power\_To\_Be\_Installed} = \text{Spec\_Therm\_En\_Cons} \times \text{Max\_Input\_Sludge\_Flow} \times 3600$$

[kW-th] (350)

8.3 Output water quality data

Hydrated lime solution to be injected in the sludge and water dilution factor (V1/V3/V4/V5/V6/V7)

$$\text{Hyd\_Lime\_Solution\_Quantity} = \frac{\text{Hyd\_Lime\_Quantity}}{\text{Hyd\_Lime\_Concentration}}$$

[kg of hydrated lime solution] (351)

$$\text{Water\_Dilution\_Factor} = \frac{\text{Input\_Sludge}}{\text{Input\_Sludge} + \text{Hyd\_Lime\_Solution\_Quantity}}$$

[no unit] (352)

Precipitated salts before and after addition of the lime

The quantity of salt precipitates ($Fe(OH)_3$, MnO_2, $Al(OH)_3$, SiO_2 and $CaCO_3$), before and after liming, are stored in two dedicated variables : *Prec_Salts_Bef_Lim, Prec_Salts_Aft_Lim*. The dissolved and total salt concentrations are changed due to the chemical reaction. The quantity of salt precipitates is normally increased due to the addition of hydrated lime and it generates an increase of suspended matter that must be taken into account.

$$\begin{aligned}\text{Prec\_Salts} &= 1.91\times(\text{Fe\_Total - Fe\_Dissolved}) + 1.58\times(\text{Mn\_Total - Mn\_Dissolved})\\ &+ 2.89\times(\text{Al\_Total - Al\_Dissolved}) + 2.14\times(\text{Si\_Total - Si\_Dissolved})\\ &+ \min[(2.5\times(\text{Ca\_Total - Ca\_Dissolved}));(8.33\times(\text{C\_Total - C\_Dissolved}))]\end{aligned}$$

[mg/L] (353)

In the model version 2 (i.e. sludge flotation), the quantity of salt precipitates stays unchanged, since there is no hydrated lime added to the sludge under treatment. The two variables *Prec_Salts_Bef_Lim* and *Prec_Salts_Aft_Lim* are then equal so that the following calculations are consistent even for this model version.

Mineral composition, TAC, TH and pH of the liquid phase of the treated sludge (V1/V3/V4/V5/V6/V7)

The mineral composition, the complete alkalinity titration TAC, the total hardness TH and the pH of the liquid phase of the treated sludge (i.e. the sludge overflow) are modified due to the addition of hydrated lime. Based on the user-defined lime dose *HLD* that is added to the sludge, these water quality data are calculated by the function *Reactant_Addition* (except for the model version 2).

Dry matter flows (V1/V2/V3/V4/V5/V6)

The dry matter flows in the input sludge, output sludge and in the sludge overflow are calculated from the quantity of precipitated salts (their increase has been previously calculated) and thanks to the recovery rate efficiency (parameter *RR_NU*).

$$\text{Input\_Sld\_DMF} = \frac{\text{Input\_Sludge\_Flow}\times\text{Input\_Sludge\_SM}\times 10^3}{\text{Input\_Sludge\_Density}}$$

[mgSM/s] (354)

$$\text{Prec\_Salts\_Increase} = \frac{\text{Input\_Sludge\_Flow} \times 10^3 \times (\text{Prec\_Salts\_Aft\_Lim} - \text{Prec\_Salts\_Bef\_Lim})}{\text{Input\_Sludge\_Density}} \quad [\text{mgSM/s}] \qquad (355)$$

$$\text{Sld\_Overflow\_DMF} = \text{Input\_Sludge\_DMF} \times (1 - \text{RR\_NU}) \quad [\text{mgSM/s}] \qquad (356)$$

$$\text{Output\_Sludge\_DMF} = \text{Input\_Sludge\_DMF} + \text{Prec\_Salts\_Increase} - \text{Sld\_Overflow\_DMF} \quad [\text{mgSM/s}] \qquad (357)$$

<u>Flows of output sludge and sludge overflow (V1/V2/V3/V4/V5/V6)</u>

$$\text{Output\_Sludge\_Flow} = \frac{\text{Output\_Sludge\_DMF} \times \text{Output\_Sludge\_Density}}{\text{SLC} \times 1000} \quad [\text{kg/s}] \qquad (358)$$

$$\text{Sld\_Overflow\_Flow} = \text{Input\_Sludge\_Flow} + \frac{\text{Hyd\_Lime\_Flow}}{\text{Hyd\_Lime\_Concentration}} + \text{Floc\_Flow} - \text{Output\_Sludge\_Flow} \quad [\text{kg/s}] \qquad (359)$$

<u>Process conversion rate (V1/V2/V3/V4/V5/V6)</u>

$$\text{Conversion\_Rate} = \frac{\text{Sld\_Overflow\_Flow}}{\text{Input\_Sludge\_Flow}} \quad [\text{dec.\%}] \qquad (360)$$

<u>Maximum flows of output sludge and sludge overflow (V1/V2/V3/V4/V5/V6)</u>

$$\text{Max\_Sld\_Overflow\_Flow} = \text{Max\_Input\_Sludge\_Flow} \times \text{Conversion\_Rate} \quad [\text{kg/s}] \qquad (361)$$

$$\text{Max\_Output\_Sludge\_Flow} = \text{Max\_Input\_Sludge\_Flow} - \text{Max\_Sld\_Overflow\_Flow} \quad [\text{kg/s}] \qquad (362)$$

<u>Output sludge and sludge overflow quantities (V1/V2/V3/V4/V5/V6)</u>

$$\text{Sld\_Overflow} = \text{Input\_Sludge} \times \text{Conversion\_Rate} \quad [\text{kg}] \qquad (363)$$

$$\text{Output\_Sludge} = \text{Input\_Sludge} - \text{Sld\_Overflow} \quad [\text{kg}] \qquad (364)$$

<u>Elimination ratio (V1/V2/V3/V4/V5/V6)</u>

This is a ratio between the suspended matter SM concentration of the sludge overflow and that of the input sludge.

Assumption : The sludge overflow has a density of 1000 kg/m^3 because of its high water content.

$$\text{Sld\_Overflow\_SM} = \frac{\text{Sld\_Overflow\_DMF}}{\text{Sld\_Overflow\_Flow}} \qquad [\text{mgSM/L}] \qquad (365)$$

$$\text{SM\_Elimination\_Ratio} = \frac{\text{Sld\_Overflow\_SM}}{\text{Input\_Sludge\_SM}} \qquad [\text{dec.\%}] \qquad (366)$$

<u>Turbidity and organic matter in the sludge overflow (V1/V2/V3/V4/V5/V6)</u>

The non-dissolved compounds (i.e. particulate compounds) are assumed to be removed by the unit processes under consideration in the same proportion as the suspended matter (i.e. *SM_Elimination_Ratio*). The concentration of the dissolved compounds stays unchanged.

$$\text{Sld\_Overflow\_Turbidity} = \frac{\text{Sld\_Overflow\_SM}}{\text{SM\_Turbidity\_Ratio}} \qquad [\text{NTU}] \qquad (367)$$

$$\text{Sld\_Overflow\_POC} = \text{SM\_Elimination\_Ratio} \times \text{POC} \qquad [\text{mg/L}] \qquad (368)$$

$$\text{Sld\_Overflow\_DOC} = \text{DOC} \qquad [\text{mg/L}] \qquad (369)$$

$$\text{Sld\_Overflow\_TOC} = \text{Sld\_Overflow\_POC} + \text{Sld\_Overflow\_DOC} \qquad [\text{mg/L}] \qquad (370)$$

$$\text{Sld\_Overflow\_UVA} = \text{UVA} \qquad [\text{m}^{-1}] \qquad (371)$$

$$\text{Sld\_Overflow\_COD} = \text{Sld\_Overflow\_TOC} \times \text{COD\_TOC\_Ratio} \qquad [\text{mgO}_2\text{/L}] \qquad (372)$$

$$\text{Sld\_Overflow\_BOD5} = \frac{\text{Sld\_Overflow\_COD}}{\text{COD\_BOD5\_Ratio}} \qquad [\text{mgO}_2\text{/L}] \qquad (373)$$

$$\text{Sld\_Overflow\_BOD} = \frac{\text{Sld\_Overflow\_BOD5}}{\text{BOD5\_BOD\_Ratio}} \qquad [\text{mgO}_2\text{/L}] \qquad (374)$$

$$\text{Sld\_Overflow\_DOC\_TOC\_Ratio} = \frac{\text{Sld\_Overflow\_DOC}}{\text{Sld\_Overflow\_TOC}} \qquad [\text{mgDOC/mgTOC}] \qquad (375)$$

$$\text{Sld\_Overflow\_Color} = \frac{\text{Sld\_Overflow\_UVA}}{\text{UVA\_Color\_Ratio}} \qquad [\text{mg Pt-Co/L}] \qquad (376)$$

<u>Concentration of pathogenic micro-organisms in the sludge overflow (V1/V2/V3/V4/V5/V6)</u>

The pathogenic microorganisms are assumed to be removed in the same proportion as the suspended matter. The following equation shows the calculation in a generic manner.

$$\text{Sld\_Overflow\_Microorganism} = \text{Input\_Sludge\_Microorganism} \times \text{SM\_Elimination\_Ratio} \qquad [\text{nb/L}] \qquad (377)$$

Concentration of salt precipitates in the sludge overflow (V1/V2/V3/V4/V5/V6)

The salt precipitates are assumed to be removed in the same proportion as the suspended matter. The following equation shows the calculation in a generic manner.

$$\begin{aligned}&\text{Sld\_Overflow\_X\_Total} = \text{Input\_Water\_X\_Dissolved}\\&+\left(\left(\text{Input\_Water\_X\_Total - Input\_Water\_X\_Dissolved}\right)\times\text{SM\_Elimination\_Ratio}\right)\end{aligned}$$

[mg/L] (378)

PAC concentration in the sludge overflow (V1/V2/V3/V4/V5/V6)

$$\text{Sld\_Overflow\_PAC} = \text{SM\_Elimination\_Ratio}\times\text{Input\_Water\_PAC}\quad\text{[mg/L]}\quad(379)$$

Concentration of dissolved compounds in the sludge overflow (V1/V2/V3/V4/V5/V6)

The concentration of dissolved compounds (e.g. micropollutants or disinfection by-products) is supposed to stay unchanged since all the unit processes for sludge treatment consist in a physical separation of particulate compounds.

Water quality data of the output sludge (V1/V2/V3/V4/V5/V6)

At this point, the water quality data of the input sludge and those of the sludge overflow are known. Therefore, the water quality data of the output sludge are calculated based on conventional mass balances as shown in the following generic equation.

$$\text{Output\_Sld\_X} = \frac{\left(\left(\text{Input\_Sludge\_Flow}\times\text{Input\_Sld\_X}\right)-\left(\text{Sld\_Overflow\_Flow}\times\text{Sld\_Overf\_X}\right)\right)}{\text{Output\_Sludge\_Flow}}$$

[Unit corresponding to the water quality under consideration] (380)

- $Output\_Sld\_X$: Value of the water quality data in the output sludge.
- $Input\_Sld\_X$: Value of the water quality data in the input sludge.
- Sld_Overf_X : Value of the water quality data in the sludge overflow.

Dry matter flows (V7)

Assumption 1 : The water is vaporized and all the water compounds stay in the sludge. Therefore, all the water compounds are concentrated.

Assumption 2 : The sludge drying process involves high temperature that could possibly affect some of the water compounds but it will be assumed that they are not, mainly for want of better information. This is not the objective of the process, so it does not really matter at this point of the treatment.

$$\text{Input\_Sld\_DMF} = \frac{\text{Input\_Sludge\_Flow} \times \text{Input\_Sludge\_SM} \times 10^3}{\text{Input\_Sludge\_Density}}$$

[mgSM/s] (381)

$$\text{Prec\_Salts\_Flow} = \frac{\text{Input\_Sludge\_Flow} \times 10^3 \times (\text{Prec\_Salts\_Aft\_Lim} - \text{Prec\_Salts\_Bef\_Lim})}{\text{Input\_Sludge\_Density}}$$

[mgSM/s] (382)

$$\text{Output\_Sludge\_DMF} = \text{Input\_Sludge\_DMF} + \text{Prec\_Salts\_Increase}$$

[mgSM/s] (383)

Output sludge nominal and maximum flows (V7)

$$\text{Output\_Sludge\_Flow} = \frac{\text{Output\_Sludge\_DMF}}{\text{ODSC} \times 10^6}$$ [kg/s] (384)

$$\text{Max\_Output\_Sludge\_Flow} = \text{Output\_Sludge\_Flow} \times \frac{\text{Max\_Input\_Sludge\_Flow}}{\text{Input\_Sludge\_Flow}}$$

[kg/s] (385)

Output sludge quantity (V7)

$$\text{Prec\_Salts\_Quantity} = \frac{\text{Input\_Sludge} \times 10^3 \times (\text{Prec\_Salts\_Aft\_Lim} - \text{Prec\_Salts\_Bef\_Lim})}{\text{Input\_Sludge\_Density}} \times 10^6$$

[kg] (386)

$$\text{Input\_DSC} = \frac{\text{Input\_Sludge\_SM}}{\text{Input\_Sludge\_Density} \times 10^3}$$

[dec.% - kgSM/kg of sludge] (387)

$$\text{Output\_Sludge} = \frac{(\text{Input\_Sludge} \times \text{Input\_DSC}) + \text{Prec\_Salts\_Quantity}}{\text{ODSC}}$$

[kg] (388)

Sludge concentration factor (V7)

$$\text{Sludge\_Concentration\_Factor} = \frac{\text{Input\_Sludge\_Flow}}{\text{Input\_Sludge\_Density}} \times \frac{\text{Output\_Sludge\_Density}}{\text{Output\_Sludge\_Flow}}$$

[dec.%] (389)

Water quality data of the output sludge (V7)

At this point, the water quality data of the input sludge and the concentration factor due to the drying process are known. This process does not generate two output flows but only one. Both dissolved and non-dissolved compounds are assumed to stay in the sludge, i.e. no compounds leave the sludge with the vaporized water.

The suspended matter SM and the turbidity of the output sludge are calculated from the following equations.

$$\text{Output\_Sludge\_SM} = \frac{\text{Output\_Sludge\_DMF} \times \text{Output\_Sludge\_Density}}{\text{Output\_Sludge\_Flow} \times 10^3} \quad [\text{mgSM/L}] \qquad (390)$$

$$\text{Output\_Sludge\_Turbidity} = \frac{\text{Output\_Sludge\_SM}}{\text{SM\_Turbifity\_Ratio}} \quad [\text{NTU}] \qquad (391)$$

Then, all the other water quality data of the output sludge are calculated based on the concentration factor as shown in the following generic equation.

$$\text{Output\_Sld\_X} = \text{Input\_Sld\_X} \times \text{Sludge\_Concentration\_Factor} \quad [\text{Unit corresponding to the water quality under consideration}] \qquad (392)$$

- *Output_Sld_X* : Value of the water quality data in the output sludge.
- *Input_ Sld _X* : Value of the water quality data in the input sludge.

8.4 Engineering design facts

Engineering design facts of the sludge settling/flotation process (V1/V2)

- Numbers of tanks installed [no unit]
- Numbers of tanks in use [no unit]
- Hydraulic residence time [h]
- Tank height [m]
- Total surface in use [m^2]
- Total surface really needed regarding the maximum flow [m^2]
- Total surface really needed regarding the treated flow [m^2]

- User-defined surface SM charge [kgSM/(m^2.day)]
- Real surface SM charge [kgSM/(m^2.day)]
- Suspended matter surface flow [kgSM/(m^2.day)] (only for V1)

Engineering design facts of the belt filtration process (V3)

- Numbers of belt filter(s) installed [no unit]
- Numbers of belt filter(s) in use [no unit]
- Total belt filtration length needed regarding the maximum flow [m]
- Total belt filtration length in use [m]
- User-defined length SM charge [kgSM/(m.day)]
- Real Length SM Charge [kgSM/(m.day)]
- Cleaning water flow [kg/s]
- Percentage of cleaning water in relation to the treated sludge [kgH_2O/kg of input sludge]

Engineering design facts of the (press or vacuum) filtration process (V5/V6)

- Numbers of filters installed [no unit]
- Numbers of filters in use [no unit]
- Total filtration surface needed regarding the maximum flow [m^2]
- Total filtration surface in use [m^2]
- User-defined surface SM charge [kgSM/(m^2.day)]
- Real surface SM charge [kgSM/(m^2.day)]
- Cleaning water flow [kg/s] (only for V6)
- Percentage of cleaning water in relation to the treated sludge [kgH_2O/kg of input sludge] (only for V6)

Engineering design facts of the settling process (V7)

- Ratio of vaporized water in relation to the input sludge [kg of vaporized water/kg of input sludge]
- Quantity of vaporized water [kg]
- Contact surface required for heat transfer [m^2]

Characteristics of the output sludge

- Output Sludge Flow [kg/s]
- Maximum Output Sludge Flow [kg/s]
- Output Sludge Concentration [g/L]

Polymer flocculant - Consumption and flow demand

- Specific flocculant consumption [kg/tSM]
- Specific flocculant consumption [kg/kg of input sludge]
- Flocculant flow demand [kg/s]
- Flocculant quantity in relation to the functional unit [kg]

Hydrated lime - Consumption and flow demand (V1/V3/V4/V5/V6/V7)

- Specific hydrated lime consumption [kg/tSM]
- Specific hydrated lime (solution) consumption [kg/kg of input sludge]
- Hydrated lime (solution) flow demand [kg/s]
- Pure hydrated lime quantity in relation to the functional unit [kg$Ca(OH)_2$]

Electrical power and electricity consumption for sludge treatment

- Specific electricity consumption for sludge treatment [kWh-el/kg of input sludge]
- Total electricity consumption for sludge treatment [kWh-el]
- Electrical power used to treat the nominal flow [kW-el]
- Electrical power to be installed to treat the maximum flow [kW-el]

Thermal power and heat consumption for sludge treatment (V7)

- Specific heat for sludge treatment [kWh-th/kg of input sludge]
- Total heat for sludge treatment [kWh-th]
- Thermal power used to treat the nominal flow [kW-th]
- Thermal power to be installed to treat the maximum flow [kW-th]

9. Flows mixing and flows divider

Two very simple models have been created to simulate the junction or the separation of water flows. They are required, for instance, to model the division of the water flow in parallel process lines (*division of water flow into two separated water flows*) or the recirculation of backwash waters at the beginning of a main treatment line (*junction of two water flows*).

The model *Flow_Divider* does not perform any calculations regarding energy and chemical consumptions, water quality or engineering design. It only uses a model parameter *FFDP* (First Flow Decimal Percentage) which defines the proportion of the input flow going in the first output flow. Then the separation of the mass, nominal and maximum flow is calculated. The water quality is obviously the same in both output flows and in the input flow.

The model *Flows_Mixer* uses the function *Flows_Mixing* (defined in chapter 3). The results of this model is the mass of water, the nominal and maximum water flow, and the water quality of the output flow resulting from the mixing of the two input flows.

Appendix 4-1. Supporting Information of the chapter 4.

1. Unit process modules involved in the plant's model and related parameters

All the UP modules are stored in the EVALEAU library with default (recommended or average) parameter values. Default values can be changed for specific case study through the parameter window in Umberto. The full list of process parameters is provided in table 1.

Table 1. Parameters of the unit process modules (the parameters selected for the sensitivity analysis are in bold)

Module	Parameters Names	Unit
Pumping	Absolute roughness of the pipe(s)	m
	Diameter of the pipe(s)	m
	Height to be pumped	m
	Length to be pumped	m
	Pump efficiency	decimal %
Pre-Ozonation **or** **Inter-Ozonation**	CT - Contact Time x Chlorine Residual	mg.min/L
	Intake pumped height	m
	Intake pump(s) efficiency	decimal %
	Ozone transfer efficiency	**decimal %**
	Percentage of pure oxygen in the feed gas	**%**
	Hydraulic/Contact residence time	min
	Ratio T10/T	**No unit**
Al2SO43 Coagulation	**Coagulation mixing duration (theoretical)**	**min**
	Coagulation dose	**ppm**
	Coagulation contact time (theoretical)	min
	Coagulation velocity gradient	**s-1**
	Flocculation dose	**ppm**
	Flocculation contact time (theoretical)	min
	Flocculation mixing duration (theoretical)	**min**
	Flocculation velocity gradient - Part 1 - Mixing water and flocculant	**s-1**
	Flocculation velocity gradient - Part 2 - Water circulation	**s-1**
	Intake pumped height	m
	Intake pump(s) efficiency	decimal %
	Stirrer(s) efficiency	decimal %
Settling	Hydraulic residence time	min

	Intake pumped height	m
	Intake pump(s) efficiency	decimal %
	Surface hydraulic charge	m3/(m2/h)
	Sludge concentration	g/L
	Suspended matter removal efficiency	decimal %
	Single settling tank surface	m2
Rapid_Biolite_Filtration	Air compressor(s) efficiency	decimal
	Biolite apparent density	kg/m3
	Backwash air flow - Phase 1	Nm3/h
	Backwash air flow - Phase 2	Nm3/h
	Biolite annual replacing rate	decimal
	Biolite density	kg/m3
	Backwash duration - Phase 1	min
	Backwash duration - Phase 2	min
	Backwash duration - Phase 3	min
	Biolite height in the filter(s)	m
	Backwash water flow - Phase 2	m3/h
	Backwash water flow - Phase 3	m3/h
	Backwash pump(s) efficiency	decimal %
	Filtration cycle duration	**days**
	Filtration nominal speed	m/h
	Filter(s) surface	m2
	Intake pumped height	m
	Intake pump(s) efficiency	decimal %
	Maximum filtered water in one cycle by one filter.	m3
	Maximum water height in the filter(s)	m
	Optimisation of the number of filters - 0 for no and 1 for yes	No unit
	Theoretical Filter Capacity	g/m3
	Turbidity filtration efficiency	decimal %
	Water height in the filter(s)	m
Rapid_GAC_Filtration	Air compressor(s) efficiency	decimal %
	Backwash air flow - Phase 1	Nm3/h
	Backwash air flow - Phase 2	Nm3/h
	Backwash duration - Phase 1	min
	Backwash duration - Phase 2	min
	Backwash duration - Phase 3	min
	Backwash water flow - Phase 2	m3/h
	Backwash water flow - Phase 3	m3/h
	Backwash pump(s) efficiency	decimal
	Filtration cycle duration	**days**
	Filtration nominal speed	m/h
	Filter(s) surface	m2
	Filter working rate	**See here**
	GAC apparent density	kg/m3
	GAC density	kg/m3
	GAC height in the filter(s)	m
	GAC regeneration duration	days
	GAC regeneration frequency	**See here**
	GAC replacing rate after each regeneration	decimal %
	Intake pumped height	m
	Intake pump(s) efficiency	decimal %
	Maximum filtered water in one cycle by one filter.	m3
	Maximum water height in the filter(s)	m

	Optimisation of the number of filters - 0 for no and 1 for yes	No unit
	Theoretical Filter Capacity	g/m3
	Turbidity filtration efficiency	decimal %
	Water height in the filter(s)	m
Final_NaOCl	CT - Contact Time x Chlorine Residual	mg.min/L
	Intake pumped height	m
	Intake pump(s) efficiency	decimal
	Pre-treatment index	No unit
	Hydraulic/Contact residence time	min
	Ratio T10/T	**No unit**

2. Sensitivity analysis

The script for sensitivity analysis of the process parameters is based on the Morris method (Campolongo et al. 2007; ; Morris 1991) and allows identifying the key parameters affecting the environmental impact results .

The parameters are design choices and operation conditions which are associated to intervals (from design expert opinion, based on their physical meaning, or from other considerations like costs, feasibility, etc.). In the test bed case, table 1 indicates (in bold) the parameters considered in the sensitivity analysis. These are operation and design parameters which could be effectively changed in the existing plant.

3. Application case

3.1 LCI results

Material and energy consumptions, as recorded at plant, are presented in table 2. This inventory corresponds to the system boundaries defined in the LCA study (i.e. infrastructure was not considered, the offsite treatment of sludge was not considered because of lack of information).

Table 3 presents the modelled inventory by unit process (recorded data at plant are not available for individual processes).

Table 2. Inventory at plant (on site measurements) and corresponding LCI taken from Ecoinvent (or other sources).

UF: 1m^3 potable water		
Material	**Value for 1 UF**	**Ecoinvent process and LCI**
Electricity [kWh/m3]	0.896	Electricity, low voltage, at grid [FR]
Polymer [g/m3]	0.174	Acrylic acid, at plant [RER]
Sodium hypochlorite [g/m3]	5.92	Sodium hypochlorite, 15% in H2O, at plant [RER]
Aluminum sulfate [g/m3]	62.9	Aluminum sulphate, powder, at plant [RER]
GAC [g/m3]	6	from Meier, 1997 *

* new GAC is used on site for each adsorption cycle, no regeneration and no reuse on site is considered

Table 3. Inventory by unit process - modeling results

	Electricity [kWh/m3]	Polymer [g/m3]	Sodium hypochlorite [g/m3]	Aluminium sulfate [g/m3]	GAC [g/m3]
Pumping	3.04E-01				
Pre-Ozonation	3.52E-01				
Coagulation	4.43E-02	0.17		62.8	
Settling	9.69E-05				
RBF	1.42E-03				
Inter-Ozonation	1.21E-01				
RGACF	8.03E-04				
Final NaOCl	3.29E-10		5.50		6.59
total by plant	8.24E-01	0.17	5.50	62.8	6.59

3.2 LCIA results

LCIA results obtained with Impact2002+ method are presented in figure 2, for midpoint impact categories expressed in points at endpoint (European normalization, [16]). The main components of the endpoint categories are: “non-renewable energy (R)”, “respiratory effects (HH)”, “terrestrial ecotoxicity (EQ)”, “climate change (CC)”. This clearly shows that the main impact source of the plant life cycle (within the defined boundaries) is the fossil fuels consumption (included in electricity production processes), which generates climate change and respiratory effects.

The comparison of the conventional LCA and PM-LCA results shows a good agreement of the modelling approach. The relative differences calculated by impact category don’t exceed 10%.

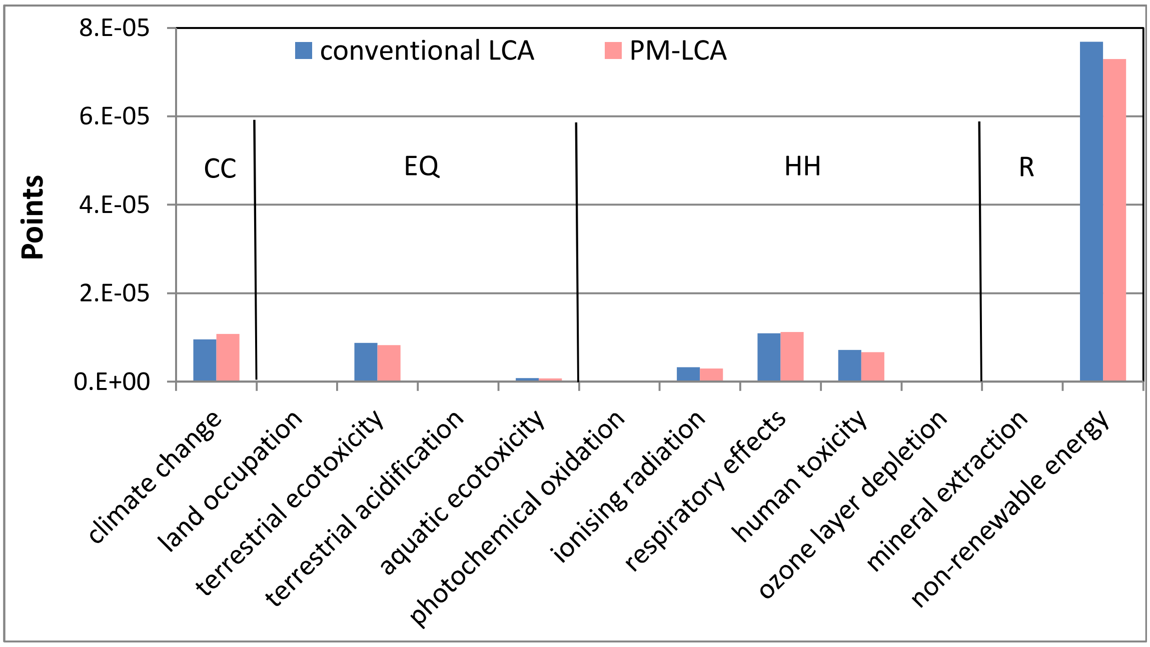


Figure 2. Plant life-cycle: mid-point impact categories calculated with the normalization at endpoint, within each endpoint category (CC =climate change, EQ = ecosystem quality, HH = human health, R=resources).

Figures 3 and 4 give a detailed picture of the LCIA results obtained by PM-LCA. No data were available on site for doing such detailed analysis by conventional LCA.

Figure 3 shows the contribution of unit process life cycle on the endpoint categories (climate change, ecosystem quality, resource depletion, human health). The tendency is the same, with a major contribution of ozonation processes, pumping and then coagulation. A more detailed analysis with the midpoint categories revealed the same behaviour for all impact categories calculated by Impact2002+ . Figure 4 shows three of them. Contribution analysis results corroborate with the plant global results since ozonation operations (and pumping) are intensive energy consuming with repercussion on the main impacts indicators of the plant: resources (non-renewable energy), respiratory effects, climate change.

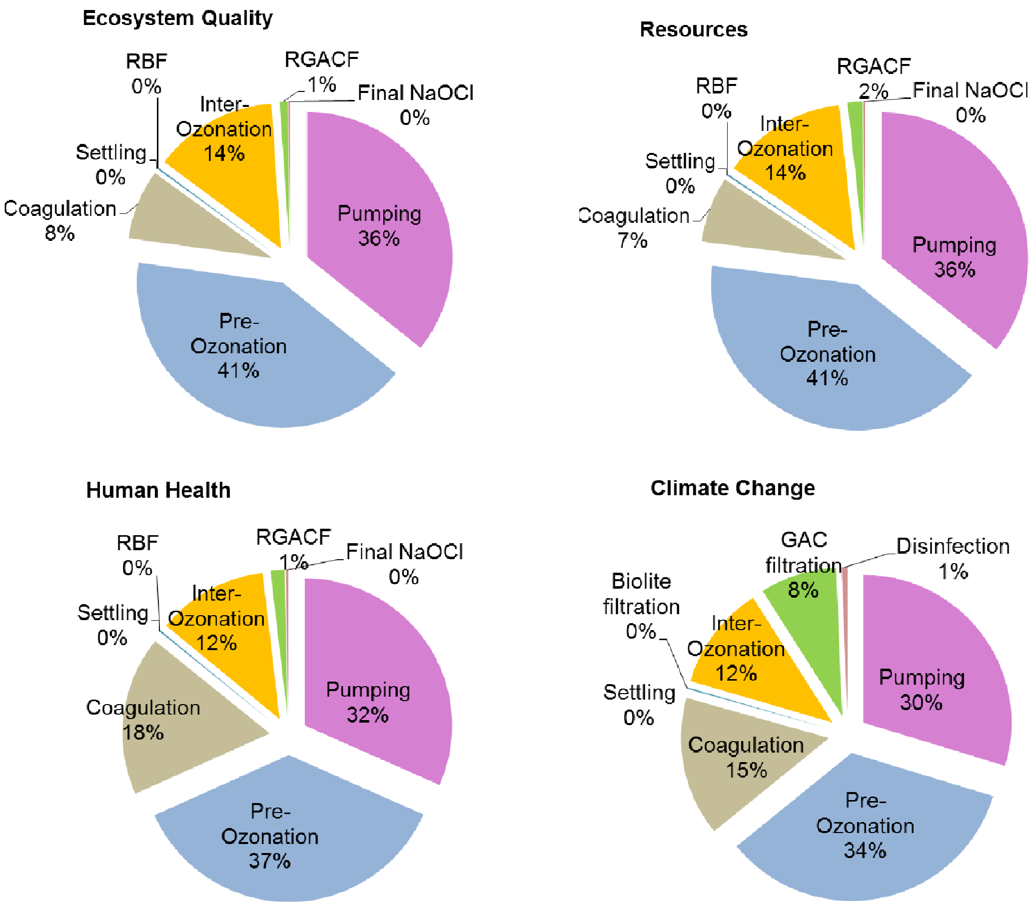


Figure 3. Contribution analysis: unit process life cycle contribution on Endpoint categories.

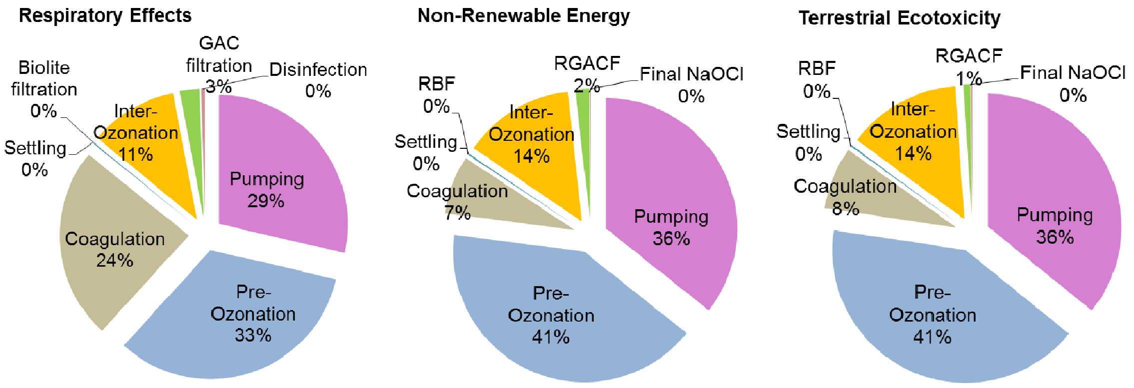


Figure 4. Contribution analysis - unit process life cycle contribution on selected Mid-point impacts.

Appendix 5-1. Parameterisation of the plant model in the retrofit approach.

1. Process Line for the Pre-Treatment

Parameter name	*Default value*	*User-defined value*	*Unit*
Importing WQD			
WF	500	**1329 (to get 1321 at the end)**	kg/s
WTI	1		no unit
MAXWF	750	**2500**	kg/s
Intake Pumping			
NU	0.8		decimal %
H	1	**15**	m
L	10	**150**	m
D	0.5	**1.2**	m
ABS_K	0.0008	**0.0015**	m
Pre-Chlorination			
SMPD	20000	**0**	Pa
IP_NU	0.8		decimal %
T	60	**1.75**	min
PTI	1		no unit
IPH	3	**0**	m
Cl2_D	2	**0.5 (0.5 - 3.0)**	ppm or g/m^3
T10_T	0.5		no unit
H2SO4 Addition			
SMPD	20000	**0**	Pa
IP_NU	0.8		decimal %
IPH	1	**0**	m
CH_D	100	**7.016**	ppm or g/m^3
HRT	0.1	**1.75**	min

CH_CI	1		no unit

H3PO4 Addition

ST_NU	0.7		decimal %
IP_NU	0.8		decimal %
IPH	3	**0**	m
CH_D	100	**0.113**	ppm or g/m^3
TVG	700	**2000**	s^{-1}
HRT	5	**1.75**	min
MIXD	1	**0.0875 ((HRT / 20) 1.75 / 20)**	min
CH_CI	1	**3**	no unit

PAC Addition

SMPD	20000	**0**	Pa
IP_NU	0.8		decimal %
IPH	1	**0**	m
PAC_D	10	**4.213**	ppm or g/m^3
HRT	0.1	**1.75**	min

Coagulation

C_CI	1		no unit
ST_NU	0.7		decimal %
IP_NU	0.8		decimal %
IPH	3	**0**	m
FVG2	60		s^{-1}
FVG1	550	**480**	s^{-1}
FMIXD	1		min
FLOCT	20		min
FLOCD	0.1	**0.1398**	ppm or g/m^3
COAGD	80	**84.55**	ppm or g/m^3
CVG	700	**0**	s^{-1}
COAGT	3		min
CMIXD	1	**0**	min

2. Process Line 1

Parameter name	*Default value*	*User-defined value*	*Unit*
Settling - Process Line 1			
SM_NU	0.95		decimal %
SHC	10	**5**	m.h
SLC	20	**3**	g/L
IPH	4	**0**	m.h
IP_NU	0.8		decimal %
HRT	60	**50**	min
SSTS	100	**590**	m^2
GAC Filtration - Process Line 1			
GACRF	50	**584 (2 years with FCD = 1.25 days)**	Number of filtration cycles before regeneration
TFC	1000		g/m^3
NOFO	0		no unit
IPH	2	**0**	m
MAXFW	12000		m^3
IP_NU	0.8		decimal %
GACRD	15		days
GACH	1	**0.96**	m
WH	1		m
MAXWH	1.8		m
FS	40	**58.2**	m^2
GACAD	480	**300**	kg/m^3
GACD	1200		kg/m^3
GACRR	0.08		decimal %
GACSR	0.25	**0**	decimal %
TUEFF	0.833		decimal %
FNS	10	**10 (7-20)**	m/h
FCD	8	**1.25 (1-1.5)**	days
BDP1	5		min
BDP2	3		min
BDP3	10		min
BAF1	2200	**3000**	Nm^3/h
BAF2	2200	**3000**	Nm^3/h
BWF2	800	**1000**	m^3/h
BWF3	800	**1000**	m^3/h
BWPNU	0.8		decimal %
AC_NU	0.1		decimal %

FWR	6	**4.5**	$m^3$of water / (m^3 of GAC . h)

Inter-Ozonation - Process Line 1

IP_NU	0.8		decimal %
T	60	**16**	min
POPFG	0		decimal %
GT_NU	0.85	**0.969**	decimal %
IPH	5	**0**	m
O3_D	2	**1.986**	ppm or g/m^3
T10_T	0.5	**0.7**	no unit

3. Process Line 2

Parameter name *Default value* *User-defined value* *Unit*

Settling - Process Line 2

Parameter name	*Default value*	*User-defined value*	*Unit*
SM_NU	0.95		decimal %
SHC	10	**9**	m.h
SLC	20	**5**	g/L
IPH	4	**0**	m
IP_NU	0.8		decimal %
HRT	60	**50**	min
SSTS	100	**320**	m^2

Sand Filtration - Process Line 2

SH	0.8	**1.2**	m
WH	0.35		m
MAXWH	1		m
FS	39.55	**63**	m^2
SAD	1460		kg/m^3
SD	2600		kg/m^3
SARR	0.005	**0**	decimal %
TUEFF	0.833		decimal %
FNS	3.5	**14**	m/h
FCD	4	**1.25 (1-1.5)**	days
BDP1	3		min
BDP2	8		min

BDP3	5		min
BAF1	2400		Nm^3/h
BAF2	2400		Nm^3/h
BWF2	260		m^3/h
BWF3	800		m^3/h
NOFO	0		no unit
IPH	1.15	**0**	m
MAXFW	15000		m^3
IP_NU	0.8		decimal %
BWPNU	0.8		decimal %
AC_NU	0.1		decimal %
TFC	1000		g/m^3

Ozonation Pumping - Process Line 2

NU	0.8		decimal %
H	1	**12**	m
L	10	**120**	m
D	0.5	**1.2**	m
ABS_K	0.0008	**0.0015**	m

Inter-Ozonation - Process Line 2

IP_NU	0.8		decimal %
T	60	**16.5**	min
POPFG	0		decimal %
GT_NU	0.85	**0.963**	decimal %
IPH	5	**0**	m
O3_D	1.6	**1.813**	ppm or g/m^3
T10_T	0.5	**0.7**	no unit

GAC Filtration - Process Line 2

GACRD	15		days
GACH	1	**1.2**	m
WH	1	**1.2**	m
MAXWH	1.8		m
FS	40	**63**	m^2
GACAD	480	**300**	kg/m^3
GACD	1200		kg/m^3
GACRR	0.08		decimal %
GACSR	0.25	**1**	decimal %
TUEFF	0.833		decimal %

FNS	10	**14**	m/h
FCD	8	**1.366 (7 days reduced)**	days
BDP1	5		min
BDP2	3		min
BDP3	10		min
BAF1	2200	**3000**	Nm^3/h
BAF2	2200	**3000**	Nm^3/h
BWF2	800	**1000**	m^3/h
BWF3	800	**1000**	m^3/h
NOFO	0		no unit
IPH	2	**0**	m
MAXFW	12000		m^3
IP_NU	0.8		decimal %
BWPNU	0.8		decimal %
AC_NU	0.1		decimal %
FWR	6	**4.5**	$m^3$of water / (m^3 of GAC . h)
GACRF	50	**535 (2 years with FCD = 1.366 days)**	Number of filtration cycles before regeneration
TFC	1000		g/m^3

4. Process Line 3

Parameter name	*Default value*	*User-defined value*	*Unit*

Settling - Process Line 3

SM_NU	0.95		decimal %
SHC	10	**15**	m.h
SLC	20	**35 (30-40)**	g/L
IPH	4	**0**	m
IP_NU	0.8		decimal %
HRT	60	**50**	min
SSTS	100	**182**	m^2

Sand Filtration - Process Line 3

SH	0.8	**1.1**	m

WH	0.35		m
MAXWH	1		m
FS	39.55	**49.2**	m^2
SAD	1460		kg/m^3
SD	2600		kg/m^3
SARR	0.005	**0**	decimal %
TUEFF	0.833		decimal %
FNS	3.5	**12**	m/h
FCD	4	**1.25 (1-1.5)**	days
BDP1	3		min
BDP2	8		min
BDP3	5		min
BAF1	2400		Nm^3/h
BAF2	2400		Nm^3/h
BWF2	260		m^3/h
BWF3	800		m^3/h
NOFO	0		no unit
IPH	1.15	**0**	m
MAXFW	15000		m^3
IP_NU	0.8		decimal %
BWPNU	0.8		decimal %
AC_NU	0.1		decimal %
TFC	1000		g/m^3

Ozonation Pumping -Process Line 3

NU	0.8		decimal %
H	1	**12**	m
L	10	**120**	m
D	0.5	**1.2**	m
ABS_K	0.0008	**0.0015**	m

Inter-Ozonation - Process Line 3

IP_NU	0.8		decimal %
T	60	**15.4**	min
POPFG	0		decimal %
GT_NU	0.85	**0.873**	decimal %
IPH	5	**0**	m
O3_D	2	**1.535**	ppm or g/m^3
T10_T	0.5	**0.5**	no unit

GAC Filtration - Process Line 3

GACRD	15		days
GACH	1	**1.2**	m
WH	1	**1.2**	m
MAXWH	1.8		m
FS	40	**49.2**	m^2
GACAD	480	**300**	kg/m^3
GACD	1200		kg/m^3
GACRR	0.08		decimal %
GACSR	0.25	**0**	decimal %
TUEFF	0.833		decimal %
FNS	10	**12**	m/h
FCD	8	**1.745 (7 days reduced)**	days
BDP1	5		min
BDP2	3		min
BDP3	10		min
BAF1	2200	**3000**	Nm^3/h
BAF2	2200	**3000**	Nm^3/h
BWF2	800	**1000**	m^3/h
BWF3	800	**1000**	m^3/h
NOFO	0		no unit
IPH	2	**0**	m
MAXFW	12000		m^3
IP_NU	0.8		decimal %
BWPNU	0.8		decimal %
AC_NU	0.1		decimal %
FWR	6	**5.7**	m^{3}of water / (m^3 of GAC . h)
GACRF	50	**628 (3 years with FCD = 1.745 days)**	Number of filtration cycles before regeneration
TFC	1000		g/m^3

5. Backwash Waters Recirculation

Parameter name	*Default value*	*User-defined value*	*Unit*

Recirculation Pumping

NU	0.8		decimal %
H	1	**10.3**	m
L	10	**103**	m
D	0.5	**1.2**	m
ABS_K	0.0008	**0.0015**	m

6. Process Line for the Final Treatment

Parameter name	*Default value*	*User-defined value*	*Unit*

Final Chlorination

IPH	3	**0**	m
CT	15		mg.min/L
T10_T	0.5		no unit
SMPD	20000	**0**	Pa
IP_NU	0.8		decimal %
T	60		min
PTI	1	**3**	no unit

NaOH Addition (pH Adjustment)

CH_CI	1	**11**	no unit
CH_D	100	**23.19**	ppm or g/m^3
HRT	0.1		min
SMPD	20000	**0**	Pa
IP_NU	0.8		decimal %
IPH	1	**0**	m

Distribution Pumping

NU	0.8		decimal %
H	1	**114**	m
L	10	**1140**	m
D	0.5	**1.2**	m
ABS_K	0.0008	**0.0015**	m

7. Process Line for Sludge Treatment

Parameter name	*Default value*	*User-defined value*	*Unit*
Sludge Settling			
SLC	30		g/L
SSTS	25	**250**	m^2
HLD	300	**0**	ppm or g/m^3
HRT	24		h
RR_NU	0.9		decimal %
SSMC	50		$kg/(m^2.day)$
PFD	2	**0**	ppm or g/m^3
Sludge Filter Press			
SFPS	50		m^2
SSMC	60		$kg/(m^2.day)$
SLC	350		g/L
HLD	300	**259**	ppm or g/m^3
RR_NU	0.9		decimal %
PFD	5	**0.942**	ppm or g/m^3

Appendix 5-2. Parameterisation of the plant model in the predictive approach.

Note : the red values are the ones different from the retrofit modelling scenario or (mostly) new parameters (process objectives).

1. Process Line for the Pre-Treatment

Parameter name	*Default value*	*User-defined value*	*Unit*
Importing WQD			
WF	500	**1329 (to get 1321 at the end)**	kg/s
WTI	1		no unit
MAXWF	750	**2500**	kg/s
Intake Pumping			
NU	0.8		decimal %
H	1	**15**	m
L	10	**150**	m
D	0.5	**1.2**	m
ABS_K	0.0008	**0.0015**	m
Pre-Chlorination			
SMPD	20000	**0**	Pa
IP_NU	0.8		decimal %
T	60	**1.75**	min
PTI	1		no unit
IPH	3	**0**	m
Cl2_D	2	**0.5 (0.5 - 3.0)**	ppm or g/m^3
T10_T	0.5		no unit
PAC Addition			
TVG	700	**2000**	Pa

IP_NU	0.8		decimal %
IPH	3	**0**	m
DOC_R	0.2	**0.16525**	decimal %
MIXD	1	**0.0875 (HRT/20)**	min
ST_NU	0.7		decimal %
HRT	3	**1.75**	min

Coagulation

C_CI	1		no unit
ST_NU	0.7		decimal %
IP_NU	0.8		decimal %
IPH	3	**0**	m
FVG2	60		s^{-1}
FVG1	550	**480**	s^{-1}
FMIXD	1		min
FLOCT	20		min
FLOCD	0.1	**0.1398**	ppm or g/m^3
DOC_R	0.33	**0.41**	decimal %
CVG	700	**0**	s^{-1}
COAGT	3		min
CMIXD	1	**0**	min

2. Process Line 1

Parameter name	*Default value*	*User-defined value*	*Unit*
Settling - Process Line 1			
SM_NU	0.95		decimal %
SHC	10	**5**	m.h
SLC	20	**3**	g/L
IPH	4	**0**	m.h
IP_NU	0.8		decimal %
HRT	60	**50**	min
SSTS	100	**590**	m^2
GAC Filtration - Process Line 1			
GACRF	50	**584 (2 years with FCD = 1.25 days)**	Number of filtration cycles before

			regeneration
TFC	1000		g/m^3
NOFO	0		no unit
IPH	2	**0**	m
MAXFW	12000		m^3
IP_NU	0.8		decimal %
GACRD	15		days
GACH	1	**0.96**	m
WH	1		m
MAXWH	1.8		m
FS	40	**58.2**	m^2
GACAD	480	**300**	kg/m^3
GACD	1200		kg/m^3
GACRR	0.08		decimal %
GACSR	0.25	**0**	decimal %
TUEFF	0.833		decimal %
FNS	10	**10 (7-20)**	m/h
FCD	8	**1.25 (1-1.5)**	days
BDP1	5		min
BDP2	3		min
BDP3	10		min
BAF1	2200	**3000**	Nm^3/h
BAF2	2200	**3000**	Nm^3/h
BWF2	800	**1000**	m^3/h
BWF3	800	**1000**	m^3/h
BWPNU	0.8		decimal %
AC_NU	0.1		decimal %
FWR	6	**4.5**	m^{3}of water / (m^3 of GAC . h)

Inter-Ozonation - Process Line 1

IP_NU	0.8		decimal %
T	60	**16**	min
POPFG	0		decimal %
GT_NU	0.85	**0.95**	decimal %
IPH	5	**0**	m
CT	1.6	**5.6**	mg.min/L
SMPD	2000	**0**	Pa
T10_T	0.5	**0.7**	no unit

3. Process Line 2

Settling - Process Line 2

Parameter name	*Default value*	*User-defined value*	*Unit*
SM_NU	0.95		decimal %
SHC	10	**9**	m.h
SLC	20	**5**	g/L
IPH	4	**0**	m
IP_NU	0.8		decimal %
HRT	60	**50**	min
SSTS	100	**320**	m^2

Sand Filtration - Process Line 2

Parameter name	*Default value*	*User-defined value*	*Unit*
SH	0.8	**1.2**	m
WH	0.35		m
MAXWH	1		m
FS	39.55	**63**	m^2
SAD	1460		kg/m^3
SD	2600		kg/m^3
SARR	0.005	**0**	decimal %
TUEFF	0.833		decimal %
FNS	3.5	**14**	m/h
FCD	4	**1.25 (1-1.5)**	days
BDP1	3		min
BDP2	8		min
BDP3	5		min
BAF1	2400		Nm^3/h
BAF2	2400		Nm^3/h
BWF2	260		m^3/h
BWF3	800		m^3/h
NOFO	0		no unit
IPH	1.15	**0**	m
MAXFW	15000		m^3
IP_NU	0.8		decimal %
BWPNU	0.8		decimal %
AC_NU	0.1		decimal %
TFC	1000		g/m^3

Ozonation Pumping - Process Line 2

NU	0.8		decimal %
H	1	**12**	m
L	10	**120**	m
D	0.5	**1.2**	m
ABS_K	0.0008	**0.0015**	m

Inter-Ozonation - Process Line 2

IP_NU	0.8		decimal %
T	60	**16.5**	min
POPFG	0		decimal %
GT_NU	0.85	**0.95**	decimal %
IPH	5	**0**	m
SMPD	2000	**0**	Pa
CT	1.6	**5.775**	mg.min/L
T10_T	0.5	**0.7**	no unit

GAC Filtration - Process Line 2

GACRD	15		days
GACH	1	**1.2**	m
WH	1	**1.2**	m
MAXWH	1.8		m
FS	40	**63**	m^2
GACAD	480	**300**	kg/m^3
GACD	1200		kg/m^3
GACRR	0.08		decimal %
GACSR	0.25	**1**	decimal %
TUEFF	0.833		decimal %
FNS	10	**14**	m/h
FCD	8	**1.366 (7 days reduced)**	days
BDP1	5		min
BDP2	3		min
BDP3	10		min
BAF1	2200	**3000**	Nm^3/h
BAF2	2200	**3000**	Nm^3/h
BWF2	800	**1000**	m^3/h
BWF3	800	**1000**	m^3/h
NOFO	0		no unit

IPH	2	**0**	m
MAXFW	12000		m^3
IP_NU	0.8		decimal %
BWPNU	0.8		decimal %
AC_NU	0.1		decimal %
FWR	6	**4.5**	m^{3}of water / (m^3 of GAC . h)
GACRF	50	**535 (2 years with FCD = 1.366 days)**	Number of filtration cycles before regeneration
TFC	1000		g/m^3

4. Process Line 3

Parameter name	*Default value*	*User-defined value*	*Unit*
Settling - Process Line 3			
SM_NU	0.95		decimal %
SHC	10	**15**	m.h
SLC	20	**35 (30-40)**	g/L
IPH	4	**0**	m
IP_NU	0.8		decimal %
HRT	60	**50**	min
SSTS	100	**182**	m^2

Sand Filtration - Process Line 3

SH	0.8	**1.1**	m
WH	0.35		m
MAXWH	1		m
FS	39.55	**49.2**	m^2
SAD	1460		kg/m^3
SD	2600		kg/m^3
SARR	0.005	**0**	decimal %
TUEFF	0.833		decimal %
FNS	3.5	**12**	m/h
FCD	4	**1.25 (1-1.5)**	days
BDP1	3		min
BDP2	8		min

BDP3	5		min
BAF1	2400		Nm^3/h
BAF2	2400		Nm^3/h
BWF2	260		m^3/h
BWF3	800		m^3/h
NOFO	0		no unit
IPH	1.15	**0**	m
MAXFW	15000		m^3
IP_NU	0.8		decimal %
BWPNU	0.8		decimal %
AC_NU	0.1		decimal %
TFC	1000		g/m^3

Ozonation Pumping -Process Line 3

NU	0.8		decimal %
H	1	**12**	m
L	10	**120**	m
D	0.5	**1.2**	m
ABS_K	0.0008	**0.0015**	m

Inter-Ozonation - Process Line 3

IP_NU	0.8		decimal %
T	60	**15.4**	min
POPFG	0		decimal %
GT_NU	0.85	**0.9**	decimal %
IPH	5	**0**	m
CT	1.6	**3.85**	mg.min/L
SMPD	2000	**0**	Pa
T10_T	0.5	**0.5**	no unit

GAC Filtration - Process Line 3

GACRD	15		days
GACH	1	**1.2**	m
WH	1	**1.2**	m
MAXWH	1.8		m
FS	40	**49.2**	m^2
GACAD	480	**300**	kg/m^3
GACD	1200		kg/m^3
GACRR	0.08		decimal %
GACSR	0.25	**0**	decimal %

TUEFF	0.833		decimal %
FNS	10	**12**	m/h
FCD	8	**1.745 (7 days reduced)**	days
BDP1	5		min
BDP2	3		min
BDP3	10		min
BAF1	2200	**3000**	Nm^3/h
BAF2	2200	**3000**	Nm^3/h
BWF2	800	**1000**	m^3/h
BWF3	800	**1000**	m^3/h
NOFO	0		no unit
IPH	2	**0**	m
MAXFW	12000		m^3
IP_NU	0.8		decimal %
BWPNU	0.8		decimal %
AC_NU	0.1		decimal %
FWR	6	**5.7**	$m^3$of water / (m^3 of GAC . h)
GACRF	50	**628 (3 years with FCD = 1.745 days)**	Number of filtration cycles before regeneration
TFC	1000		g/m^3

5. Backwash Waters Recirculation

Parameter name	*Default value*	*User-defined value*	*Unit*
Recirculation Pumping			
NU	0.8		decimal %
H	1	**10.3**	m
L	10	**103**	m
D	0.5	**1.2**	m
ABS_K	0.0008	**0.0015**	m

6. Process Line for the Final Treatment

Parameter name	*Default value*	*User-defined value*	*Unit*
Final Chlorination			
IPH	3	**0**	m
CT	15		mg.min/L
T10_T	0.5		no unit
SMPD	20000	**0**	Pa
IP_NU	0.8		decimal %
T	60		min
PTI	1	**3**	no unit

Parameter name	*Default value*	*User-defined value*	*Unit*
NaOH Addition (pH Adjustment)			
A_CI	1	**1**	no unit
B_D	1	**3**	no unit
HRT	0.1		min
SMPD	20000	**0**	Pa
IP_NU	0.8		decimal %
IPH	1	**0**	m
T_PH	7.0	**7.7**	no unit

Parameter name	*Default value*	*User-defined value*	*Unit*
Distribution Pumping			
NU	0.8		decimal %
H	1	**114**	m
L	10	**1140**	m
D	0.5	**1.2**	m
ABS_K	0.0008	**0.0015**	m

7. Process Line for Sludge Treatment

Parameter name	*Default value*	*User-defined value*	*Unit*
Sludge Settling			
SLC	30		g/L
SSTS	25	**250**	m^2
HLD	300	**0**	ppm or g/m^3
HRT	24		h
RR_NU	0.9		decimal %

SSMC	50		kg/(m^2.day)
PFD	2	**0**	ppm or g/m^3

Sludge Filter Press

SFPS	50		m^2
SSMC	60		kg/(m^2.day)
SLC	350		g/L
HLD	300	**259**	ppm or g/m^3
RR_NU	0.9		decimal %
PFD	5	**0.942**	ppm or g/m^3

Appendix 5-3. Predictive model results with varying coagulation pH.

The numerical experiments consist in running the predictive model with a constant DOC removal objective during coagulation and a varying coagulation pH. Chemical doses are not constant in these simulations (coagulant, acid and base). Normally, when the coagulation process is operated at a lower pH, the required coagulant dose is lower but acid must then be added to lower the pH. The aim of these numerical experiments is to understand if the coagulation process is really enhanced by acid addition in this situation.

The coagulation pH of 6.79 is the one obtained with no acid or base addition (standard coagulation) and this is the optimum coagulation pH for all considered model results ("Climate Change" impact category, EndPoint scores with the Recipe evaluation method and operational costs). So in this situation, the best technical option is standard coagulation according to the results presented on figures 1, 2 and 3.

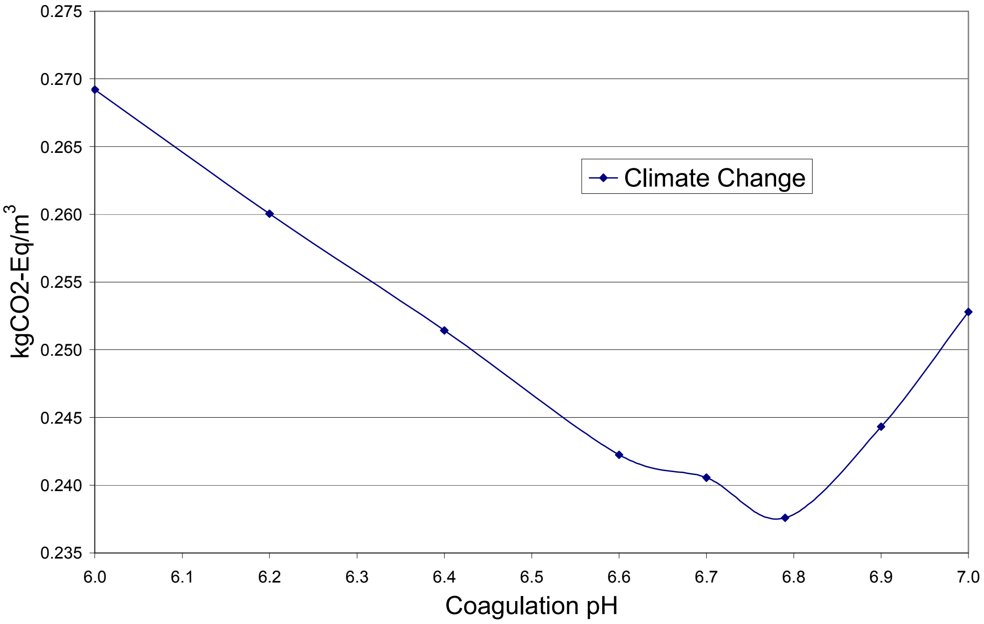


Figure 1. Climate Change (Recipe MidPoint) depending on the coagulation pH.

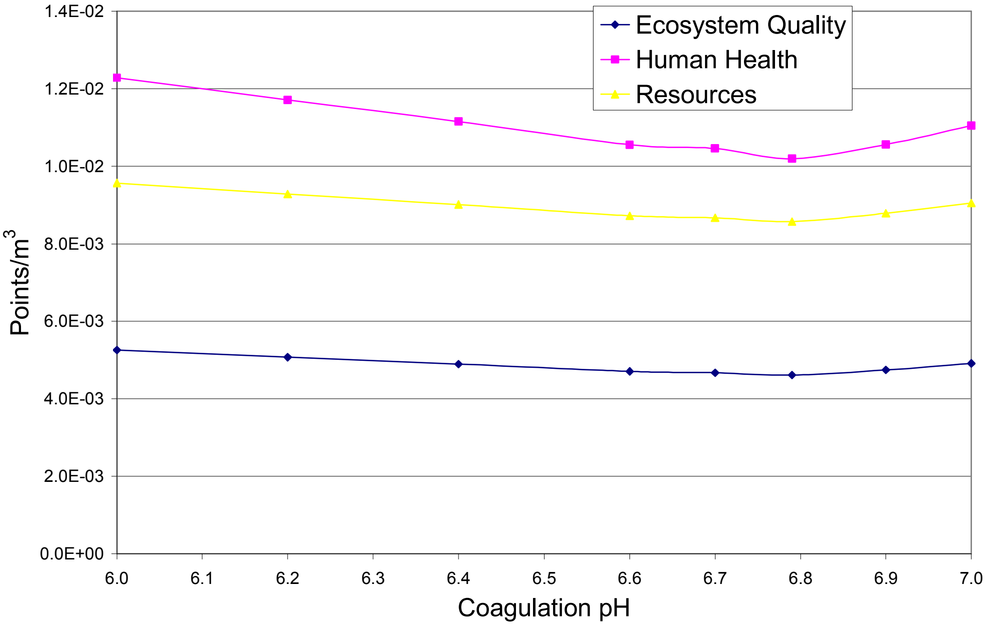


Figure 2. LCIA results (Recipe EndPoint) depending on the coagulation pH.

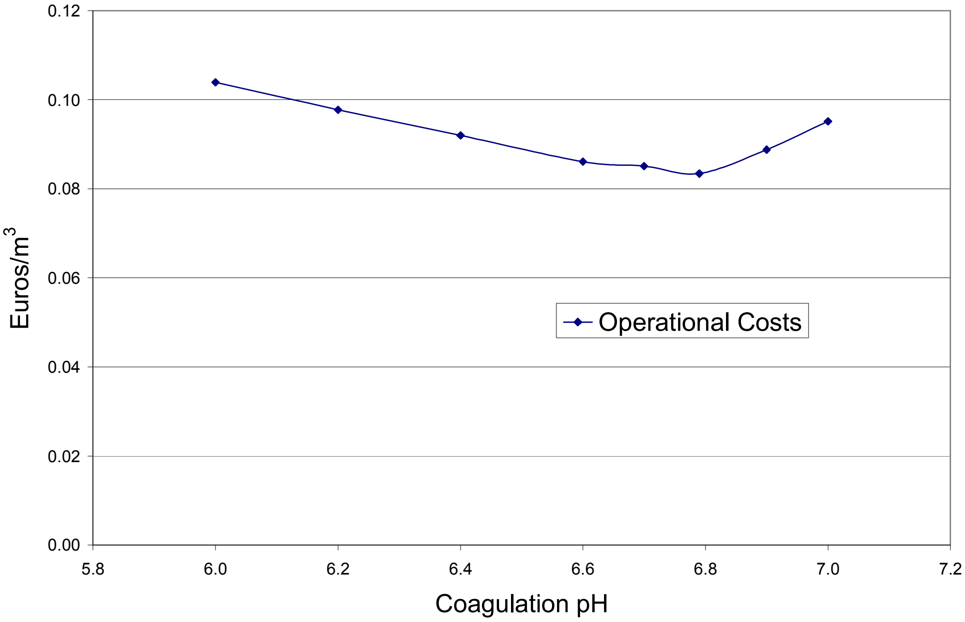


Figure 3. Operational costs depending on the coagulation pH.

Appendix 5-4. Energy and chemical inventory for production and regeneration of (powdered or granular) activated carbon.

Inventory for the production of activated carbon (1 kg)

Chemical / Energy	Quantity / Physical unit
hard coal mix, at regional storage [UCTE]	1 kg
transport, lorry 16-32t, EURO3 [RER]	0.6 tkm
hydrochloric acid, 30% in H2O, at plant [RER]	0.04 kg
natural gas, burned in industrial furnace >100kW [RER]	196 MJ
steam, for chemical processes, at plant [RER]	3 kg
hard coal, burned in industrial furnace 1-10MW [RER]	30.4 MJ
electricity, medium voltage, production UCTE, at grid [UCTE]	0.021 kWh

Inventory for the regeneration of activated carbon (1 kg)

Chemical / Energy	Quantity / Physical unit
hard coal, burned in industrial furnace 1-10MW [RER]	3 MJ
electricity, medium voltage, production UCTE, at grid [UCTE]	0.001 kWh
steam, for chemical processes, at plant [RER]	0.3 kg
natural gas, burned in industrial furnace >100kW [RER]	108 MJ
transport, lorry 16-32t, EURO3 [RER]	2.542 tkm

Note : It must be noted that the regeneration of activated carbon often implies some losses of activated carbon that must be replaced with newly produced activated carbon. This is taken into consideration in the concerned unit process models from the EVALEAU library.

Appendix 5-5. Parameter set considered for sensitivity analysis on LCIA results.

Unit process	Parameter	Lower bound	Upper bound
Tank_PAC_Add	TVG	500	2000
Tank_PAC_Add	MIXD	0.0875	0.6
Tank_PAC_Add	DOC_R	0.15	0.3
Tk_Std_Coag	FVG1	300	700
Tk_Std_Coag	FMIXD	0.5	2
Tk_Std_Coag	DOC_R	0.3	0.45
Oz_O3_Dis_PL1	T	12	20
Oz_O3_Dis_PL1	POPFG	0	1
Oz_O3_Dis_PL1	GT_NU	0.75	0.95
Oz_O3_Dis_PL1	CT	4.2	7
Oz_O3_Dis_PL1	T10_T	0.3	0.8
Oz_O3_Dis_PL2	T	12.375	20.625
Oz_O3_Dis_PL2	POPFG	0	1
Oz_O3_Dis_PL2	GT_NU	0.75	0.95
Oz_O3_Dis_PL2	CT	4.33125	7.21875
Oz_O3_Dis_PL2	T10_T	0.3	0.8
Oz_O3_Dis_PL3	T10_T	0.3	0.8
Oz_O3_Dis_PL3	T	11.55	19.25
Oz_O3_Dis_PL3	POPFG	0	1
Oz_O3_Dis_PL3	GT_NU	0.75	0.95
Oz_O3_Dis_PL3	CT	2.8875	4.8125
Chlr_Cl2_Dis_EL	T	45	75
Chlr_Cl2_Dis_EL	CT	11.25	18.75
Chlr_Cl2_Dis_EL	T10_T	0.3	0.8
Pipe_pH_Adj	T_PH	7	8

Appendix 5-6. Electricity and chemical costs.

Note 1 : The chemical prices presented in this appendix are average prices given for reference but they change depending on several factors.

Note 2 : The electricity price presented in this appendix is an average price over the reference year. In fact, a contract with the electricity supplier makes the electricity pricing more complex than one single number as given in this appendix. The plant operators are purchasing low and medium voltage electricity, and their price is time-varying.

Chemicals actually used on-site

	Aluminium Sulfate	Sulfuric acid	Soda	Chlorine	Hydrated lime
Price [€/ton]	220	180	350	1000	150

	Flocculant	New GAC	Regenerated GAC	PAC
Price [€/ton]	2200	700	300	700

Chemicals used for alternative treatment solutions

	Bleach	Pure Oxygen
Price [€/ton]	220	10

Average electricity price over the reference year

	Electricity
Price [€/kWh]	0.0591